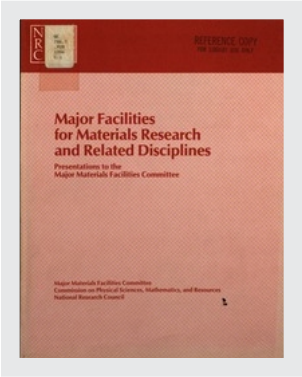

Major Facilities for Materials Research and Related Disciplines: Presentations to the Major Materials Facilities Committee

DETAILS

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MAJOR FACILITIES FOR MATERIALS RESEARCH AND RELATED DISCIPLINES

Presentations to the Major Materials Facilities Committee

Major Materials Facilities Committee
Commission on Physical Sciences,
Mathematics, and Resources
National Research Council

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This report has been reviewed by a group other than the authors according to procedures approved by a Report Review Committee consisting of members of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine.

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FOREWORD

In their preface to the report on Major Facilities for Materials Research and Related Disciplines, Dean E. Eastman and Frederick Seitz wrote that "the report was the result of six months of extremely intensive efforts...." A main part of these efforts was devoted by the Committee to assuring itself that it was thoroughly versed in the scientific opportunities offered by more powerful and versatile facilities for neutron scattering and synchrotron radiation. It also sought to gain a thorough understanding of both the existing and needed technological capabilities for building new facilities.

This appendix documents how the Committee explored these scientific and technological issues. It contains the reports given to the Committee, mainly at a three-day workshop held in March 1984, to assist it in addressing its charge: to assess priorities for major facilities for materials research. Aside from clarifying the bases of the Committee's conclusions, these papers indicate the depth and complexity of materials research in the United States, ranging from condensed matter physics to chemistry, biology, and medicine.

Finally, the Committee extends its gratitude to those who made this volume possible. The efforts involved in preparing these papers, presenting them to the Committee, and answering its questions were considerable. That they were made testifies to the health of materials science in particular and to the common dedication by all--whether or not they ultimately agreed with the Committee's recommendations--to offering the federal government sound and well-documented advice for maintaining the nation's strength in a vital scientific endeavor.

Not included in this Appendix, yet useful to the Committee, were presentations by William D. Nix on the materials research laboratory program at Stanford University, and Brian Fender, Institut Laue Langevin, on the scientific opportunities in chemistry with neutrons, and presentations made to the neutron scattering, synchrotron radiation, and other specialized materials facilities panels.

CONTENTS

FOREWORD vii

PART I: THE WORKSHOP: MARCH 17-19, 1984

INTRODUCTION

Probing Matter with Electrons, Photons, and Neutrons - J. D. Litster, Massachusetts Institute of Technology 1

SCIENTIFIC OPPORTUNITIES WITH SYNCHROTRON RADIATION - D. W. Lynch, Iowa State University, Chairman

1. Physics Research Opportunities with Synchrotron X-Radiation - D. Moncton, Brookhaven National Laboratory 15

2. Scientific Opportunities with Vacuum Ultraviolet (Soft X-Ray) Synchrotron Radiation from Insertion Devices - J. Stohr, Exxon Research and Engineering Company 45

3. X-Ray Microprobe Characterization of Materials: The Case for Undulators on Advanced Storage Rings - C. Sparks, Oak Ridge National Laboratory 91

4. Synchrotron Radiation Research in Biology and Medicine - K. Hodgson, Stanford University 127

SCIENTIFIC OPPORTUNITIES WITH NEUTRONS - R. J. Birgeneau, Massachusetts Institute of Technology, Chairman

1. Physics - J. Axe, Brookhaven National Laboratory 149

2. Scientific Opportunities with Neutrons in Materials Science - J. Weertman, Northwestern University 177

3. Application of Neutron Beam Research in Biology and Medicine - P. Moore, Yale University 197

OVERVIEW OF RELATED REPORTS

1. Current Status of Neutron Scattering Research and Facilities in the United States - S. A. Werner, University of Missouri 211

2. Planning Study for Advanced National Synchrotron-Radiation Facilities - M. L. Knotek, Sandia National Laboratory 235

PROPOSED NEW AND UPGRADED FACILITIES FOR SYNCHROTRON RADIATION RESEARCH - D. W. Lynch, Chairman

1. Proposal for a 6-GeV Synchrotron Source 253
Argonne National Laboratory
Presented by K. L. Kliewer

2. Planned Evolution of NSLS 265
Brookhaven National Laboratory
Presented by D. Moncton

3. Prospectus for a 6 GeV Dedicated Synchrotron Radiation Facility at Cornell University 317
Cornell High Energy Synchrotron Source
Presented by B. McDaniel

4. The Advanced Light Source: Scientific Opportunities 331
Lawrence Berkeley Laboratory
Presented by H. Grunder

5. SSRL's Planning for a New Synchrotron Radiation Facility including a 6 GeV Storage Ring 391
Stanford Synchrotron Radiation Laboratory
Presented by A. Bienenstock

PROPOSED NEW AND UPGRADED FACILITIES FOR NEUTRON SCATTERING - R. J. Birgeneau, Chairman

1. The Argonne Neutron Plan 411
Argonne National Laboratory
Presented by G. Lander

2. Guide Hall Construction at the High Flux Beam Reactor 433
Brookhaven National Laboratory
Presented by B. Schoenborn

3. WNR/PSR Experimental Hall Expansion 455
Los Alamos National Laboratory
Presented by J. Browne

4. NBS Center for Cold Neutron Research 477
National Bureau of Standards
Presented by M. Rowe

5. ORNL Presentation to the MMF Committee 501
Oak Ridge National Laboratory
Presented by R. Moon

PROBING MATTER
WITH
ELECTRONS, PHOTONS, AND NEUTRONS

A Simple-Minded Overview by

J. D. Litster

March 17, 1984

Contents

I. Introduction 1

II. Absorption Spectroscopy. 3

A. Auger Electrons. 3

B. Photoemission. 4

C. EXAFS. 7

III. Scattering Spectroscopy. 9

A. Relation to Real Space Studies 9

B. General Scattering Concepts. 9

C. Electron Scattering. 10

D. Neutron Scattering 11

E. X-Ray Scattering 12

I. INTRODUCTORY REMARKS

A. Momentum

$\vec{p} = \hbar\vec{k}$ $\qquad k = 2\pi/\lambda$

$k = mv/\hbar$ $\qquad$ particle

$k = \omega/c$ $\qquad$ photon

B. Kinetic Energy

$E = p^2/2m = \hbar^2k^2/2m$ $\qquad$ particle

$= \hbar\omega = \hbar ck$ $\qquad$ photon

C. Some Values

electron at 1eV: $\qquad k = 5.1 \times 10^7$ cm^{-1}

$\lambda = 12$Å

$v = 6 \times 10^7$ cm sec^{-1}

neutron at 1ev $\qquad k = 2.3 \times 10^9$ cm^{-1}

$\lambda = 0.28$Å

$v = 1.4 \times 10^6$ cm sec^{-1}

KBT at room temp. = $\qquad 0.025$ eV

visible photon $\qquad \hbar\omega = 2$eV

$\lambda = 6000$Å

$\nu = \omega/2\pi = 5 \times 10^{14}$ Hz

soft x-ray photon $\qquad \hbar\omega = 240$ eV

$\lambda = 50$Å

$\nu = 6 \times 10^{16}$ Hz

Hard x-ray photon $\qquad \hbar\omega = 8$ keV

$\lambda = 50$Å

$\nu = 2 \times 10^{18}$ Hz

D. Source Properties

Intensity or flux: particles cm^{-2} sec^{-1} in the beam

Brightness: particles cm^{-2} sec^{-1} into a unit solid angle - important for experiments where collimation matters.

E. Some Energy Units

1 meV = 0.001 eV = 8.066 cm^{-1}

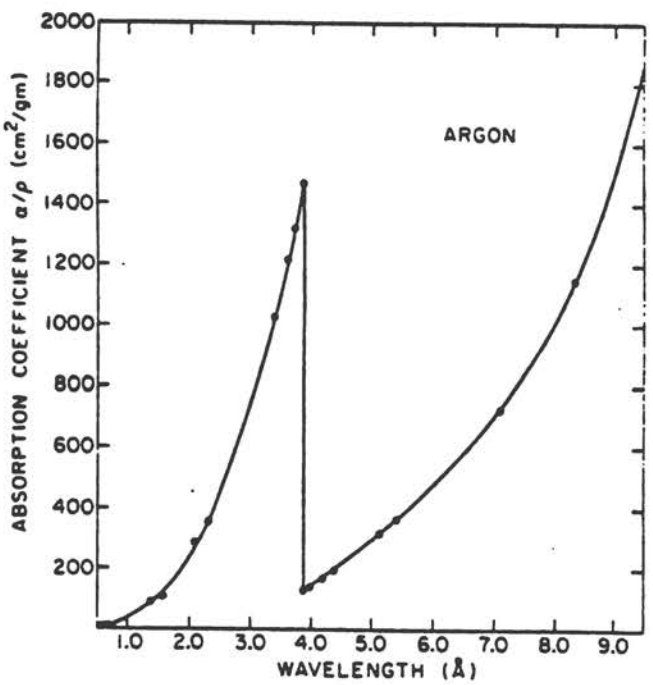
= 11.606 K

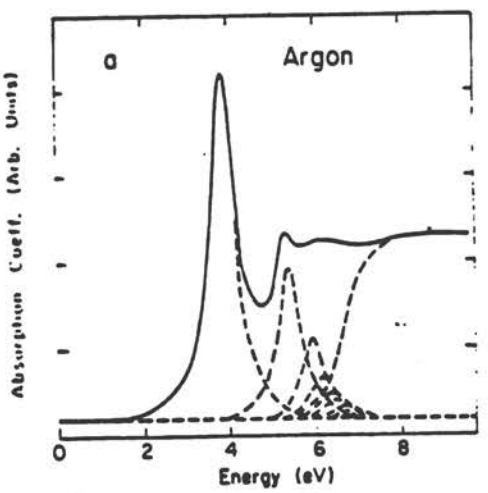
= 242 GHz

F. Interaction of Photons with matter:

Absorption may be followed by

- heat
- fluorescence (chemical analysis)
- photelectron emission
- Auger electron emission
- photo ionization or dissociation





K edge of argon gas. [From A. H. Compton and S. K. Allison. *X-rays in Theory and Experiment*, Van Nostrand-Reinhold, Princeton, New Jersey (1949).]

Scattering may be

- inelastic (e.g. Compton effect)
- elastic (Thompson scattering; scattered and incident waves are coherent).

F. Interaction of Particles with Matter:

Particles can be absorbed and excitation of fluorescence by electrons is a common analytical tool, but we are mostly interested in scattering of particles.

II. ABSORPTION SPECTROSCOPY

Momentum and energy always conserved, but the nucleus or crystal lattice can take up some momentum in many cases.

A. Auger Electrons

A photon may excite an inner (e.g. K shell) electron. The atom may return to the ground state in two ways:

(i) emit a photon - fluorescence
(ii) an electron from a higher state (e.g. L shell) drops to the vacant K shell while simultaneously, another electron is ejected from the atom. Its kinetic energy is equal to the energy difference between the two states.

This is not a radiative or photoelectric process and the angular distribution of Auger electrons is isotropic.

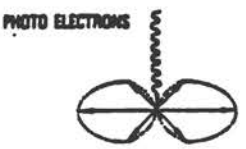
In either case, the fluorescent photon or Auger electron energy is characteristic of the atom, so this can be used for chemical analysis. Fluorescence yield increases with atomic number, approximately as Z^4, so Auger spectroscopy is more important for lighter elements.

K-Shell Core-Hole Widths and Radiative Decay Branching Ratios for a Selection of Elements[a]

Atom	Z	K absorption energy(keV)	Full width (eV)	Fluorescence efficiency
P	15	1.839	0.50	0.058
Ca	20	4.038	0.77	0.16
Fe	26	7.112	1.15	0.34
Cu	28	8.333	1.23	0.45
Ge	32	11.104	1.83	0.55
Kr	35	14.322	2.57	0.66
Mo	42	19.999	4.29	0.77
Ag	47	25.514	6.42	0.84

B. Photoemission

This is not isotropic. Probability goes like $\cos^2 \theta$, if θ is angle between polarization of incident photon and direction of emitted electron.



The anisotropies of the material that the electron comes from also effect the dependence of photoelectron emission on direction.

The input photon can range from a few eV (for studying the emission of weakly bound electrons) to KeV for core electrons.

The energy of the photon goes into first removing the photo-electron from the surface of the material, then giving it kinetic energy. By measuring the electron kinetic energy, you know what energy level it came from in the material. Measurement of the number of photoelectrons gives information on the density of the states.

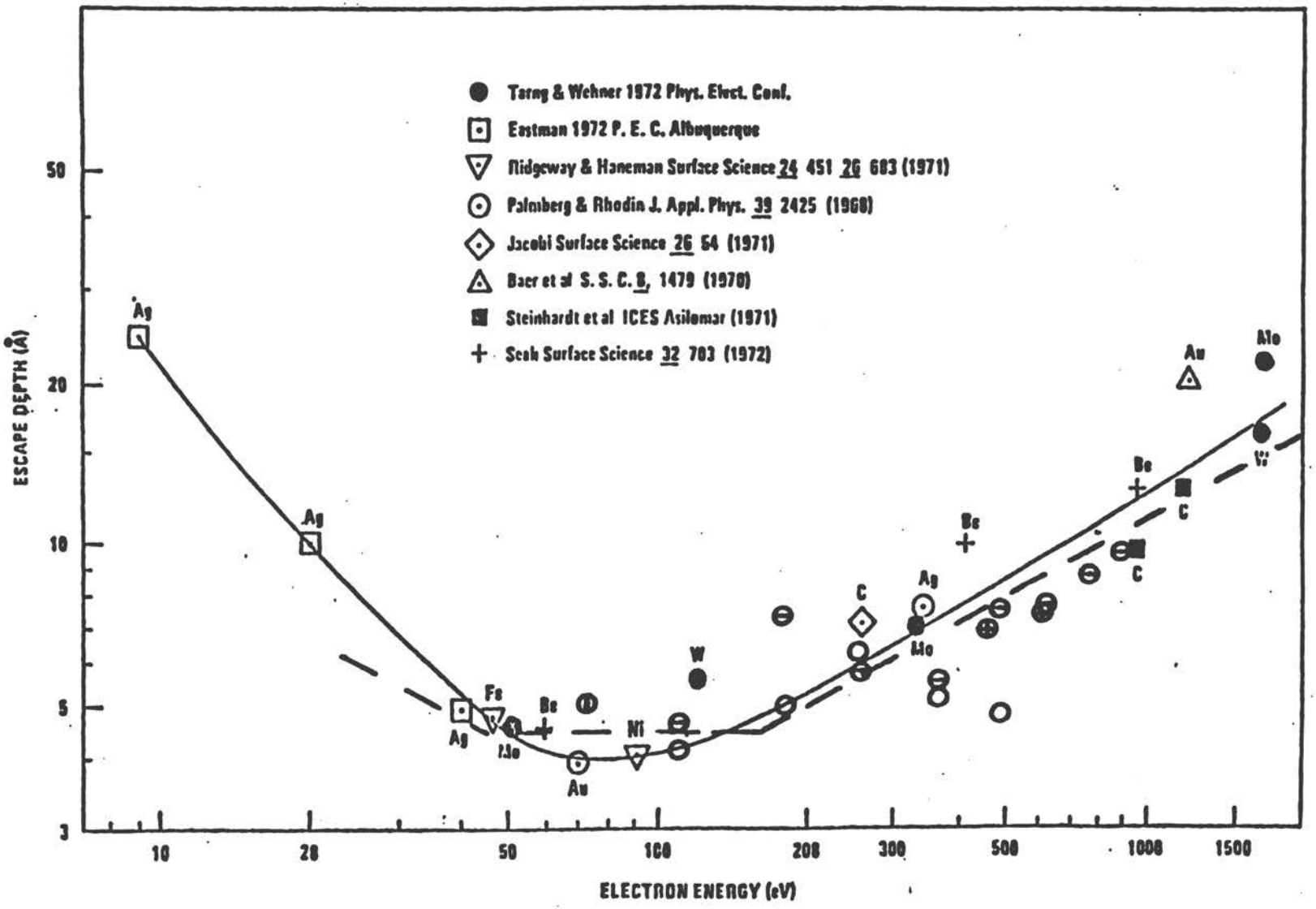
For valence band electron studies:

Photons: $h\nu \sim$ 10's of eV (vacuum u.v.)

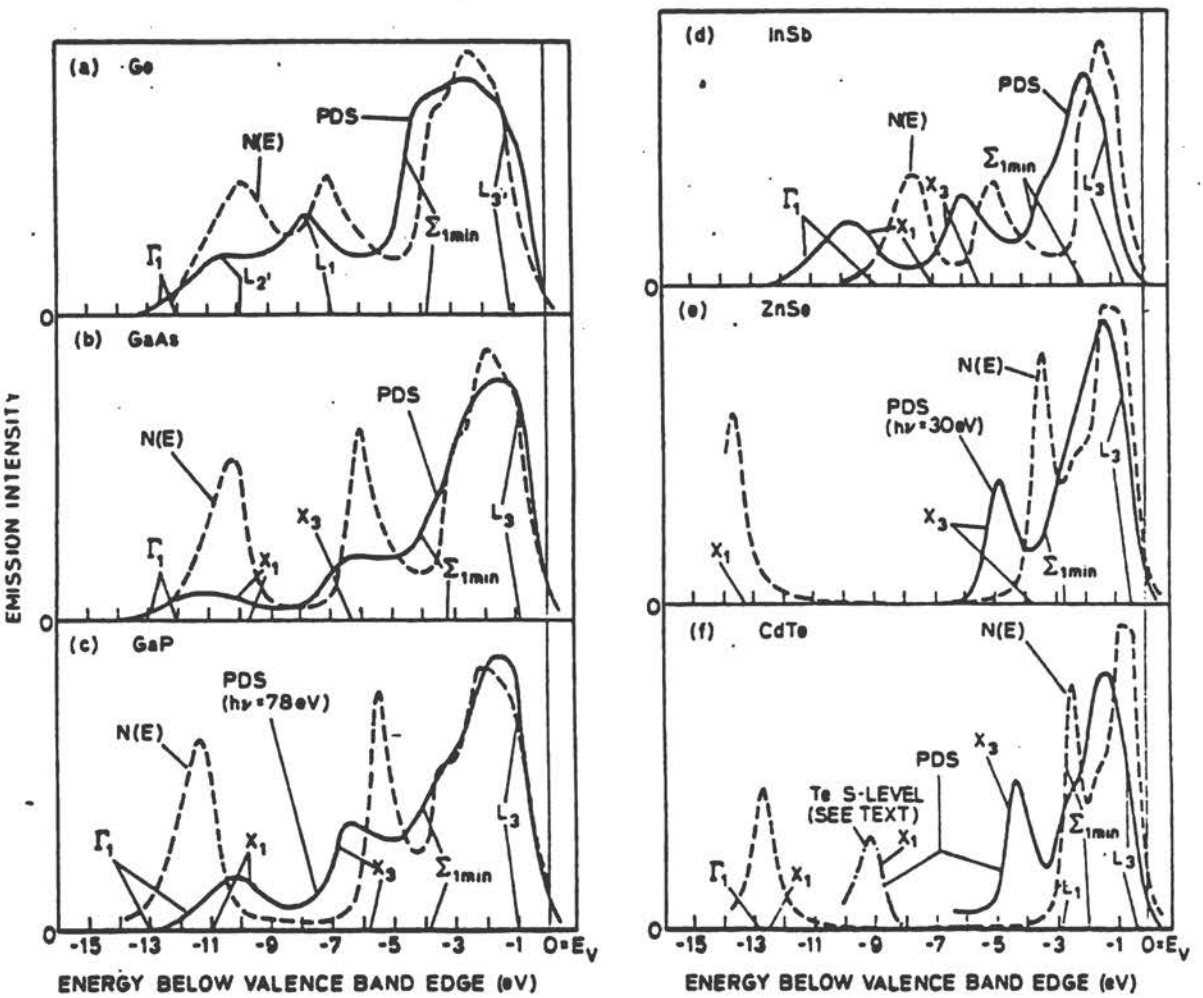
Can be line sources, but synchrotron is tunable; monochromators have resolution of 0.1Å (0.005 eV) typically.

Electrons: spectrometers have energy resolution as good as 0.01 eV.

An important feature of these experiments is that the photoelectrons must get out of the material. This makes them sensitive to material within $\lesssim$ 100Å of the surface. Varying the photon/electron energies gives some control as the figure on the next page shows. It is possible to measure bulk densities of states or to do experiments where only 1 or 2 atomic surface layers are probed.


Tarng & Wehner 1972 Phys. Elect. Conf.
Eastman 1972 P. E. C. Albuquerque
Ridgeway & Haneman Surface Science 24 451 26 683 (1971)
Palmberg & Rhodin J. Appl. Phys. 39 2425 (1968)
Jacobi Surface Science 26 64 (1971)
Baer et al S. S. C. 8, 1479 (1970)
Steinhardt et al ICES Asilomar (1971)
Seah Surface Science 32 703 (1972)
ESCAPE DEPTH (Å)
ELECTRON ENERGY (eV)
50
20
10
5
3
10
20
50
100
200
300
500
1000
1500
Ag
Mo
Au
W
Fe
Be
Ni
C

The data below are typical of the kind of results that first demonstrated densities of states ten years ago (Dean Eastman's data). Quantitative interpretation of the data is not trivial, and theoretical calculations are also difficult, so agreement between theory and experiment tends to be qualitative.

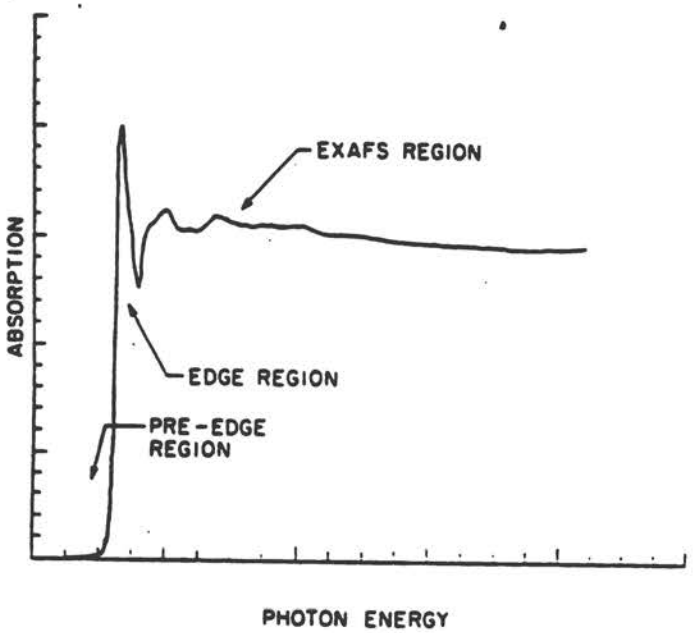


A comparison of energy distribution curves (the background of secondary electrons has been subtracted) for six semiconductors with the calculated density of states according to the empirical pseudopotential method (EPM)

Angle resolved photoemission can be used to study anisotropies in either bulk or surface energy states and can also be used to determine the orientation of molecules adsorbed on the surface.

C. EXAFS (Extended X-Ray Absorption Fine structure)

An examination of the details of the absorption near absorption edges can provide much useful information; the high flux of tuneable radiation from synchrotrons has been essential to the development of this field.



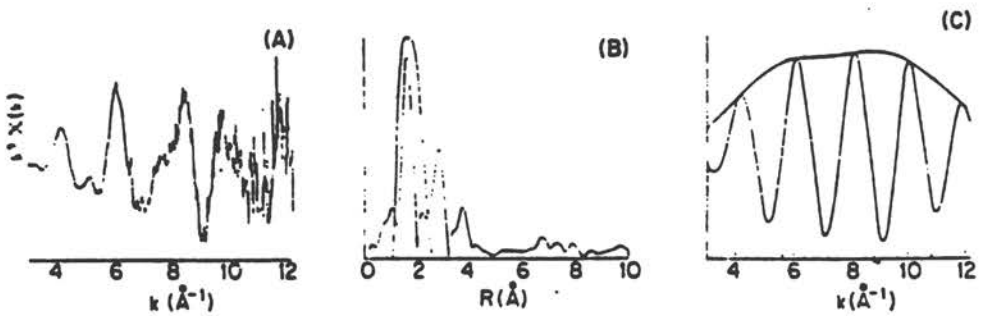
Photon energies needed are those near and up to about 100-1000 eV above the absorption edge of the element being studied.

The structure in the EXAFS region of the spectrum can give quantitative information about the local structure and environment surrounding the atom. Experimentally, if $\hbar\omega > 3$ keV, a beryllium window can separate the sample from the machine vacuum so the sample can be in an air or helium atmosphere.

The physical ideas behind EXAFS are simple. The excited photoelectrons leaving the atom are matter waves and can be scattered back by surrounding atoms. It is the interference between outgoing and back-scattered waves that modulates the absorption. Information on near-neighbour and often further coordination distances can be obtained. The energy resolution needed in the incident photon beam is a few eV, which is readily obtained by a double crystal monochromator. A simple ionization chamber usually serves as a broad-band detector for the radiation transmitted by the sample.

Analysis of the data is not trivial, since one needs to know electron wave functions quite well. One must also know the amplitude and phase of the back-scattered photoelectrons. Inelastic processes and thermal motion of the atoms add further complications. Many of these difficulties have been overcome and near-neighbor distances can be measured with a precision of 0.01Å. The technique works for crystals, amorphous materials, liquids, and any other state of matter.

As an example, Eisenberger and his colleagues have measured the Fe-N distance in the porphyrin ring of oxy and de-oxy states of hemoglobin.



(A) The oscillating part of the absorption spectrum of a concentrated solution of oxyhemoglobin (~25 mM in heme), after conversion to k space, multiplication by k^3, and background removal. Measurements were made by fluorescence. The Fourier transform of (A) is shown in (B), where the large peak contains contributions from the 4Fe-N in-plane ligands and the oxygen and nitrogen axial ligands. The filter window is applied to the transformed data (B) and the inverse transform is computed. The resulting filtered data are shown (C). The Fourier transform technique also yields the amplitude (C) and phase (not shown) of the filtered data. Further analysis, described in the text, removes the contributions of the axial ligands from the phase function, making it possible to determine the in-plane Fe-N distance to ±0.01 Å.

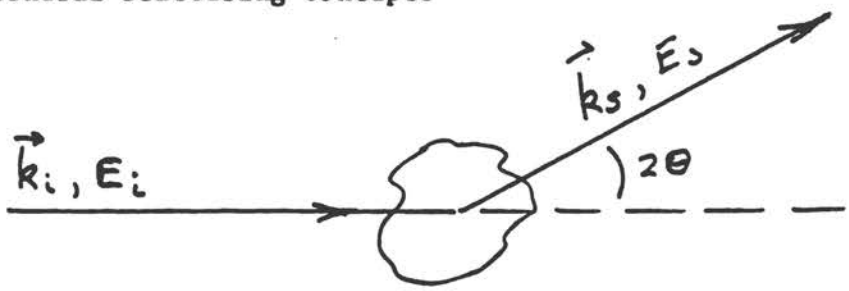
It is also possible to use EXAFS to determine the local structure of biological materials, such as enzyme nitrogenase.

III. SCATTERING SPECTROSCOPY

A. Relation to Real Space Studies

One approach to study the structure of matter is by real space imaging - microscopes and their relatives. One cannot see details finer than the wavelength of the probe used, but good electron microscopes can give resolution approaching 1 Å. There is not much work done to study dynamical behavior with real space imaging, but there is overlap in the details of structure which can be observed with real space imaging and scattering - which measures the Fourier transform of the real space image.

B. General Scattering Concepts



$\vec{q} = \vec{k}_i - \vec{k}_s$ momentum transferred to sample

$\hbar\omega = E_i - E_s$ energy transferred to sample

When $k_i = k_s = k$

$$q = 2k \sin\theta \qquad \text{(Bragg's Law)}$$

Scattering is by spatial Fourier component of property that causes probe to interact with matter; wave length is $2\pi/q$ and ranges from very long, as $\theta \to 0$, to half wavelength of probing particle, as $\theta \to 180°$.

The table below gives what one observes with typical scattering probes.

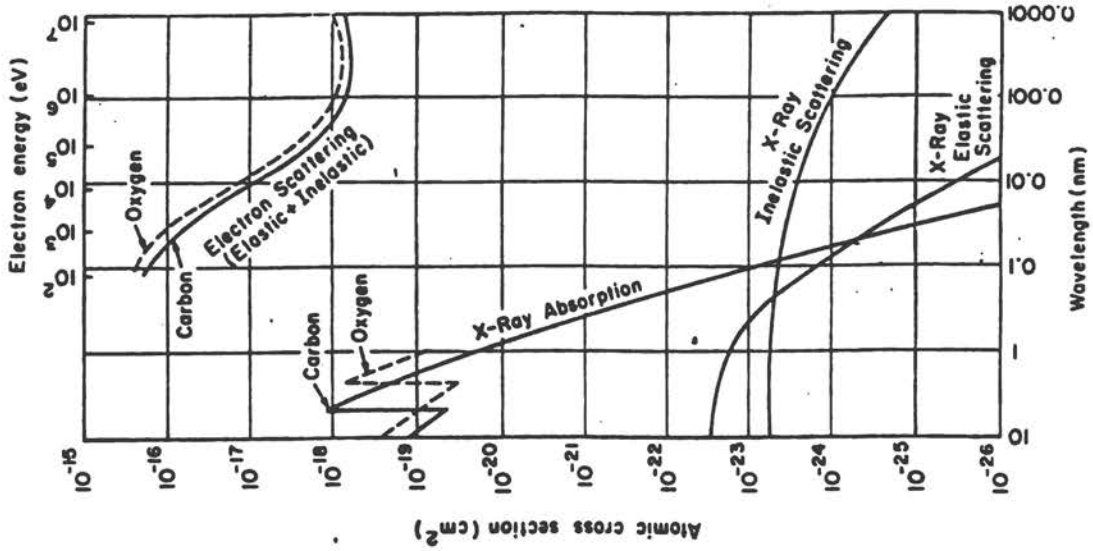
Probe	Sees Spacial Fluctuations in:
electrons	charge density
neutrons	mass density, magnetization
visible photon	dielectric constant
x-ray photon	electron density (= mass density)

The wavelength of the probe determines the smallest scale on which structure can be seen. Another important variable is the momentum space resolution in the scattering process; better resolution means the ability to see if order extends over longer distances. Thermal fluctuations in condensed matter are determined by the degrees of freedom, symmetries, normal modes and response functions of the matter. Fluctuations frequently determine what phases are allowed to exist in nature and their properties. Scattering spectroscopy probes these directly, which is why it has become such an important tool.

C. Electron Scattering

Basic interaction is Coulomb, hence measures charge distribution. Complicated by relativistic and exchange effects. One can probe "bulk" properties with energies Ei ~ 300 kV; at small scattering angles, fast electrons, exchange effects are small. The major use of electron scattering up to now has been low energy electron diff-raction (LEED). Choose Ei so that $\lambda i \approx 1\text{Å}$; this allows probing struc-ture on an atomic scale. The electrons of these energies (few 10's of volts) do not penetrate beyond the surface. Cross sections are large, as the graph on the following page shows. Thus LEED is a very sensitive probe for revealing the structure of surface layers. The momentum space resolution is moderate; one can determine the range of order if less than a few hundred Angstrams.

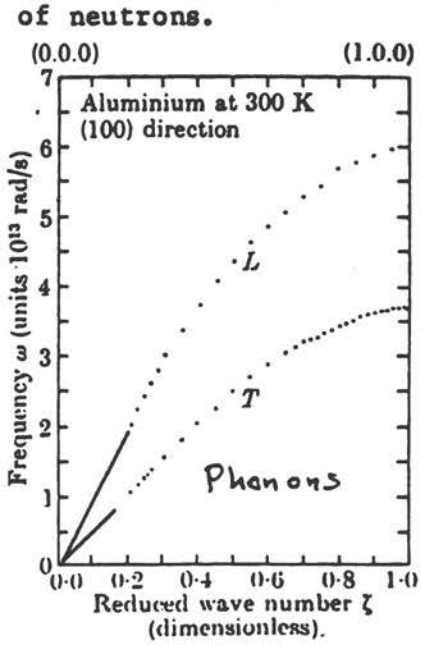
The main difficulty with LEED measurements comes from the strong interactions which make it so sensitive. Multiple scattering is common and quantitative interpretation is difficult.

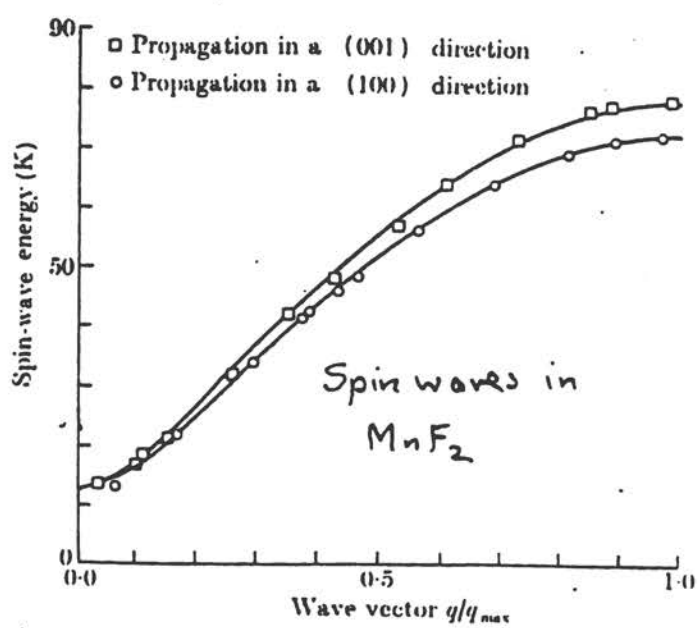


D. Neutron Scattering

One uses neutrons that have been "thermalized" to a Maxwellian distribution of momenta corresponding to the temperature of the moderator, ~ 30 meV for room temperature. This gives $\lambda \sim 1.6$ Å, ideal for probing details on an atomic scale. Since the neutron energies as well as the energy of thermal fluctuations in condensed phases are about the same, there is an ideal energy match for the study of dynamical behavior by means of energy transfer to the scatterer. Neutrons are scattered by magnetic interactions as well as collisions with nuclei. They can be used to study magnetic ordering as well as positional ordering in condensed matter.

Energy and momentum resolution is usually accomplished by Bragg scattering from crystals; graphite is commonly used. Momentum space resolution is modest, the range of order up to about 500 Å or so can be studied. Energy shifts of less than 1 meV are readily detected in scattering experiments. Time of flight can also be used to measure energies and is especially useful with pulsed sources of neutrons.





The two figures on the previous page show some classical things measured by neutron scattering - phonon and spin wave dispersion curves. Neutrons have also been very important in studying phase transitions and critical phenomena, especially in magnetic materials.

E. X-Ray Scattering

This has, and will continue to be, revolutionized by synchrotron sources - when compared with the best available conventional sources. The x-ray flux emerging from a storage ring or insertion device is naturally collimated, by relativistic effects, to about 10^{-4} radian in the vertical plane. Mirrors can be used to focus in the horizontal plane and several hundred watts of x-rays are thus available. By trading photons for resolution, collimation to the Darwin width of perfect Ge or Si crystals (about 0.005 degrees) is readily obtained. With a probe whose k_i is 4Å^{-1} ($\lambda \simeq 1.5\text{Å}$), a momentum space resolution of 5×10^{-4} Å^{-1} is thus obtained. With this, the range of order can be followed on length scales exceeding 1 μm. By grazing angle incidence (the refraction index of most materials to x-rays is slightly less than one, so total external reflection can occur), x-ray scattering can be made surface sensitive. The flux is often sufficient to observe scattering from less than one monolayer of adsorbed atoms or from hydrocarbon films two molecules thick. As an example of these kind of results, below I show data of Moncton, et.al, from December 1982 Phys. Rev. Letters for x-ray scattering from a liquid crystal film two molecules thick.

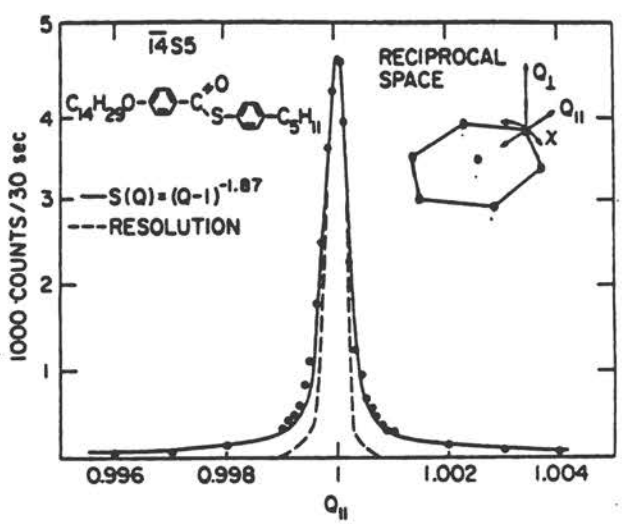


FIG. 1. High-resolution longitudinal scan taken at 65°C in an $N = 2$ film of $\overline{14}$S5 showing the fit to a two-dimensional power-law structure factor $S(Q) \approx (Q-1)^{-2+\eta}$ where $\eta = 0.13$. The resolution is shown by the dashed line. The in-plane momentum transfer $Q_\parallel$ is in units of $2\pi/a = 1.4177$ Å^{-1} $- (6.6 \times 10^{-4}$ Å^{-1} deg$^{-1})(T - T_{AB})$ for $T > T_{AB} = 66.5$ °C. Inset: the general scattering geometry.

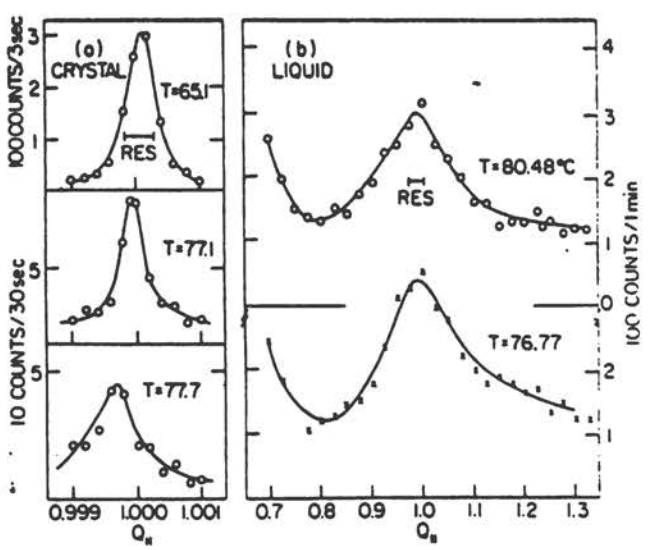
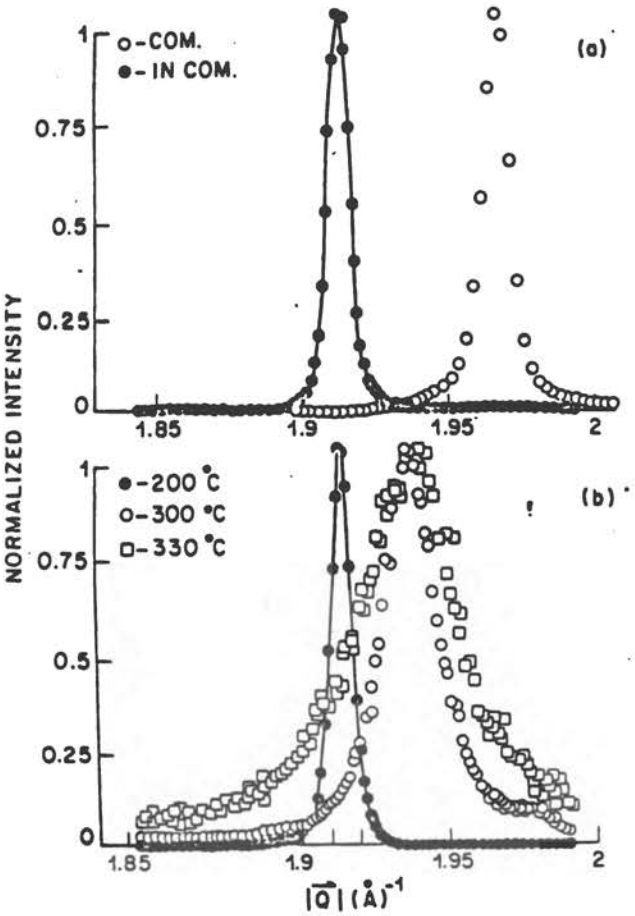


FIG. 2. Longitudinal scans in an $N = 2$ film taken as a function of $Q_\parallel$ (the in-plane momentum transfer) at temperatures approaching the melting transition (a) from below and (b) from above.



The figure at the left shows measurements by Marra, Fuoss, and Eisenberger of the melting of a monolayer of lead on a copper crystal substrate. The greatest shortcoming of x-ray scattering is the lack of energy resolution. Typical photon energies are ~ 8 keV and energy shifts of 1eV can be measured. To study dynamical behavior in condensed matter, energy shifts of 10^{-3} eV should be detected. Because they integrate over energy, present x-ray scattering experiments measure instantaneous electron-electron correlation functions; they give us an instantaneous or "snapshot" picture of the material. There is potential for improving this situation. With bright sources, the x-rays can be focused to very small areas so that quite small samples of matter can be studied - samples less than 0.05 mm x 0.05 mm are possible. Because the x-rays are produced from bunches of electrons circulating in the storage ring, they arrive in pulses of a fraction of a nanosecond duration. The use of time-resolved x-ray scattering to study dynamical behavior on nanosecond or slower time scales is just beginning to be explored.

PHYSICS RESEARCH OPPORTUNITIES WITH SYNCHROTRON X-RADIATION

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ABSTRACT

New X-ray sources of substantially increased brilliance would be available from undulator magnets operating on a new-generation 6 GeV storage ring. To understand what research opportunities would be provided by such improved sources, a number of existing x-ray scattering techniques are briefly described with a qualitative analysis of their requirements for source brilliance. In addition to improvements of existing techniques which will permit application to a generally broader range of problems, new opportunities for magnetic and inelastic x-ray scattering are discussed.

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A revolution in x-ray research has resulted from the availability of synchrotron radiation from storage ring bending magnets and recently from wiggler magnets.[1-3] Another extraordinary improvement in source brilliance is anticipated when undulator magnets begin to produce coherent x-ray beams on the next generation of higher energy (6 GeV) storage rings.[4] These new devices will provide many new opportunities for x-ray research not possible with current sources.

There are two basic classes of synchrotron x-ray experiments — scattering and spectroscopy. Both of these techniques will be considerably improved by the next generation of sources of increased brilliance. In this paper, the emphasis will be on the research frontiers and particularly the impact of brilliance.

The history of x-ray source brilliance, with is defined as the number of photons per second per unit source area per unit source divergence per 0.1% bandwidth, is shown in Figure 1. The brilliance of a conventional x-ray tube is on the order of 10^7 photons/sec x mm^2 x $mrad^2$ x 0.1%BW. The introduction of rotating anodes increased brilliances in the early sixties by an order of magnitude. The introduction of synchrotron sources produced the first qualitative improvement in brilliance over the x-ray tube; effective brilliance was increased by some four to six orders of magnitude. Although there is an enormous difference (about two orders of magnitude) between using a bending magnet during parasitic beam time at the Stanford Synchrotron Radiation Laboratory, and using the 54-pole wiggler[3] during dedicated operation, these are quantitative increases when viewed in this historical perspective. The brilliance potentially available from an undulator on a 6 GeV ring represents a further increase of five to six orders of magnitude, and it will drive the next generation of synchrotron x-ray science.

Figure 2 describes the properties of synchrotron radiation. It shows the fundamental relationships between the critical wavelength produced by a bending magnet which provides a continuous spectrum as a function of wavelength and energy, and the undulator on which the new generation of experiments will be based. The undulator produces a peaked spectrum in which the photon wavelength, λ_p^m, depends on the harmonic number m, the magnetic period of the device λ_u, the electron energy γ (in units of mc^2), and a factor which includes the K parameter of the undulator device. This parameter is simply the magnetic field strength times its period, that is $K = 0.93\ B(T)\lambda_u(cm)$. One can tune an undulator over a small (say 10%) range by varying the magnetic field by changing the gap between the permanent magnet poles. A better way to tune it would be changing the magnetic period, but the technical aspects associated with this technique have not yet been studied in any detail.

The performance of an x-ray undulator on a 6 GeV machine running at some 100 milli-amps is shown in Figure 3. At a photon wavelength of 1Å this device would produce an approximately isotropic cone of radiation, emitting into a solid angle $(\Delta\theta)^2$ given by two times the photon wavelength over the length of the undulator. For a device 2 meters in

length, $\Delta\theta \approx 10^{-5}$ radians. All the radiation of the fundamental wavelength would be transmitted by a pinhole 10 microradians in angular size; at 20 meters from the source this aperture would be 200 microns in diameter. The flux at the fundamental wavelength would be approximately 10^{15} photons/sec x 0.1% BW, and the brilliance about 10^{19} photons/sec x mm^2 x $mrad^2$ x 0.1%BW.

Having described the characteristics of undulator radiation, it is appropriate to provide a general overview of the new research opportunities before discussing specific examples. Figure 4 shows a general space-time plane which can be used to locate various physical phenomena. The ordinate denotes momentum transfer (in inverse angstroms) going to successively smaller resolutions, and distance (in millimeters) going to successively smaller length scales. The abscissa denotes energy, in volts, going to successively smaller energy scales and time, in picoseconds, going to successively smaller time scales. Currently, experiments with x-rays are generally done outside the central region. That is, they are done with energy-transfer resolution of less than 1 eV. They are done with momentum-transfer resolution generally poorer than 10^{-3} inverse angstroms. They are done with real-space resolution generally poorer than 10 microns, and they are done with time resolution generally longer than about a nanosecond. These are not hard boundaries. There are experiments which penetrate in various ways, but they are exceptions. The x-ray undulator, however, will permit us to work routinely in the central region. It is also very exciting to note that there will be possible overlaps. It will be possible to do both diffraction and microscopy simultaneously. It will be possible to do inelastic scattering and time-resolved scattering.

The principal techniques using synchrotron radiation in the x-ray region are based either on spectroscopic or diffraction techniques. Absorption spectroscopy[5], of course, is the technique that grew along with the development of synchrotron radiation. It grew increasingly more sophisticated as synchrotron sources grew more sophisticated, and it is an example which demonstrates very nicely how increases in flux and in brilliance have impact on the quality of science that is possible. Today, absorption spectroscopy experiments are routine and they have been used in many different areas. The following papers on materials science and biological applications will describe some of the most interesting applications. The present discussion is concentrated entirely on scattering: elastic scattering and inelastic scattering. Research based on these techniques constitutes the strongest case for the high-brilliance devices which will be available on the next generation of high-energy (6 GeV) storage rings.

Elastic scattering experiments are extraordinarily well-matched to synchrotron sources primarily because the natural opening angle of the radiation is on the order of a Darwin width of a perfect crystal. Thus, a momentum-transfer resolution on the order of 10^{-3} to 10^{-4} inverse angstroms is naturally achieved. Conventionally, such scattering instruments[6] have an energy resolution on the order of 1 eV. The energy resolution is not particularly important in an elastic scattering experi-

ment except to reject Compton and fluorescent background. Later in this paper possibilities will be discussed for inelastic scattering experiments which will improve the energy resolution in order to access the region of thermal excitations in condensed matter.

Concentrating on elastic scattering experiments, there are a variety of different types of techniques: high Q-resolution, time-resolved diffraction, small angle scattering, anomalous scattering, standing wave diffraction, white-beam techniques, and grazing incidence scattering. Examples of each of these techniques will be described below to show in general what experimental work is being pursued and how these techniques would each individually benefit from the brilliance of the new generation of sources. Note also that there are new opportunities and new techniques such as magnetic x-ray scattering which will be impossible without the flux and brilliance of new sources. Similarly, diffraction microscopy would represent an important opportunity available with the new sources.

Before discussing the specific techniques, let me review the important general elements of brilliance. As described above, brilliance is the number of photons per sec per unit solid angle and unit area of the source. Scattering experiments require flux, collimation, and small beam size in varying degrees. Flux is necessary for studying lower-Z materials, for studying samples with few scattering particles (such as atomic microclusters), and for performing time-resolved experiments. Collimation is necessary in scattering experiments to study long-range coherence. In some cases collimation in only one angular direction is adequate, and the broad fan of highly collimated radiation from bending magnets and wigglers is utilized. But in other cases, such as in small-angle scattering and in some applications in wide-angle scattering (e.g., glancing angle scattering and transmission experiments in two-dimensional systems) it is exceedingly important to have a beam collimated in both spatial dimensions. Finally, the requirements for beam size: for studying small crystals; for restricted access as in a high-pressure experiment in a diamond-anvil cell; for investigating atomic clusters in narrow beams;and for diffraction microscopy. All of these applications involve sample dimensions on the 10- to 100-micron size scale. To summarize the impact of brilliance, if a technique or experiment has a requirement in each one of these categories - flux, collimation, beam size — it benefits directly from a high brilliance source. It is possible with an optical element, to trade collimation for beam size, but one can only improve both with sources of increased brilliance.

Now let me turn to specific examples. Figure 5 shows a diamond-anvil cell used in high-pressure diffraction experiments.[7] In order to access the crystal, which is typically on the order of 10-100 microns in size, one needs to get the radiation in and out through a relatively narrow angle defined by the gaskets. The diffraction experiment requires high collimation. Therefore, source brilliance will be the determining factor. Continuing on the theme of high pressure, it is important to mention that undulators proposed for a 6 GeV ring would produce fundamental radiation up to 20-kilovolt energy range. Such high-energy pho-

tons are one of the important advantages of these proposed high-energy machines. High-pressure experiments demand high-energy photons for penetrating the diamond cell. The signal measured in an experiment is a combination of the intensity, the transmission, and the reflecting power. Calculations[7] show that maximum signals are achieved at about 15 keV (λ = 0.8 Å).

The standing wave method[8] is another technique demanding brilliance. In these experiments a highly collimated x-ray beam is Bragg-reflected from the surface, as shown in Figure 6. During the process of dynamical reflection, a standing wave field penetrates the surface and atoms on or in the surface layers are excited into fluorescence. This signal depends on the atoms' location relative to the standing wave field, allowing the determination of the atommic positions. This technique requires a highly collimated incident beam to precisely define the incident angle. Furthermore, to look at a reasonably small area on the surface, a beam with relatively small size is necessary. Therefore, this technique benefits directly from brilliance. The best example of this research so far is the study of bromine on the surface of silicon. Figure 6 shows a scan of the crystal through its Darwin curve and the fluorescence from bromine. The location of the fluorescence peak relative to the rocking curve determines the position of the Br atom above the surface.

Grazing-incidence scattering[9-11] is another technique for getting information on the surface structure of materials, as shown in Figure 7. This method has been developed over the last few years, and it is a good example of the importance of brilliance. Grazing incidence scattering requires very high collimation in both the vertical and horizontal directions. High collimation is necessary in the diffraction plane in order to get high-resolution diffraction information. But high collimation is also necessary in the grazing-incidence direction in order to define the angle-of-incidence with adequate precision, since the angle-of-incidence is directly related to the penetration depth. Therefore, collimation in both spatial directions is extremely important. Again, small beam sizes are required because at glancing angles the sample does not have a large effective area. The requirements for both vertical and horizontal resolution, for small beam size, and for large flux (e.g., if it is a low-Z material) are precisely the requirements for brilliance. Using these grazing-incidence techniques, a variety of experiments have been done. One example is the study[10] of the commensurate-incommensurate transition of monolayers of lead on copper as shown in Figure 8. A study of the reconstruction of Germanium (100) has also been undertaken.[11] In favorable cases, for example Au(110),[12] rotating anode fluxes are adequate to do glancing-angle experiments, with signals of 10 counts a second. But for Si(111) 7x7, the signals are 10^4 weaker and it is impossible to use a laboratory source. The first Si(111) 7x7 reconstruction peaks were recently observed at SSRL.[13] We see an increasing number of surface structural problems where good x-ray structural information is already available or should be shortly. Ultimately, synchrotron x-ray techniques will permit the determination of the structures of surfaces with a degree of certainty that has been available for standard three-dimensional crystallography for some time.

The next example chosen is a variant of the glancing-angle technique using a liquid sample, as shown in Figure 9. This is very difficult diffraction geometry since the liquid surface must be kept horizontal. Note that this experiment is also very demanding in collimation as well as flux. Using surface reflection scans, such as shown in the Figure, direct measurements have been made of the surface-induced smectic A phase above the nematic to smectic A phase transition in liquid crystals.[14]

Surface diffraction[15-17] studies can often be done to advantage in a transmission geometry, which also requires two-dimensional collimation. If the incident wave-vector is very well defined in its divergence in the diffraction plane one can measure long coherence lengths. However, if this radiation comes from a bending magnet or a wiggler, it will have a large divergence perpendicular to the plane, which will mean that the resolution function is elongated. Two-dimensional scattering is a rod in reciprocal space, as shown in the inset to Fig. 10, and it is oriented perpendicular to the resolution function in the transmission geometry. The anisotropy of the resolution function is such that failure to match the resolution with the scattering profile reduces the signal by up to a factor of 100. With an x-ray undulator, which would provide a very highly collimated beam in both spatial directions, one would have an isotropic resolution function. As a result, transmission-geometry experiments, which are favorable for many cases, could be performed without paying this large price in signal.

Figure 10 shows some results from an experiment[15] that was done without the advantages of resolution focusing. This experiment demonstrates the lack of long-range order in two-dimensional crystal systems confirming theoretical predictions made decades ago, and helping to establish the basis for the study of 2D melting. Another approach to the study of 2D phase transitions involves graphite substrates. A whole family of measurements on phase transitions of various types has been made using exfoliated graphite samples.[16] Recently data from monolayers on single crystal graphite has been obtained[17], as shown for krypton in Figure 11. The signal rates are reasonably substantial, on the order of 1000 counts per second, using an 8-pole wiggler at SSRL. However, if one is considering a more ambitious experiment, considerably more flux is necessary. One experiment that is very interesting is the behavior of monolayer helium.[18] Scaling the krypton data shown in Figure 11, one would predict a count rate of 1 count/sec with existing sources. The improvement anticipated at the new facilities would be about an order of magnitude more flux, using an instrument which could provide wave vector resolution of about 10^{-4} $\AA^{-1}$. Large bandwidth multilayer monochromators could be used to gain an additional factor of 100 in signal at the expense of resolution. This trade-off would be advantageous for studying the 2D crystal-to-superfluid transition.

Time-resolved diffraction studies are also in the category of flux-demanding experiments. Figure 12 displays some results from time-resolved experiments[19] done at Cornell in the last few years looking at the properties of silicon and germanium during laser annealing. In this experiment, the diffraction pattern is measured as a function of angle.

The x-ray beam is synchronized with the laser-annealing pulse to follow the behavior of the surface structure as a function of time after the initiating laser pulse. As shown in Figure 12 the Bragg peak is extended, showing the thermal heating of the surface. From these data it is possible to determine a precise thermal profile of the surface and follow in detail the process of recrystallization following the laser pulse. In this work, the time resolution was on the order of 5 nanoseconds.

There are interesting time-resolved experiments spanning a wide range of time scales, and an example of data taken on the scale of minutes is shown in Figure 13. This particular experiment involves small-angle scattering studies of phase separation in borate glass.[20] Although such experiments are possible on the time scale of minutes, one has a great deal more flexibility in choice of problem (that is, shorter time-scale) if more photon flux is available. Note also that small-angle scattering experiments are experiments which need two-dimensional collimation, so x-ray undulators are the ideal sources.

I would like to turn now to a discussion of prospects for new kinds of experiments which have not yet been undertaken on existing storage rings. One of these is magnetic scattering.[21] There is a relativistic term in the interaction of the x-rays with matter that couples the electromagnetic field of the photon to the magnetization of the solid. The scattering structure factor is down by two to three orders of magnitude and the cross-section for iron, for example, is down by about 10^6. Although these cross-sections are small, scattering should be easily measured with available fluxes from storage rings.

The opportunity exists to do experiments that are not in the traditional area for neutron research, for example very high Q-resolution magnetic scattering. Wave vector resolutions of 10^{-4} A^{-1} come naturally with a synchrotron x-ray scattering instrument. It turns out that there are terms in the magnetic cross-section which differentiate the spin and the orbit. There are anomalous magnetic-scattering effects. Unlike neutron scattering, small samples are perfectly adequate for x-ray experiments. One could study magnetic materials which have high neutron-absorption cross-sections and, most interestingly, it should be possible to study surfaces. Surface-enhanced magnetism is an interesting field and very little good data are available on the magnetic structure of surfaces. There should be magnetic analogues to the surface-reconstruction problems, and these could potentially be seen with the high-brilliance sources.

A second example of new techniques which demand brilliance is inelastic scattering, with energy resolution on the order of thermal (meV) energies. Inelastic scattering experiments have been done, although not to a great extent, with ≈1 eV energy resolution.[22] Moving into the regime of a few millivolts[23] would greatly increase the range of study of physical phenomena of interest in condensed matter physics.[24] There would be a number of potential advantages of x-rays in the range of energy and momentum transfers where interesting cooperative phenomena take

place. Of course, x-rays have the general advantage that they couple directly to the electronic charge. There are additional specific advantages in each of the three separate regions of energy and momentum transfer shown in Figure 14. In region I excitations in disordered materials can be studied without the kinematical restraints of neutron scattering. In area II, the energy transfer regime above 100 meV, x-rays techniques are ideal. A 15-keV photon can easily transfer energies in this regime, whereas the neutron flux available from reactor sources at these energies is very small. Finally, region III is the high momentum-transfer range, which is the work horse region for neutron scattering. Here x-rays would offer some complementary advantages to neutrons: small samples, neutron-absorbing materials, and perhaps the study of the dynamics of surfaces, for example.

Inelastic scattering depends, of course, on being able to get energy resolutions in the millivolt range. It is well known that using back-reflection techniques with perfect crystal monochromators one can achieve these kinds of energy resolutions. Figure 15 shows the energy resolution as a function of photon energy for various Bragg reflections in silicon. There are two curves which derive from two different types of structure factors for silicon reflections. Reflections with high Miller indices excited by photons in the 10-keV to 15-keV range will naturally provide energy resolutions below 10 meV. To implement techniques or instruments based on these ideas requires fairly elaborate engineering, particularly if the sources that will be used are not of high brilliance. One has to collect a large number of x-rays, both in the monochromatic beam and in the scattered beam. It is necesssary to bend the monochromator and analyzer crystals into a spherical shape. Bending introduces a strain which is hard to eliminate. Elaborate strain-relief schemes are being studied but the technology is difficult and such monochromators have not yet been achieved. Although we are optimistic that success will result, it has not yet been achieved. In the context of x-ray undulator sources, many advantages would be obtained for inelastic scattering with this highly collimated radiation. The technique is greatly simplified. It is not necessary to bend a crystal and no elaborate optical systems are required for focusing. Starting with a highly collimated source, one can use a flat pre-monochromator, a flat back-reflection monochromator, and another flat or cylindrically-bent back-reflection analyzer. With this instrument samples that are less than a couple of tenths of a millimeter will be adequate. Thus, it is clear that an x-ray undulator would be of great advantage for inelastic x-ray scattering.

Is millivolt resolution the limit for inelastic x-ray scattering? Probably for routine experiments that will be the limit, but other techniques are currently under discussion. One such method involves using nuclear-resonant scattering from Fe^{57} to monochromate x-rays to a level of 10^{-7} eV.[25] Using beams from the proposed 6 GeV x-ray undulator, one would have some 10^{6} to 10^{7} photons/sec. These levels are similar to beams from a standard x-ray tube, but with one part in 10^{11} monochromaticity. There are many interesting experiments which could be performed with this energy resolution, particularly in the dynamical properties of condensed matter and in iron-containing biological structures.

In conclusion it should be emphasized that it is not generally possible to predict the most exciting science that will be possible using improved sources of radiation. In this paper an attempt has been made to demonstrate the crucial importance of source brilliance in determining the limits of various current x-ray scattering methods. From this basis it is straightforward to envision the improvement of existing techniques which will result with a gain of 10^5 provided by x-ray undulators on a 6 GeV ring. Generally these involve improved resolution in real space, in reciprocal space, in time, and in energy. They involve extensions to studies of lower scattering cross-sections resulting from small sample volume, lower-Z constituents, small displacement modulations, and weak scattering processes. The range of improvement is so vast that lists of specific examples do not do justice to the scientific possibilities.

In spite of the strength of the above arguments, the most exciting science to be done at new facilities will probably not be based on existing methods but on new methods which are simply not possible with current brilliance levels. Two examples of these new techniques are x-ray holography and sub-meV inelastic x-ray scattering. Nevertheless, as strong as this argument is, the history of x-ray and neutron source development shows that even the predicted new techniques are often eclipsed in importance by unpredicted discoveries which occur as scientists begin to actually use the new sources. By providing five orders of magnitude improvement over current facilities, these new sources will undoubtedly be rich sources of scientific discovery.

In preparation of this paper I have benefitted from collaboration and conversation with colleagues too numerous to mention. I hope it will suffice to generally thank the x-ray community for their commitment to synchrotron radiation development.

References

1. "Synchrotron Radiation Research," eds. H. Winick and S. Doniach, Plenum Press, New York (1980).

2. "Handbook on Synchrotron Radiation," Vol. 1, E.-E. Koch, ed., North Holland Publishing Co., Amsterdam (1983).

3. A. Bienenstock and H. Winick, Phys. Today 36, No. 6, 48 (1983).

4. See the Proceedings of the New Rings Workshop (SSRL Report 83/02) Stanford, October 1983, K. Cantwell, ed.

5. See article by E. A. Stearn and S. M. Heald in Ref. 2, p. 955.

6. D. E. Moncton and G. S. Brown, Nucl. Instr. Meth. 208, 579 (1983).

7. B. Buras, Nucl. Instr. Meth. 208, 563 (1983).

8. J. A. Golovchenko, J. R. Patel, D. R. Kaplan, P. L. Cowan, and M. J. Bedzyk, Phys. Rev. Lett. 49, 560 (1982).

9. W. C. Marra, P. Eisenberger, and A. Cho, J. Appl. Phys. 50, 6927 (1979).

10. W. C. Marra, P. H. Fouss, and P. Eisenberger, Phys. Rev. Lett. 49, 1169 (1982).

11. P. Eisenberger and W. C. Marra, Phys. Rev. Lett. 46, 1082 (1981).

12. I. K. Robinson, Phys. Rev. Lett. 50, 1145 (1983).

13. I. K. Robinson, private communication.

14. J. Als-Nielsen and P. S. Pershan, Nucl. Instr. Meth. 208, 545 (1983).

15. D. E. Moncton, R. Pindak, S. C. Davey, and G. S. Brown, Phys. Rev. Lett. 49, 1865 (1982).

16. P. W. Stephens, P. A. Heiney, R. J. Birgeneau, P. M. Horn, D. E. Moncton, and G. S. Brown, Phys. Rev. B29, 3512 (1984); P. A. Heiney, P. W. Stephens, R. J. Birgeneau, P. M. Horn, and D. E. Moncton, Phys. Rev. B28, 6416 (1983).

17. K. L. D'Amico, D. E. Moncton, E. D. Specht, R. J. Birgeneau, S. E. Nagler, and P. M. Horn (to be published).

18. K. Carneiro, W. D. Ellenson, L. Passell, J. P. McTague, and H. Taub, Phys. Rev. Lett. 37, 1695 (1976).

19. D. M. Mills, B. C. Larson, C. W. White, and T. S. Noggle, Nucl. Instr. Meth. 208, 511 (1983).

20. S. Bras, A. Craievich, J. M. Sanchez, C. Williams, and E. D. Zanotto, Nucl. Instr. Meth. 208, 489 (1983).

21. P. M. Platzman and N. Tzoar, Phys. Rev. B2, 3556 (1970).

22. P. Eisenberger and P. M. Platzman, Phys. Rev. B13, 934 (1976).

23. J. B. Hastings, D. E. Moncton, and Y. Fujii, Proceedings of the Workshop on High-Energy Excitations in Condensed Matter, Los Alamos, February 13-15, 1984, R. Silver, ed.

24. S. Doniach, Proceedings of the Workshop on High-Energy Excitations in Condensed Matter, Los Alamos, Feb. 13-15, 1984, R. Silver, ed.

25. See article by R. L. Cohen in Ref. 1, p. 647; A. I. Chechin, N. V. Andronova, M. V. Zelepukhin, A. N. Artem'ev, and E. P. Stepanov, Pis'ma Zh. Eksp. Teor. Fiz. 37, 531 (1983).

Figure Captions

Fig. 1 The history of x-ray sources brilliance is represented by the performance of x-ray tubes including rotating anodes, and various source devices on the SPEAR storage ring. A proposed 6 GeV storage ring designed for synchrotron radiation production could achieve a brilliance of about 10^{19}.

Fig. 2 A summary of the general properties of synchrotron radiation as produced by a uniform magnetic field provided by a storage ring bending magnet and by a periodic field device known as an undulator.

Fig. 3 The properties of the radiation produced by an x-ray undulator on a 6 GeV storage ring would include very high collimation, flux, and brilliance.

Fig. 4 The fundamental physical properties of condensed matter can be categorized according to their spatial and temporal dimensions. Equivalently they are often studied in terms of their energy and wave vector dependence. Current x-ray techniques based on synchrotron radiation cannot routinely access the central region shown above. New synchrotron sources based on undulators on a 6 GeV storage would open this central region to study.

Fig. 5 The principle of a diamond-anvil high pressure cell.

Fig. 6 Schematic illustration (upper figure) of a silicon (111) surface viewed edge-on along a (110) projection. Distances A and B indicate bromine-atom positions above surface. Silicon and bromine atoms are represented by open and closed circles, respectively. The position of the relevant (111) and (220) Fourier components of the charge density are indicated by dashed lines. In the lower figure bromine fluorescence and reflectivity angular yields for (111) Bragg diffraction on a silicon (111) surface. Angular scale is in reduced units where rocking curve width is 2. Ref. 8.

Fig. 7 Grazing incidence scattering geometry.

Fig. 8 Monolayer Pb on Cu(110). Scans (top) show the commensurate (open circles) and incommensurate (filled circles) solid; scans (bottom) as a function of temperature show the changing line shapes as the solid melts. Ref. 10.

Fig. 9 Geometry for diffraction from a horizontal surface is shown in the upper figure. Total reflection ($Q/Q_0 < 0.1$), Fresnel partial reflection and diffraction from smectic A layering at the surface are shown in the lower figure. Ref. 14.

Fig. 10 A scan through the (10) Bragg rod (see reciprocal lattice shown in inset) demonstrates the lack of true long-range order in the two dimensional crystal of $\overline{14}S5$. The scattering fits the power law function (solid line) which is distinctly different from the resolution function (dashed line). Ref. 15.

Fig. 11 A scan thrugh the (10) Bragg rod of a monolayer of Kr adsorbed on a single crystal graphite surface demonstrates the signal rate and resolution obtainable with synchrotron radiation. Ref. 17.

Fig. 12 Results of an initial investigation of laser annealing of pure silicon. Extended Bragg scattering profiles were measured for two different delay times between laser and X-ray bursts; 100 ns (circles) and 195 ns (squares). The "no laser" profile indicates the instrumental resolution. Ref. 19.

Fig. 13 Time evolution of the small angle X-ray scattering at 460°C for a 80 B_2O_3-15 PbO-5 Al_2O_3 glass. The times (min) are 10.0, 18.1, 25.6, 31.1, 37.3, 46.9, 57.0, 67.2, 78.0, respectively, from the bottom to top data sets. Ref. 20.

Fig. 14 An illustration of the energy and momentum transfer regimes accessible using x-ray and neutron probes to study excitations by inelastic scattering. For 14 meV and 100 meV neutron energies, the accessible region is located within the respective inverted parabolas. For a 14.4 keV x-ray, virtually the entire energy-momentum plane is accessible except for a small region $Q(\text{Å}^{-1}) \leq 0.51 \times 10^{-6}$ E (meV). Ref. 23.

Fig. 15 The absolute resolution versus the back-scattering ($2\theta = 179°$) photon energy for the two classes of Bragg reflections in silicon. Ref. 23.

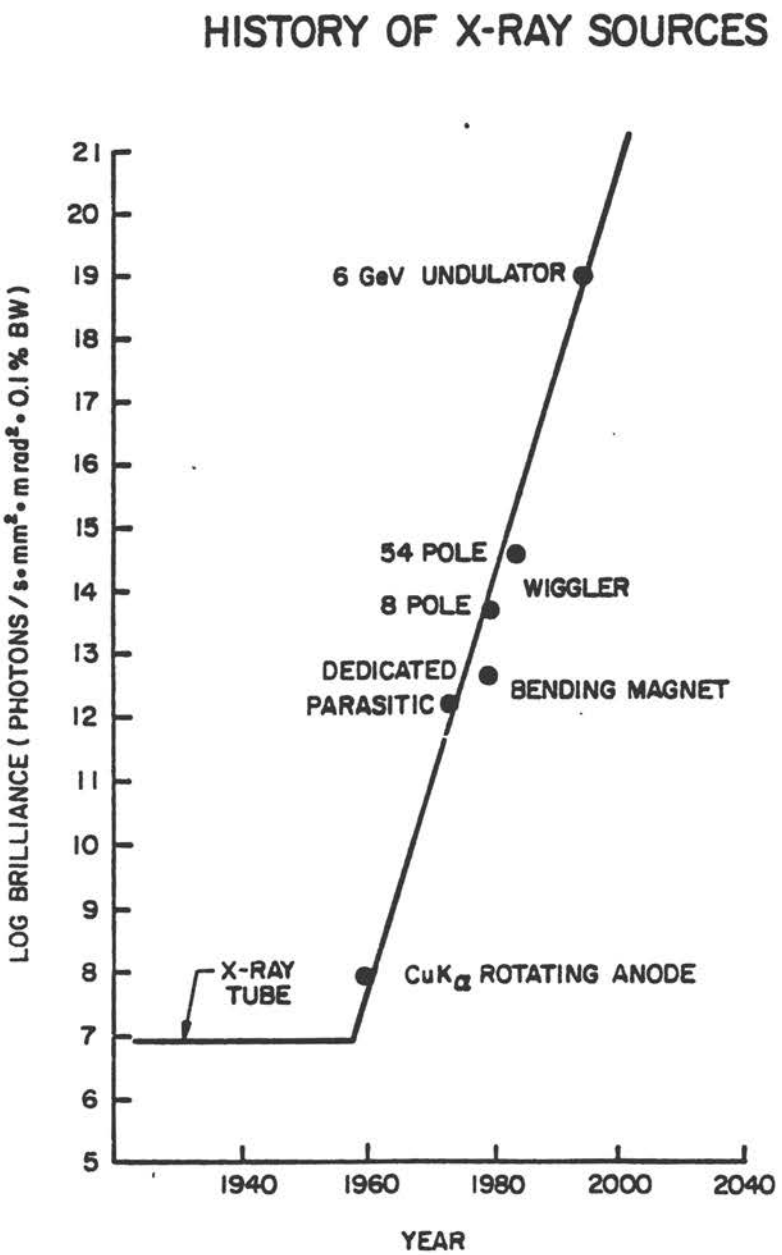
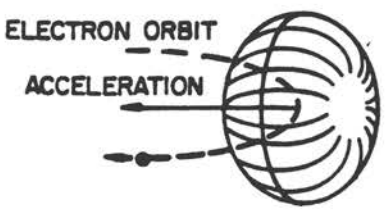
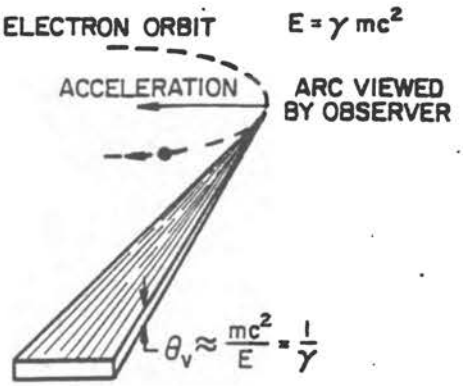

HISTORY OF X-RAY SOURCES
LOG BRILLIANCE (PHOTONS / s • mm² • m rad² • 0.1 % BW)
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
1940
1960
1980
2000
2040
YEAR
6 GeV UNDULATOR
54 POLE
WIGGLER
8 POLE
DEDICATED
PARASITIC
BENDING MAGNET
X-RAY
TUBE
CuKα ROTATING ANODE

Figure 1

SYNCHROTRON RADIATION



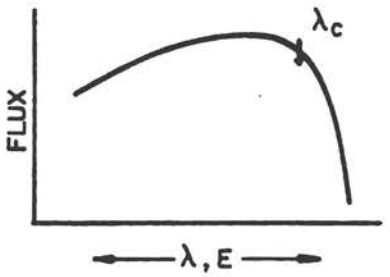


CASE I: $\frac{v}{c} << 1$

CASE II: $\frac{v}{c} \approx 1$

BENDING MAGNET

$$\lambda_c = R/\gamma^3$$



UNDULATOR

$$\lambda_p^m = \frac{\lambda_u}{2m\gamma^2}\left(1 + \frac{K^2}{2}\right)$$

$$K = 0.93\ B(T)\ \lambda_u(cm)$$

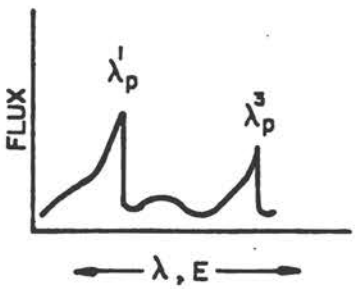


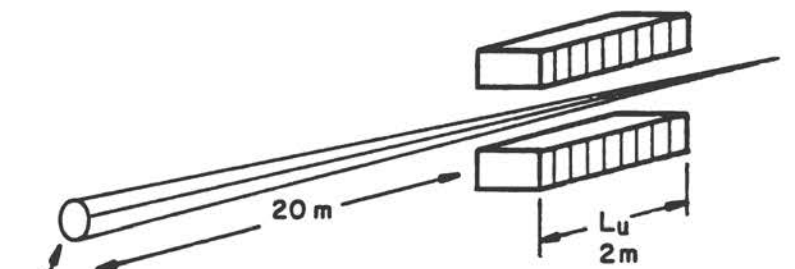
Figure 2

X-RAY UNDULATOR

$E = 6$ GeV $I = 100$ m amp

λ photon $= 1$ Å

$\Delta\theta^2 = 2\lambda_p / L_u$



PINHOLE : $\Delta\theta^2 = 10\ \mu$rad ; DIA. $= 200\ \mu$

FLUX

$\sim 10^{15}$ photons/s • 0.1% BW • 0.1 amp

BRILLIANCE

$\sim 10^{15}$ photons/s • mm^2 • m rad^2 • 0.1% BW • 0.1 amp

Figure 3

SYNCHROTRON FRONTIERS

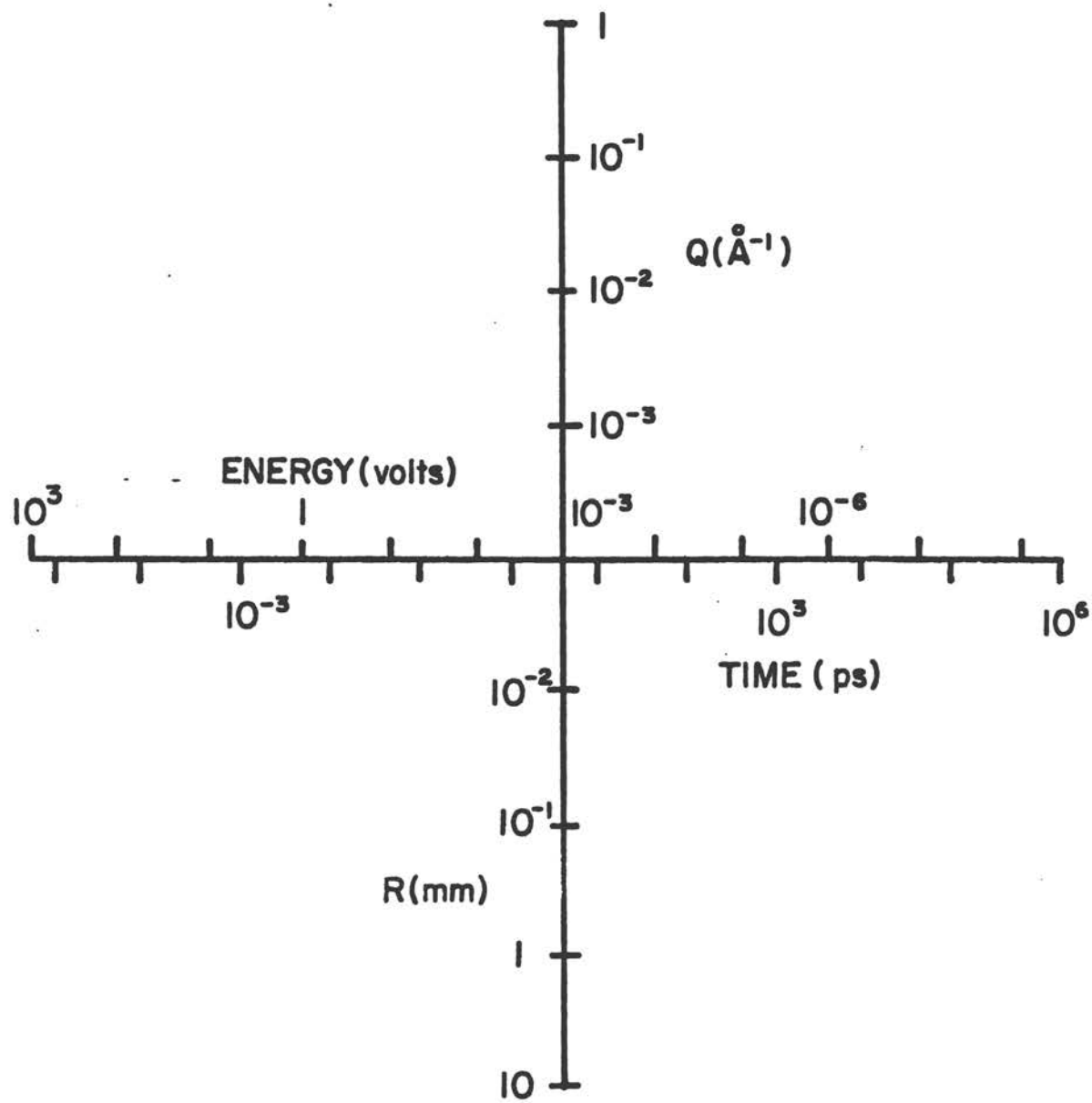


Figure 4

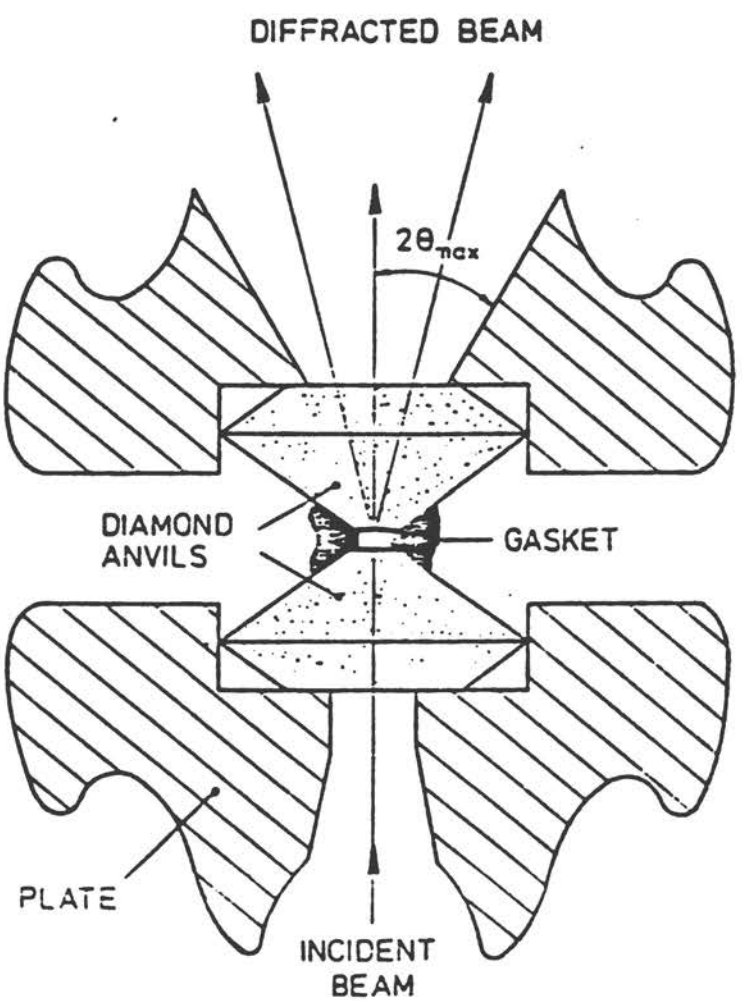
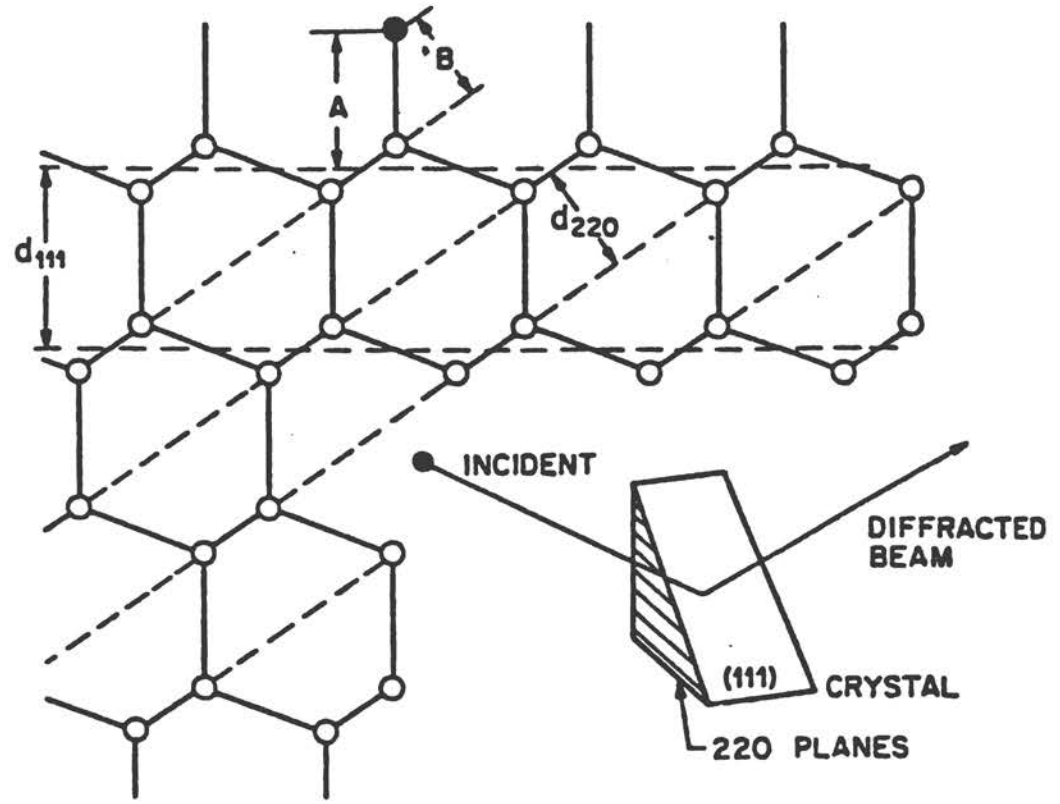

DIFFRACTED BEAM
$2\theta_{max}$
DIAMOND ANVILS
GASKET
PLATE
INCIDENT BEAM

Figure 5


A
B
d_{111}
d_{220}
INCIDENT
DIFFRACTED BEAM
(111)
CRYSTAL
220 PLANES

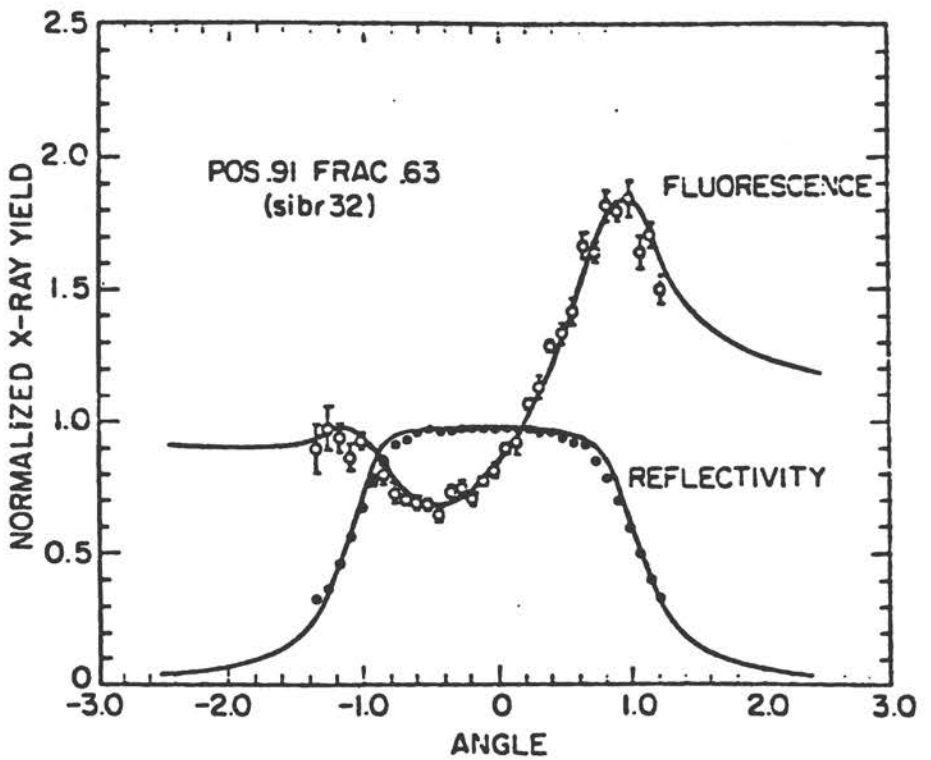

POS .91 FRAC .63
(sibr32)
FLUORESCENCE
REFLECTIVITY
NORMALIZED X-RAY YIELD
ANGLE
2.5
2.0
1.5
1.0
0.5
0
-3.0
-2.0
-1.0
0
1.0
2.0
3.0

Figure 6

GRAZING INCIDENCE SCATTERING

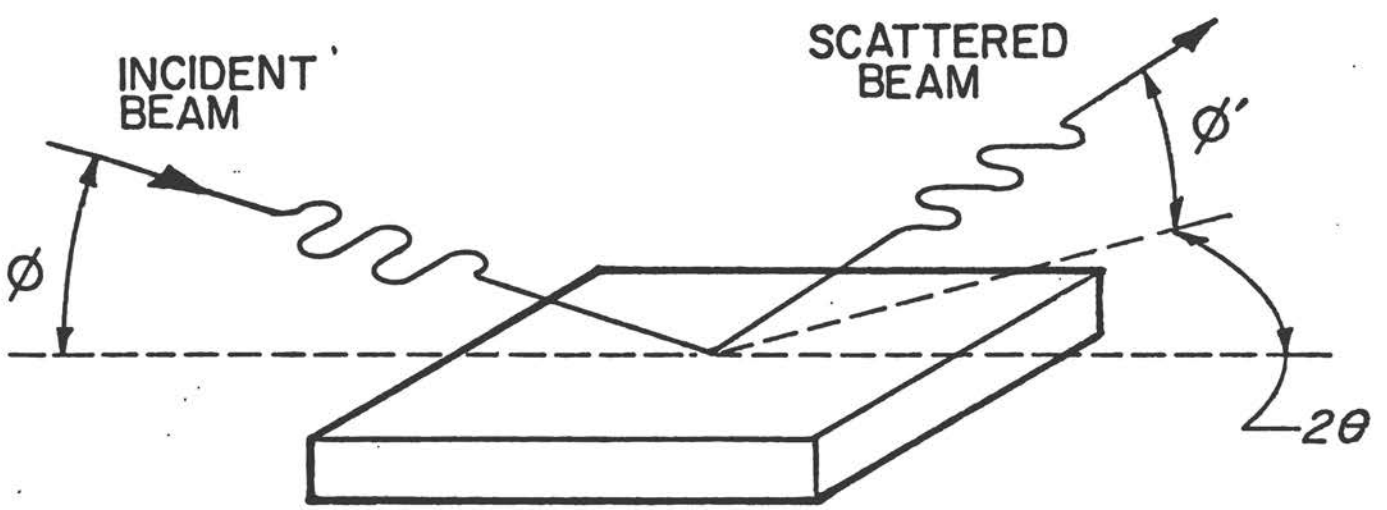


Figure 7

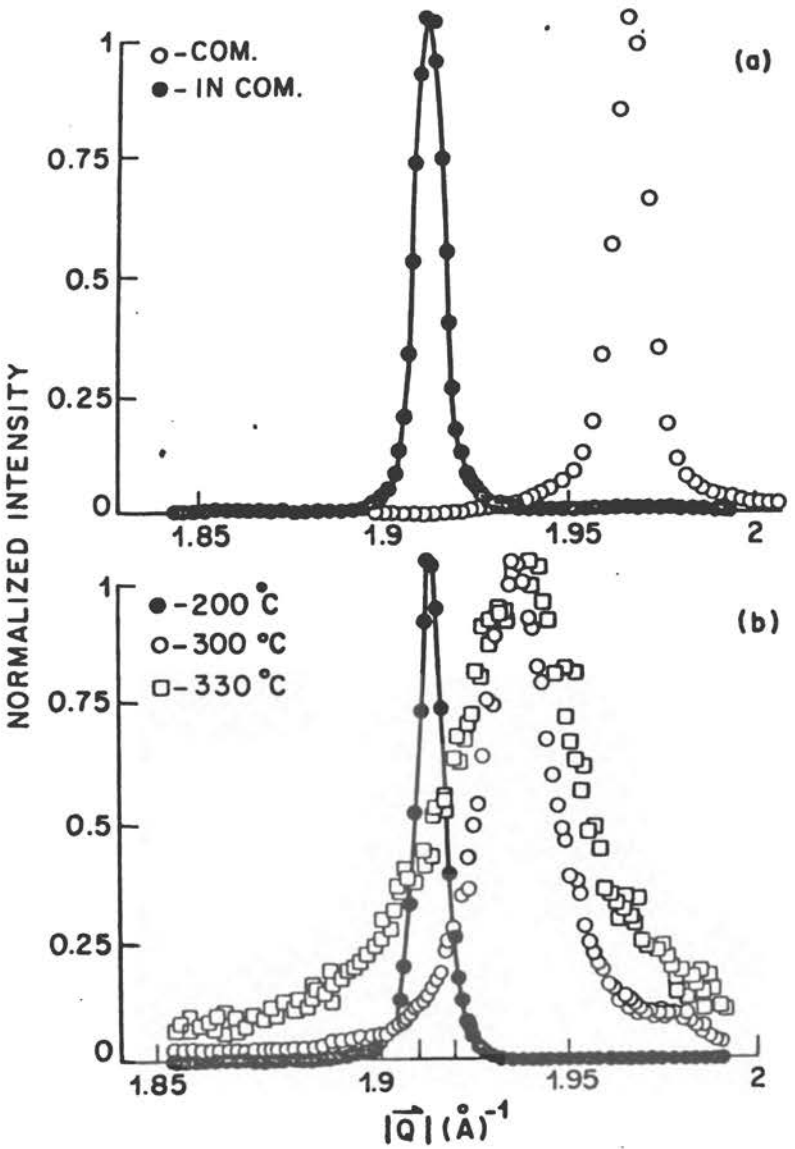
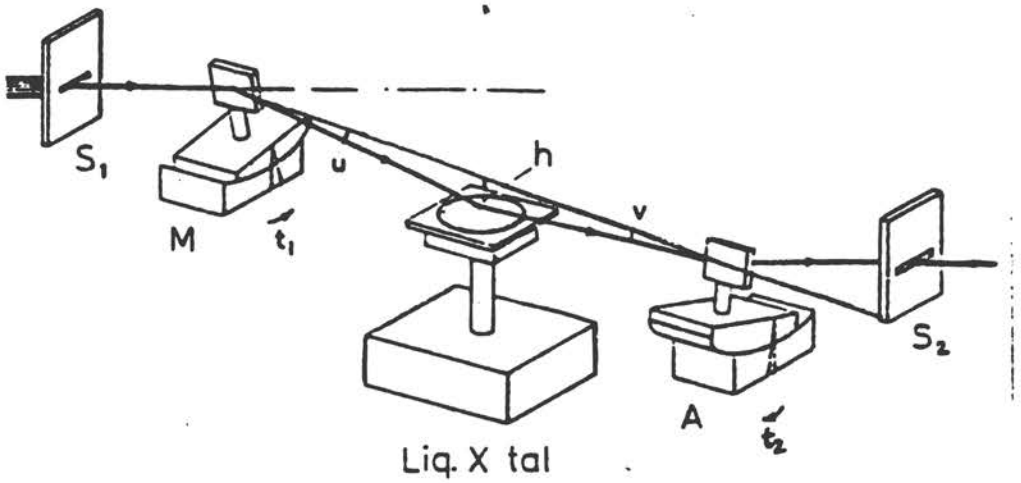

o-COM.
●- IN COM.
(a)
NORMALIZED INTENSITY
1
0.75
0.5
0.25
0
1.85
1.9
1.95
2
●-200 °C
o-300 °C
□-330 °C
(b)
|Q| (Å)⁻¹

Figure 8


S1
M
t1
u
h
v
S2
A
t2
Liq. X tal

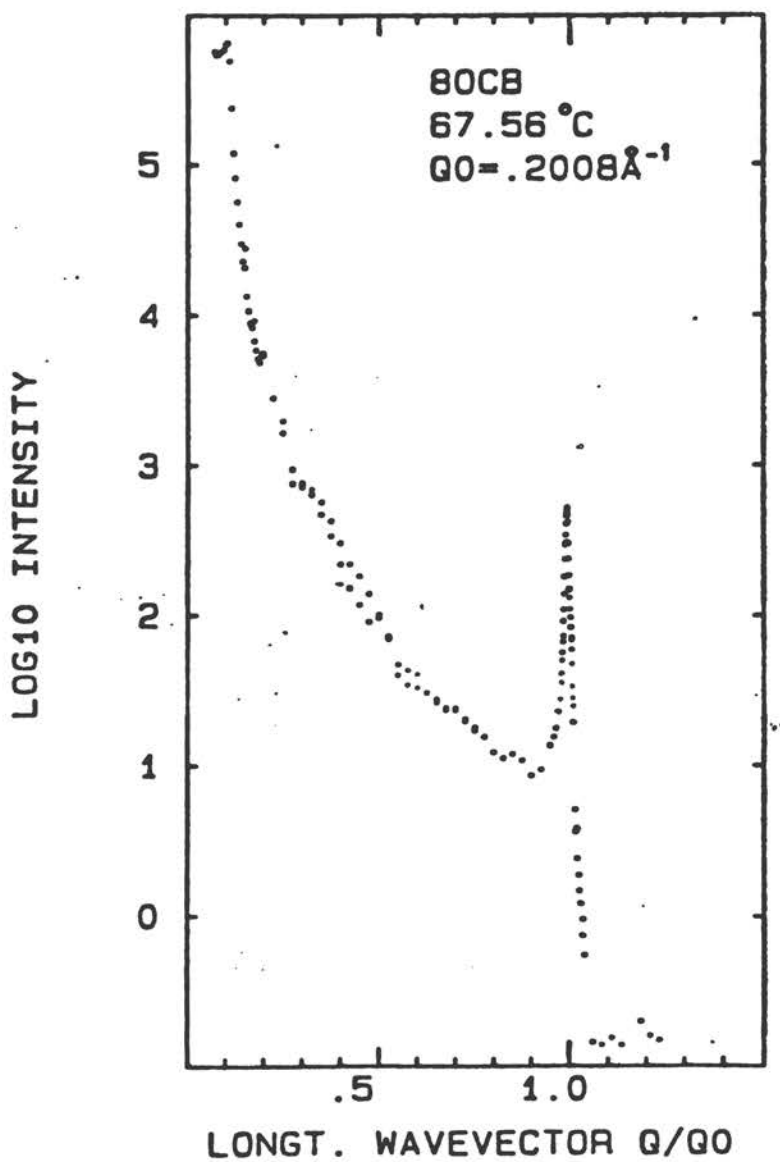

80CB
67.56 °C
Q0=.2008Å-1
LOG10 INTENSITY
5
4
3
2
1
0
.5
1.0
LONGT. WAVEVECTOR Q/Q0

Figure 9

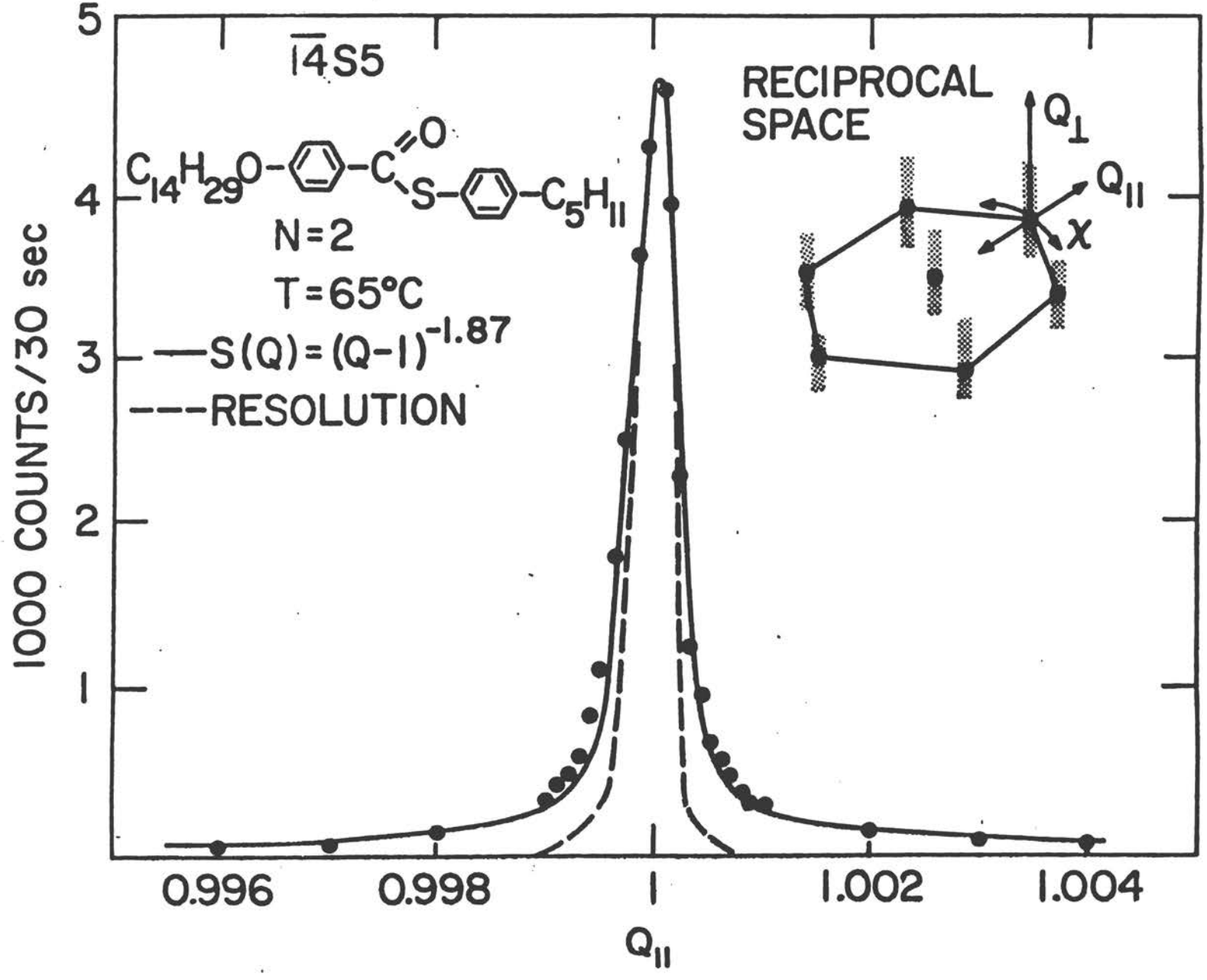

$\overline{14}$S5
$C_{14}H_{29}O-C_6H_4-C(=O)-S-C_6H_4-C_5H_{11}$
N=2
T=65°C
—S(Q)=(Q-1)$^{-1.87}$
---RESOLUTION
RECIPROCAL SPACE
$Q_\perp$
Q_{11}
X
1000 COUNTS/30 sec
5
4
3
2
1
0.996
0.998
1
1.002
1.004
Q_{11}

Figure 10

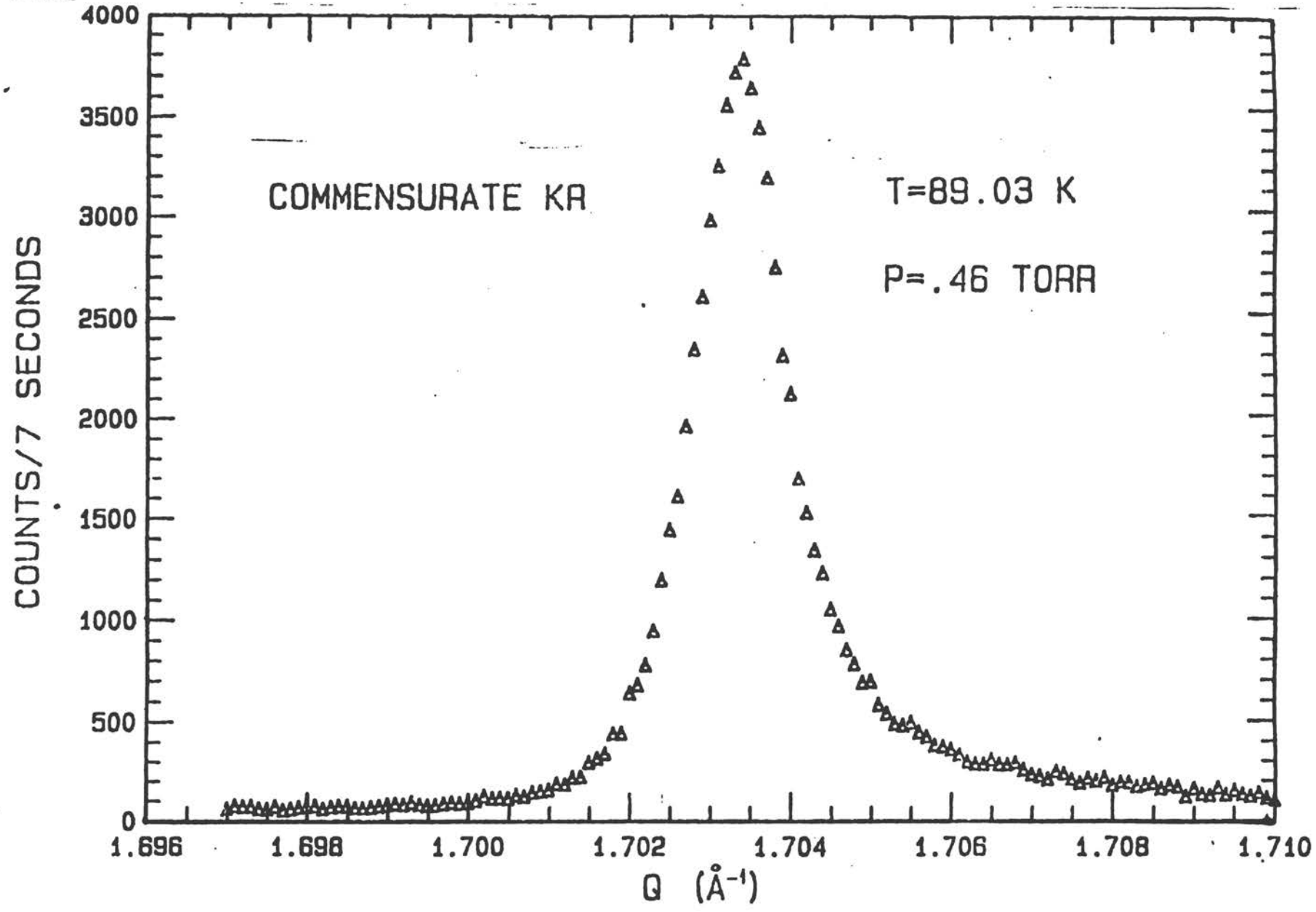
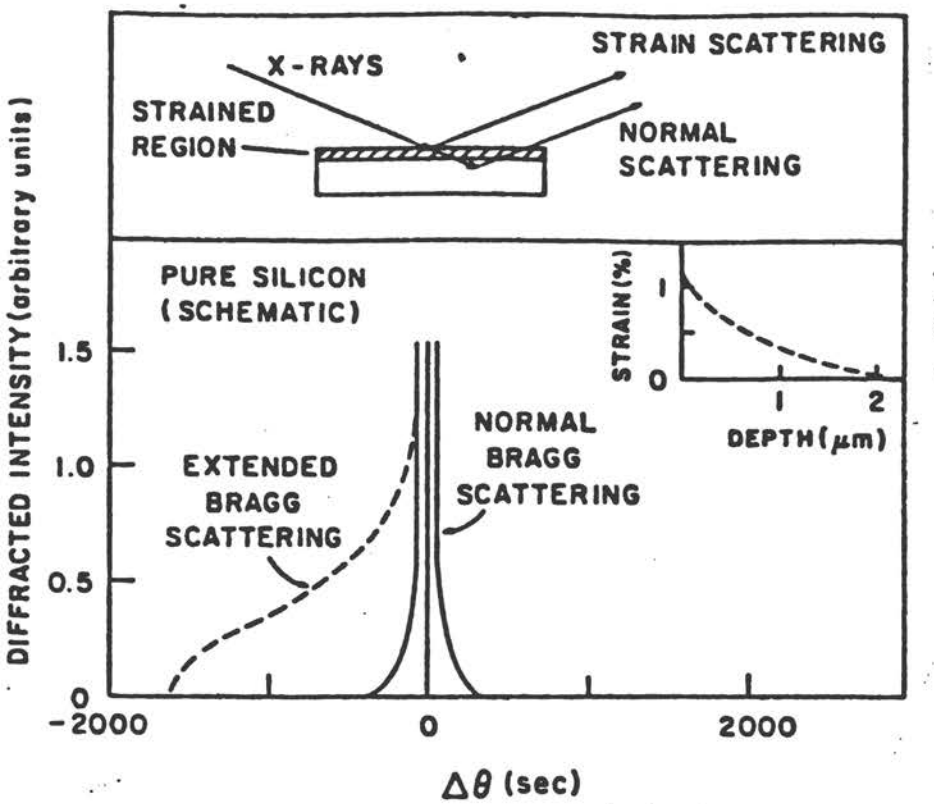

COMMENSURATE KR
T=89.03 K
P=.46 TORR
COUNTS/7 SECONDS
4000
3500
3000
2500
2000
1500
1000
500
0
1.696
1.698
1.700
1.702
1.704
1.706
1.708
1.710
Q (Å⁻¹)

Figure 11


X-RAYS
STRAIN SCATTERING
STRAINED REGION
NORMAL SCATTERING
PURE SILICON (SCHEMATIC)
STRAIN (%)
DEPTH (μm)
DIFFRACTED INTENSITY (arbitrary units)
EXTENDED BRAGG SCATTERING
NORMAL BRAGG SCATTERING
Δθ (sec)

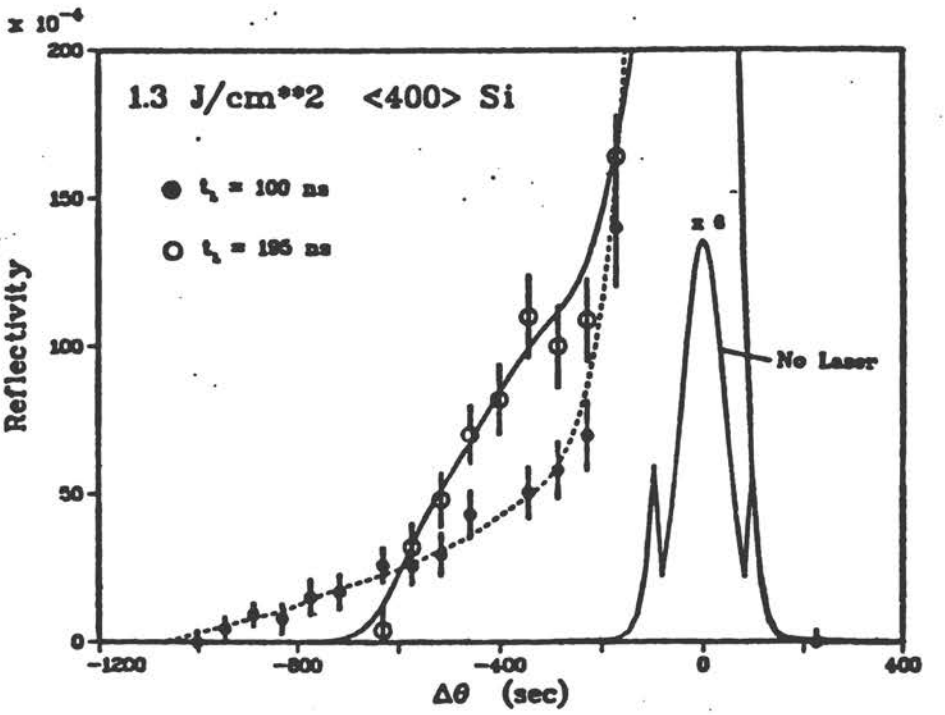

1.3 J/cm**2 <400> Si
Reflectivity
No Laser
Δθ (sec)

Figure 12

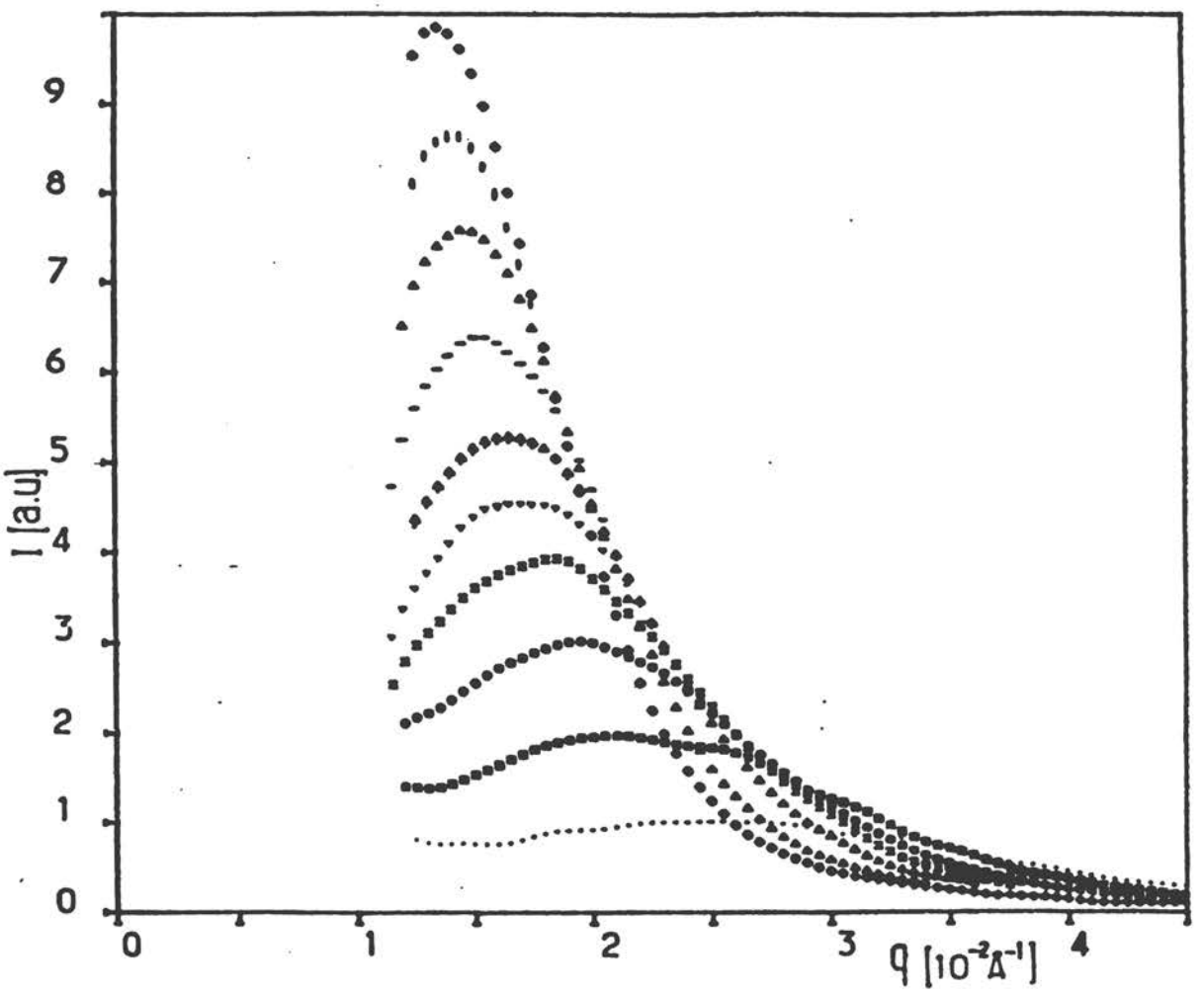


Figure 13

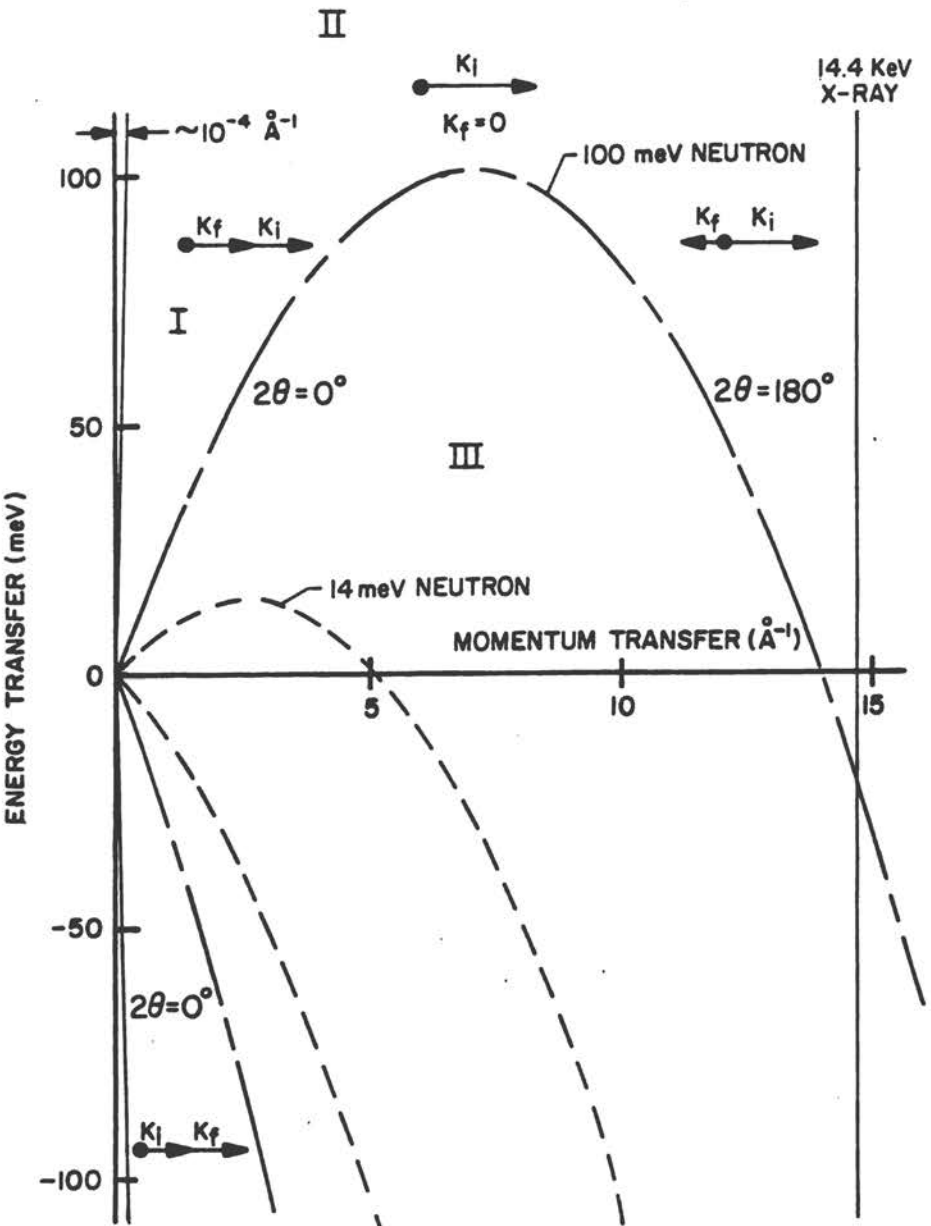

II
K_i
$K_f = 0$
14.4 KeV
X-RAY
$\sim 10^{-4}$ Å^{-1}
100 meV NEUTRON
100
K_f K_i
K_f K_i
I
$2\theta = 0°$
$2\theta = 180°$
50
III
14 meV NEUTRON
MOMENTUM TRANSFER (Å^{-1})
ENERGY TRANSFER (meV)
0
5
10
15
-50
$2\theta = 0°$
K_i K_f
-100

Figure 14

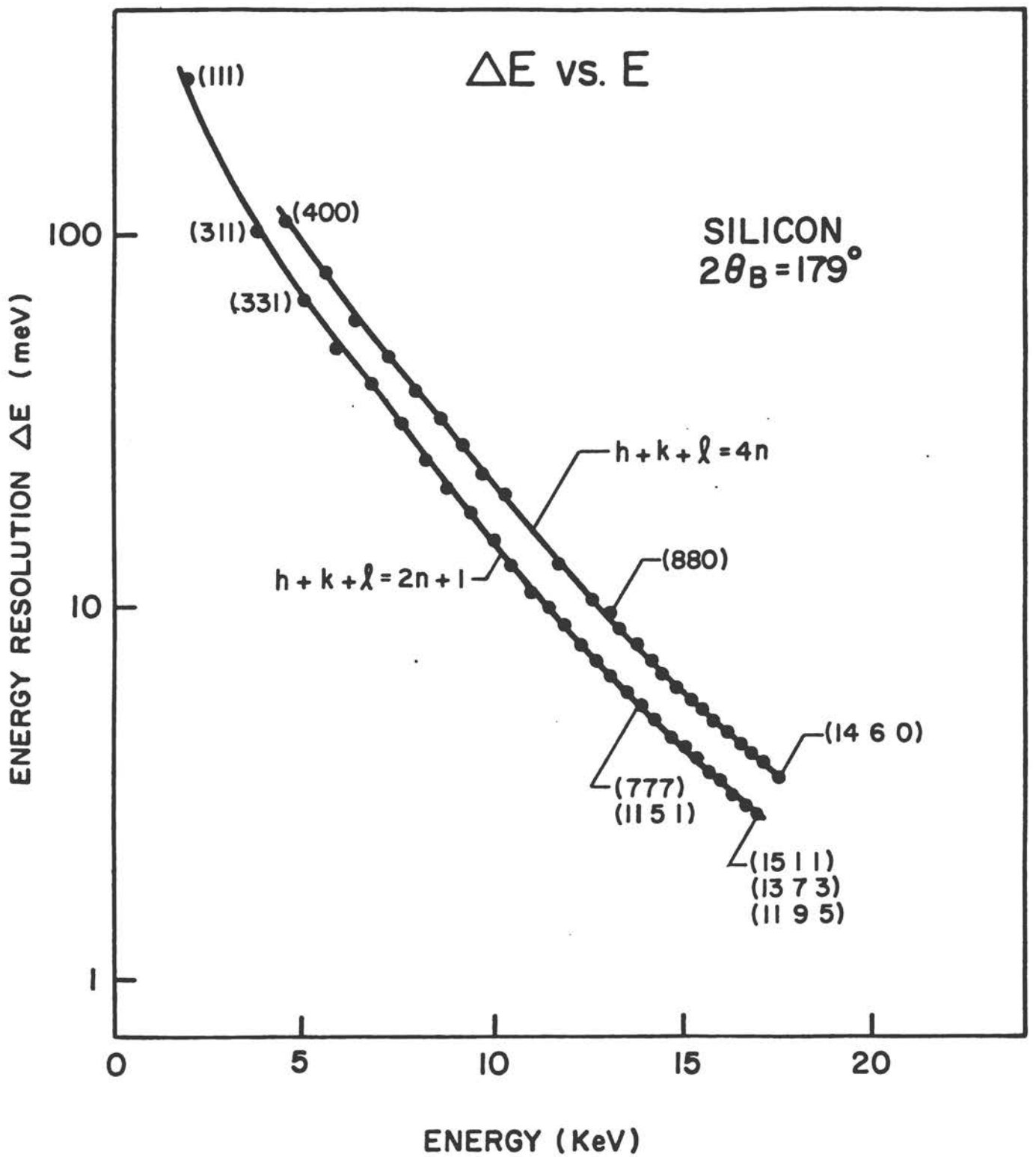

ΔE vs. E
SILICON
2θB = 179°
(111)
(400)
(311)
(331)
h + k + ℓ = 4n
h + k + ℓ = 2n + 1
(880)
(14 6 0)
(777)
(11 5 1)
(15 1 1)
(13 7 3)
(11 9 5)
100
10
1
0
5
10
15
20
ENERGY RESOLUTION ΔE (meV)
ENERGY (KeV)

Figure 15

SCIENTIFIC OPPORTUNITIES WITH VACUUM ULTRAVIOLET (SOFT X-RAY) SYNCHROTRON RADIATION FROM INSERTION DEVICES

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ABSTRACT

An assessment is presented of scientific opportunites with VUV synchrotron radiation created by the availability of next generation electron storage rings with undulator insertion devices. It is shown that such devices coupled to the same beam line optics as presently used with bending magnet sources offer gains of up to five orders of magnitude in the specific photon flux usable in certain experiments. It is argued that this enhancement can lead to qualitatively new science. Selected examples are presented of present and future experiments in three scientific fields: gas phase chemistry and physics, surface science and biology.

1. INTRODUCTION

Traditionally, the name "vacuum ultraviolet" (VUV) has referred to the large spectral range from about 2000 A (6 eV) to about 2 A (6 keV) while radiation in the 300 A (40 eV) to 2 A range has been denoted as "soft X-rays".[1] With the advent of synchrotron radiation[2] it is the spectral region 1000 A (10 eV) to 4 A (3000 eV) which plays a special role. The limits indicate the cut-off energies of typical windows (LiF at low energy, Be at high energy) which may be used to decouple the sample environment from the ultra-high vacuum (UHV) of the storage ring. Therefore, in the spectral range 10 eV to 3000 eV experiments are typically performed in an UHV environment. In the following we shall deviate from tradition and refer to this spectral range synonymously as "VUV" or "soft X-ray".

The scientific importance of the VUV range is largely based on the fact that the valence levels of all elements are accessible with large excitation cross-sections. The study of photon excitations of valence electrons yields direct information on the interaction of valence electrons to form matter (e.g., valence band structure) or on the disintegration of matter (e.g., molecular dissociation, desorption). Furthermore most atomic core levels have binding energies (BE) in the range < 3keV. Their number is more than three times larger than for those with BE's in the X-ray range > 3keV. In particular, the K (1s) shells of the most abundant and chemically and biologically most important elements (with the possible exception of hydrogen) - carbon, nitrogen and oxygen - fall into the VUV range. The K edge energies (1s BE's) for these elements are 285 eV (C), 400 eV (N) and 530 eV (O). Other important K edges in the VUV range are Si

(1840 eV), P (2150 eV) and S (2470 eV). The L edges (2s and 2p BE's) of the 3d and 4d metals and of the technologically important elements Ge, Ga and As also fall into the soft X-ray range. The importance of core level excitations lies in the ability to obtain crystallographic structure information through the scattering processes of the created photoelectron (e.g., EXAFS) in addition to electronic structure information (e.g., chemical shifts).

It is the accessibility of all these electronic energy levels which renders the VUV range of special importance. This importance is best illustrated by the fact that even at an X-ray oriented facility like the Stanford Synchrotron Radiation Laboratory (SSRL) the number of scientific publications over the last 10 years was larger for the VUV (55%) than for the X-ray (45%) spectral range.[3]

The first generation soft X-ray experiments were carried out with synchrotron radiation from bending magnet source points in the storage ring. Experiments in the 10-1000 eV range typically employed reflection grating monochromators while vacuum compatible double crystal monochromators were used in the 1-3 keV range.[4] The most powerful experimental technique used in conjunction with VUV synchrotron radiation has been photoelectron spectroscopy (PES)[5,6] in all its variants such as polarization and angle resolved ultra violet photoemission spectroscopy (PARUPS),[7] X-ray photoelectron spectroscopy (XPS),[5,6] photoelectron diffraction (PhD) and the angle resolved photoemission extended fine structure (ARPEFS).[8] Photoemission studies have been carried out on gases as well as on solids, clean surfaces and gas-solid and solid-solid interfaces yielding detailed information on the electronic and geometric structures.[5-7] Another important technique which relies on the availability of high intensity, tuneable

monochromatic synchrotron radiation is the surface version of the extended X-ray absorption fine structure technique called SEXAFS.[9] This technique is a precise structural tool which in many cases compliments the photoemission techniques. Its importance in the soft X-ray region lies in the structural determination of chemisorption geometries of C, N and O and their molecules. A closely related technique, NEXAFS[10] (for near edge X-ray absorption fine structure), is particularly suited to monitor chemical reactions of low-Z molecules (containing C, N, O, F) with surfaces. It yields information on the molecular orientation, hybridization and bond length. The technique of photon stimulated ion desorption (PSID)[11] from surfaces and its gas phase analogue the photon induced fragmentation (PIF)[12] of molecules has helped our understanding of the dissociation of matter as a consequence of electronic excitations. PSID even promises to be usable as a surface structural tool when used as the signal for NEXAFS or SEXAFS measurements.[13] Besides the utilization of soft X-rays for various spectroscopies it has become apparent that radiation in the 100-3000 eV range is ideally suited for real space imaging. This has been utilized in soft X-ray lithography[14] and microscopy,[15] two techniques which are still in a state of development but promise advantages over conventional imaging techniques by means of electron beams.

While the scientific productivity with soft X-ray synchrotron radiation has been high and gratifying, the question arises where the field is headed. Is the second generation of science expected to just consolidate what is presently done or can we hope for qualitatively new scientific opportunities? It is the purpose of this paper to demonstrate that VUV science indeed has the possibility of yet another quantum jump. This development, which may be of similar importance to the first use of synchro-

tron rather than bremsstrahlung radiation from an X-ray anode, is facilitated by the development of wiggler and especially undulator insertion devices.[16] Such devices offer improvements up to five orders of magnitude in the specific photon flux usable in certain experiments and will, therefore, lead to qualitatively new science.

In order to lay the ground work for the scientific opportunities discussed below, the present paper first reviews the spectral characteristics of bending magnet and undulator sources in section 2. We also discuss how the source characteristics affect the experimentally usable photon flux. Section 3 illustrates scientific opportunities generated by the utilization of insertion devices. Three areas are chosen: gas phase chemistry and physics, surface science and biology. A summary and scientific outlook is presented in section 4.

2. SYNCHROTRON SOURCES FOR VUV RADIATION

The important characteristics of bending magnet sources as compared to those available in the future with undulator insertion devices are summarized in Figure 1. In the following we shall make a comparison of the photon flux available from the two sources at an energy of $h\nu$ = 300 eV. This energy lies in the middle of the spectral range considered here and corresponds to an excitation energy of the important K edge of carbon. For the bending magnet source we assume the design values for the VUV ring at the National Synchrotron Light Source (NSLS):[17] source size (one-standard deviation): s_x = 0.3 mm (horizontal), s_y = 0.1 mm (vertical); beam divergence: θ_y = 0.5 mrad and θ_x = 25 mrad (maximum horizontal acceptance of most beam line optics); electron energy 750 MeV; beam current 1 Amp. We

obtain a flux $F=4\times10^{15}$ photons/sec/1% bandwidth in a 0.5 cm x 25 cm large spot at an observation point 10 m from the source. For the undulator source we choose the design values for the proposed Advanced Light Source (ALS).[18] Here s_x = 0.2 mm, s_y = 0.1 mm, θ_x = 0.06 mrad, θ_y = 0.03 mrad, and 1.3 GeV electron energy. Assuming the same electron current as for the bending magnet case (1 Amp) we obtain $F=8\times10^{16}$ photons/sec/1% bandwidth in a spot of 400 μm x 800 μm, 10 m from the source (Fig. 1).

Two parameters which characterize the different sources are the vertical (ε_y) and horizontal (ε_x) emittances. Their product defines the phase space emittance ε.

$$\varepsilon=\varepsilon_x\varepsilon_y= s_x s_y \theta_x \theta_y \qquad (1)$$

According to Liouville's theorem ε is a conserved quantity. Hence it can never be improved but only be spoiled by optics. The spectral brilliance is another characteristic source parameter and is given by,

$$B = F/\varepsilon \qquad (2)$$

With the above numbers, the emittance ε of the undulator is a factor of $\sim10^4$ smaller than that of the bending magnet source, while its spectral brilliance is a factor of $\sim10^5$ larger. While the undulator source gives us an increase of a factor of 20 in total photon flux, it offers a gigantic increase of $\sim10^5$ in specific photon flux characterized by the spectral brilliance. The question arises whether VUV science can take advantage of this latter enhancement factor in spectral brilliance.

As illustrated in Figure 2, the number of usable photons at the target depends on the phase space acceptance A of the beam line optics. If A is larger than the emittance ε of the source, all emitted radiation can be utilized. In general, specific requirements on the beam at the target like improved resolution in photon energy (ΔE) or beam size (ΔR) will require a decreased acceptance of the optics (e.g., closing of slits) and, therefore, lead to a loss in photon flux. Alternatively, if we require a certain energy resolution or spot size and can achieve it by means of optics with a certain acceptance A, we need a source of emittance $\varepsilon < A$ in order not to lose any flux. Therefore, experiments which require high spatial or energy resolution will strongly benefit from a source with a small emittance or a large spectral brilliance. They may thus benefit from enhancement factors up to 10^5 by using undulator rather than bending magnet sources.

A. Spectroscopies With High Energy Resolution

In order to illustrate the gains achievable for spectroscopies which require high energy resolution (e.g., photoemission, NEXAFS), we compare the calculated output flux available for a toroidal grating monochromator (TGM) coupled to a bending magnet versus an undulator source. We choose the TGM design optimized for a bending magnet source as discussed by Chen, Plummer and Howells,[19] and shown in Figure 3. Since the TGM has a particularly large horizontal acceptance, most other monochromator schemes would be less favorable for a bending magnet source and thus yield even larger enhancement factors for the undulator source.

Results for the gain in photon flux of undulator over bending magnet sources are summarized in Table 1 for $h\nu$ = 250 eV and 1030 eV and

two different resolution requirements, ΔE = 0.1 eV and 1 eV, respectively.[20] In order to obtain 0.1 eV resolution, only a small fraction (< 3 mrad) of the horizontal emittance of a bending magnet source can be utilized while all of the undulator radiation is usable. This reflects the fact that the acceptance of grating optical systems decreases as $h\nu$ increases due to grazing incidence angle and optical aberration considerations. We obtain photon flux enhancements up to a factor of 2×10^3 by use of an undulator. At 1 eV resolution, a larger fraction of the horizontal bending magnet fan can be used and the enhancem nt factor is reduced to less than 10^2.

An impressive example which illustrates the gain obtainable for high resolution spectroscopy by use of synchrotron radiation in general and undulators in particular is found in the application of electron spectroscopy for chemical analysis (ESCA)[21] to the C, N and O 1s core levels. Standard ESCA measurements performed with Mg or Al K_α radiation have proven to be a valuable analytical tool in gas, liquid and solid state science since their original development by Siegbahn in the late 1960's.[21] Especially designed instruments with 1 kwatt x-ray anodes and monochromatized Al K_α radiation (1486.6 eV) can provide a resolution of ΔE = 0.2 eV with a flux of about 1×10^{10} photons/sec in a 2 mm x 4 mm spot on the sample. A bending magnet source with an electron current of 500 mA and a TGM monochromator as discussed above yields 5×10^{10} photons/sec with ΔE = 0.1 eV resolution in a spot less than 1 mm^2. An undulator source with 500 mA electron current and a TGM monochromator provides 1×10^{13} photons/sec with ΔE = 0.1 eV resolution in a < 1 mm^2 spot. The results are summarized in Table 2. The bending magnet and undulator sources provide tunable radiation and the flux estimates given in Table 2 are valid within a factor of

2 over a large energy range from below the C 1s threshold (250 eV) to above the O 1s threshold (600 eV). From Table 2 we find that the bending magnet source offers an advantage of a factor of 2 in resolution and a factor of 5 in photon flux. This gain may not be sufficient to make scientists abandon their home laboratory set-up. However, the undulator source offers an enhancement of 10^3 in flux and a factor of 2 in resolution which opens the door for qualitatively different experiments than those doable with a conventional ESCA spectrometer. The above comparison does not even consider other significant advantages of the synchrotron radiation based ESC measurements. The tunability enables one to excite the C, N and O 1s levels with optimum cross-section, i.e., close to threshold, which offers more than a factor of 10 gain over excitation with $h\nu$ = 1486.6 eV.[22] For surface studies the escape depth can be minimized (~5 Å) by tuning the photon energy 50-100 eV above the core threshold, yielding a large gain (up to a factor of 10) in sensitivity.[5] Thus, in certain cases, the total gain with an undulator/TGM over a laboratory ESCA set-up approaches a factor of 10^5.

B. Experiments With Low Energy Resolution

The simplest way to use an undulator is without beam line optics. This is facilitated by the laser-like beam which can be placed on small targets without focussing and by the quasi monochromaticity of the emitted radiation as shown in Fig. 1. For an undulator with N periods the peak width of the first harmonic is $\Delta E \sim E/N$ such that it is possible to obtain an energy resolution of a few eV near the K edges of C, N and O without a monochromator. For certain experiments like x-ray lithography, contact microscopy or even (S)EXAFS this resolution is adequate. For

storage rings with an electron energy of 1-1.5 GeV the undulator parameters can be chosen such that the first harmonic falls into the VUV range and the higher harmonics are of relatively smaller intensity. Furthermore, the undulator can be continuously tuned by changing the gap between the magnetic poles such that the first harmonic moves over a substantial energy range.[18] For example, a permanent magnet undulator with N=142 periods and a length of 5m installed on a 1.3 GeV ring (ALS design) could be tuned in its first harmonic between 250 eV (K=1.9) and 650 eV (K=0.37).[18] By removing higher harmonics by a simple mirror reflection a monochromatic ($\Delta E/E \simeq 10^{-2}$) beam could be obtained with a photon flux in excess of 10^{16} photons/sec and a spot size of <1 mm^2. In comparison, a bending magnet line equipped with a grating monochromator and focussing optics at best has a transmission efficiency of a few percent. Together with its higher total flux (factor 20) the undulator would thus yield a gain in monochromatic flux of the order 10^2-10^3.

C. Imaging With High Spatial Resolution

The high spectral brilliance of an undulator is also suited for obtaining high flux in a small spot as needed for certain imaging schemes in microscopy[15] or for microprobe[23] analysis of materials. One common way to obtain small images is shown in Figure 4 where a Fresnel zone plate is used to form a demagnified image of the source. For diffraction limited performance the zone plate needs to be coherently illuminated, i.e., the path difference from a given point on the finite source to a given point on the zone plate needs to be less than the wavelength λ. For a source of height d this requires

$$d \sin\theta \sim d\,\theta < \lambda \qquad (3)$$

where θ is defined in Fig. 4. For a two-dimensional source Eq. (3) has to be satisfied for the horizontal and vertical source sizes and angular divergences and the coherence condition becomes

$$S_x S_y \theta_x \theta_y = \varepsilon < \lambda^2 \qquad (4)$$

The lateral coherence condition (4) shows that with increasing photon energy (smaller λ) smaller emittances are required to image without loss in flux. For an undulator source with the parameters listed above the emittance is sufficiently small that Eq. (4) is satisfied for $\lambda \gtrsim 60$ Å. Thus undulators have remarkable coherence properties. For radiation with $\lambda = 30$ Å, i.e., an energy above the C and below the O K edge as frequently used for microscopy of biological cells, ε needs to be reduced by a factor of 4 for an undulator source and a factor of 4×10^4 for a bending magnet source. In practice, this is done by the insertion of collimators or pinholes resulting in a loss of flux proportional to the reduction in ε. Coupled with the factor of 20 smaller total flux of a bending magnet line we find a $\sim10^5$ reduction in flux at the image relative to an undulator source. In this example, the gain factor in flux for an undulator is thus equal to the full gain in spectral brilliance.

3. SCIENTIFIC OPPORTUNITIES

In this section we shall present examples of present and possible future studies based on VUV synchrotron radiation. We have chosen three

scientific fields: gas phase chemistry and physics, surface science and biology. This choice and that of the specifically discussed experiments reflects an assessment of where the largest scientific progress is expected. During the first 10 years of VUV science the major scientific contributions have been in solid state physics and surface science. Examples are the determination of the detailed energy band and/or valence level structure of bulk solids, solid surfaces, solid-solid interfaces and chemisorbed adlayers by photoemission techniques.[7] By far the most experiments were carried out in the 10-40 eV range, less in the 40-250 eV and relatively few in the 250-3000 eV range. This distribution does not simply reflect the scientific importance of these sub-ranges but is partly due to experimental difficulties encountered at higher photon energies.[4] First, some of the existing storage rings (SURF at NBS, Tantalus at Stoughton) operated at small electron beam energies and thus only covered the lower end ($\lesssim$ 100 eV) of the VUV region. Second, grating monochromator designs which provide good resolution (< 0.1 eV), high flux and low scattered light levels become conceptually more difficult with increasing photon energy. Third, carbon contamination build-up on the optical surfaces of the beam line under exposure with high intensity radiation results in a loss of monochromatic flux above the K absorption edge of carbon ($h\nu > 280$ eV). Fourth, the 1-2 keV spectral region is difficult to cover with either grating or crystal monochromators because of scattered light and resolution problems with many grating designs, and radiation damage problems with presently available large d-spacing monochromator crystals.[4] It is for the above reasons that in the future the largest instrumental improvements will be possible in the 250-2000 eV spectral region. Also, from a scientific point of view, this spectral region is of great importance because it con-

tains the K edges of C, N and O which are of prime importance in chemistry and biology. In fact, one may speculate or hope that the second generation of VUV science will attract chemists, physical chemists and biologists in addition to physicists who, in the past, have dominated VUV science.

Because the present paper is not a review of past accomplishments, but rather an outlook into the future, we have selected below experiments and scientific problems which can presently be done only with difficulty, or not at all, and are thus waiting for the next generation undulator sources. Of course, there are many problems not discussed here which will also significantly gain from insertion device sources. Some of these will be mentioned in the final section 4.

A. GAS PHASE CHEMISTRY AND PHYSICS

In the past, gas phase investigations in the VUV have played a subordinate role to solid state and surface science. This is partly due to potential compatibility problems of such studies with the UHV environment of the storage ring and the beam line (optics). Furthermore, because of the lower atomic density as compared with solids and surfaces gas phase spectroscopies are most demanding in terms of photon flux.[24] Typically, the number of atoms (10^9-10^{10}) from which the measured signal originates corresponds to less than one thousands of a monolayer in a surface science experiment. The requirements in terms of energy resolution (~10 meV) are also higher than those for solid state studies (~100 meV). At present, many gas phase experiments are therefore limited by the available photon flux at high energy resolution.

Because of better compatibility with the UHV beam lines and the possibility of freezing out rotational and translational motions by using adiabatic expansion gas phase studies are best carried out by use of molecular beams.[25] This allows the investigations of atoms, molecules and clusters in their ground state as well as excited states with the possibility of studying reactions in crossed beam experiments.

a) Soft X-Ray Induced Fragmentation of Molecules

The first example of gas phase experiments is the photon induced fragmentation (PIF) of molecules. The experiment consists of measuring the ion fragment yield as a function of photon energy around a main absorption edge of the molecule as shown in Fig. 5 for the C K edge in acetone $(CH_3)_2CO$.[12] The total ion yield which closely follows the X-ray absorption spectrum is characterized by a structure below the 1s ionization potential (IP) and a broader edge-like feature beginning at the IP. The H^+ yield basically exhibits only the edge-like onset above the IP corresponding to 1s core electron excitations into the continuum. On the other hand, the O^+ yield is dominated by the strong pre-edge peak below the IP corresponding to a bound state transition of a 1s electron to an unfilled molecular orbital. This can be understood by the schematic in Figure 5c. Hydrogen is bonded to carbon atoms in a methyl configuration and the H^+ signal originates from a "Coulomb explosion" process following the creation of a 1s core hole on the methyl carbon atoms. The H-C bond is broken because valence electrons are removed from the bond in an Auger deexcitation process of the 1s hole on the C atom. The threshold for this Auger deexcitation process and the H^+ creation coincides with the ionization of a C 1s electron. Oxygen is bonded to a different carbon atom in a carbonyl configura-

tion. The C=O double bond character gives rise to an antibonding π^* molecular orbital. The C=O bond is preferentially broken by an excitation of a C 1s electron into this π^* orbital. The 1s → π^* transition energy is less than the IP because of the Coulomb interaction of the core hole and the π^* orbital. The O^+ yield therefore is largest at this transition energy as seen in Figure 5b. It is apparent that by tuning the photon energy either to the π^* resonance below the IP or to an energy above the IP one can selectively break different bonds of the molecule.

The next step to a detailed understanding of fragmentation processes would be to correlate the production of certain ions to specific electronic Auger deexcitation channels. This requires electron-ion coincidence measurements using Auger electrons of selected kinetic energy. Such measurements have not been carried out due to a lack of photon flux. The above measurements on acetone[12] were carried out on a bending magnet line at the NSLS with a photon energy resolution of ~1.5 eV and a counting rate for ions of ~10 counts/sec. The counting rate for energy selected Auger electrons (0.8 eV resolution) was ~1 count/sec. For future experiments one would desire a factor of ~10 better experimental resolution in photon and electron energy and a factor $\sim 10^2$-10^3 increase in count rate. Clearly, an undulator source is needed to achieve this goal.

b) Small Metal Clusters

One of the most fundamental problems in chemistry and physics is the study of the formation of matter - the transition from atomic to molecular to solid-state behavior. The elucidation of this process appears to be within our reach through the development of molecular beam sources which produce clusters ranging from isolated atoms to several hundred

atoms.[26,27] Chemists can think of using those sources to study the detailed bonding between a small number of atoms (~10 atoms) while solid state physicist who are more interested in collective phenomena will be able to look at, for example, the formation of surface and bulk energy bands (~100 atoms). Furthermore, clusters can be used as models for alloy or solid-solid interface formation and as model catalysts where a metal cluster is allowed to react with different gases. At present, however, studies of small unsupported clusters have been restricted to laser sources.

Results for nickel/aluminum alloy clusters are shown in Fig. 6.[27] The clusters were produced by laser vaporization of Ni_3Al. The vapor is entrained in a pulsed flow of helium which expands toward a vacuum region under high pressure. Cluster formation occurs before the supersonic He/cluster beam expands into vacuum. The clusters were laser ionized and the intensity of the ions was monitored by time-of-flight (TOF) mass detection. The ion intensity reveals different pure and alloy clusters like Ni_3, Ni_8Al or Ni_9Al. At low mass values peaks characteristic of pure and oxidized Al clusters are observed. The simplicity of the Ni/Al cluster spectrum is a result of the near mass coincidence of Al_2 and Ni and the lack of oxide formation for the alloy clusters. For example, the peak labelled Ni_9 also contains contributions from Ni_8Al_2 and Ni_7Al_4. In the future composite clusters from many different atomic species will be made and questions like, when does an aggregate of atoms form a metal or semiconductor, will be answered.

Using VUV radiation, one could study the formation of the interatomic bonding by photoemission, the bond lengths and structure by NEXAFS and SEXAFS and the dissociation and fragmentation by PSID and PIF. A par-

ticular cluster would be mass selected by ion TOF spectroscopy and the photoelectron or Auger electron signal would be measured in coincidence. Present VUV photoemission studies with molecular beams are carried out with about 10^9-10^{10} atoms in a typical interaction volume of 1 mm^3. It appears possible with present cluster sources to produce corresponding numbers of ~10^8 atoms, ~$5x10^6$ dimers, ~$5x10^5$ trimers and clusters with n > 3 of abundance ~$2x10^5$, each.[28] With presently used detection schemes, VUV studies of dimers and trimers would require a photon flux enhancement of 10^2-10^3. This gain could be provided by undulator sources. In addition, it appears that gains are possible in existing electron and ion detection schemes by fully utilizing the advantages of TOF detection which is made possible by the time structure of a well designed storage ring.[18]

B. SURFACE SCIENCE

The investigation of the electronic and geometric structure of solid surfaces has been one of the prominent applications of VUV synchrotron radiation. In the following we shall present examples of different techniques which will especially benefit from increased photon flux and/or energy resolution.

a) High Resolution XPS Studies

Figure 7a demonstrates the effect of different bonding configurations of carbon atoms on the C 1s binding energy for ethyl trifluoroacetate gas taken from Siegbahn's original work.[21] Depending on the charge transfer between C and its different neighbors like F, O, C or H, shown in Figure 7a, the 1s photoemission line will exhibit corresponding chemical

shifts. In Figure 7a the sequence of photoemission peaks corresponds to that of C in the molecule depicted above. Similar chemical shifts also exist for chemisorbed molecules, but almost no C, N or O 1s XPS studies with soft X-ray synchrotron radiation have been carried out so far. This is largely due to limitations in photon flux and energy resolution. Typical previous experimental conditions were ΔE = 1.5 eV at a flux of 5 x 10^9 photons/sec for C 1s spectroscopy around $h\nu$ = 350 eV with decreased flux and increased ΔE for N and O 1s spectroscopy. Comparison to the numbers listed in Table 2 for commercially available ESCA spectrometers makes it clear why chemist or chemical engineers have not used synchrotron radiation for such studies in the past.

An example of how synchrotron radiation has helped to study clean metal surfaces is shown in Figure 7b.[29] Here the $4f_{7/2}$ photoemission spectrum of a clean W(110) crystal at $h\nu$ = 70 eV is seen to clearly exhibit a chemically shifted peak for bulk and surface W atoms. The surface peak is quenched upon H_2 chemisorption because the charge distribution around the surface W atoms is no longer distinctly different from those in the bulk. Future studies of this kind will help to solve the electronic and geometric structure of clean surfaces, gas-solid and solid-solid interfaces.

b) Photoelectron Diffraction

The study of the energy dependence of a particular core photoemission peak forms the basis of two structural techniques called photoelectron diffraction (PhD) and angle resolved photoemission extended fine structure (ARPEFS).[8] Both techniques monitor modulations of the intensity of core photoemission peaks seen by an angle-resolving detector. The PhD range corresponds to excitation energies close to threshold (kinetic ener-

gies $\lesssim$100 eV) where the photoelectron intensity is modulated by multiple scattering processes involving neighbor surface atoms. The ARPEFS range corresponds to larger photoelectron kinetic energies (100-500 eV) and is dominated by single scattering processes. The distinction between PhD and ARPEFS is analogous to that between NEXAFS and (S)EXAFS. However, for these latter techniques the detector is not outside the sample but is at the site of the original excitation.

An example of a structure determination by PhD is shown in Figure 8 for CO on Ni(100).[30] The C 1s photoelectron intensity was monitored in the emission direction along the surface normal. As shown in Figure 8a, various scattered photoelectron waves interfere in the direction of the detector and cause energy dependent intensity modulations. These intensity modulations plotted over an extended energy of ~100 eV can then be compared to those calculated for different chemisorption geometries similar to the analysis of the energy dependence of low energy electron diffraction (LEED) intensities. The structure is determined from matching (R-factors) of experimental and theoretical curves (Figure 8c). For our example, CO was determined to stand up on the surface with the C atom bonded to a Ni surface atom.[30] The bond lengths are listed in Figure 8c.

Future studies can take advantage of a greatly increased energy resolution which will allow to separate chemically shifted peaks at surfaces, similar to the examples shown in Figure 7. It should then be possible to distinguish between the same atoms in different surface complexes (e.g., O 1s for H_2O, O_2 and O) which are simultaneously present and to determine their structural environment.

c) NEXAFS

Measurement of the X-ray absorption coefficient in the vicinity of one of the major absorption edges (e.g., K or L edges) of a specific atom allows to probe the structural environment of that atom. The familiar extended X-ray absorption fine structure (EXAFS) or its surface version, SEXAFS, measure the absorption coefficient at excitation energie well above ($\gtrsim$ 50 eV) the edge.[9] Recently it has become clear that the detailed structures close to the edge ($\lesssim$ 50 eV) which are ignored in the EXAFS analysis also contain important structural information.[31] This near edge X-ray absorption fine structure (NEXAFS) also referred to as XANES (for x-ray absorption near edge structure) arises from scattering processes of photoelectrons with relatively small kinetic energies ($\lesssim$ 50 eV). Therefore it is sensitive, not merely to the spacial distribution of the core potentials of neighbor atoms (i.e., nuclear positions) but also to the details of the valence electron charge distribution (i.e., the bonding). In contrast to (S)EXAFS, it does not only provide information on the local geometric structure around a selected atom, but also on the nature of the interatomic bond (e.g., hybridization).

The most pronounced near edge structures are observed for low-Z molecules where the spectra are dominated by scattering resonances which originate from the bond between C, N and O atoms (H is not seen because it does not backscatter well). The NEXAFS spectra of chemisorbed molecules are dominated by the same resonances as for the gas phase.[10,32] These intramolecular resonances dominate completely over scattering channels involving neighbor substrate atoms. It is for this reason that NEXAFS can determine changes within a given molecule like changes in hybridization, bond length or even orientation with respect to the surface.

An example which demonstrates the power of NEXAFS to monitor chemical reactions of molecules with surfaces is shown in Figure 9. NEXAFS spectra recorded near the C K edge for a monolayer (290K) of thiophene (C_4H_4S) on Pt(111)[33] exhibit various σ resonances corresponding to scattering processes between C-S, C-C and C=C neighbor pairs. In addition, a π^* resonance is observed which is characteristic of the π bonding associated with C=C double bonds. Upon annealing to 470K, the C-S resonance vanishes while all other resonances remain unchanged. Similarly, at the S $L_{2,3}$ edge, a resonance associated with the S-C bond disappears during the same annealing step. This is direct evidence for desulfurization of thiophene with increasing temperature resulting in the formation of a metallocycle where a Pt surface atom is substituted for S in the hydrocarbon ring. S remains on the surface in atomic form.[33]

It is apparent that studies of this kind can be used to monitor catalytic reactions at surfaces. In the future, it may be possible to record a whole NEXAFS spectrum in one "shot" ($\sim$ 1 sec) and thus monitor reaction kinetics. Measurement of the NEXAFS spectra using low yield K_α fluorescence from C, N or O surface atoms (rather than electron yield detection as presently done) would open the door for recording spectra under reaction conditions (e.g., H_2 atmosphere). Since for low-Z atoms fluorescence yields are small (10^{-3}-10^{-2}) compared to Auger electron yields, higher photon flux is needed.

d) Photon Stimulated Ion Desorption

Ion desorption from surfaces following electron excitation (ESD) has been studied for many years and was long thought to be the sole consequence of valence electron excitations which lead to repulsive states,

the so-called Menzel-Gomer-Redhead (MGR) mechanism.[11] The recognition that ions may desorb from surfaces following the excitation of a core electron by Knotek and Feibelman[34] and the direct demonstration of this effect by means of photon excitation near an absorption edge by Knotek, Jones and Rehn[35] laid the cornerstone for a new technique. Photon stimulated ion desorption (PSID) has since then been studied on many different surfaces. The essence of the Knotek-Feibelman desorption model is that the desorption process is linked to the probability of core electron excitation, i.e., the absorption coefficient. Excitation of a core electron gives rise to a cor hole which is filled by Auger transitions from more shallow atomic levels and finally leads to holes in the valence shell through a cascading process. The KF desorption process is the surface analog of the "Coulomb explosion" discussed earlier for the core excitation induced fragmentation of gas molecules.

The importance of PSID lies in its potential to study the bonding at and geometric structure of surfaces. Whenever desorption occurs via the KF mechanism, the yield of a particular ion will be a replica of the absorption coefficient of the corresponding atom as it sat on the surface before the desorption process. Thus, PSID can be used as a signal for SEXAFS and NEXAFS.[13]

Figure 10 gives an example of a PSID study of the H^+ yield from NH_3 molecules in different surface environments.[36] For a thick NH_3 multilayer, the H^+ yield near the N K edge closely follows the absorption coefficient. The observed H^+ yield is large and easily recordable with a photon flux of $\sim 5 \times 10^9$ photons/sec. For NH_3 molecules chemisorbed as a monolayer or less on a Ni(110) surface the H^+ yield is greatly reduced (factor $\sim 10^3$) and at present can hardly be recorded, even after hours of

data collection time, as shown in Figure 10. The low desorption cross-section is the result of enhanced reneutralization of the created valence holes on the molecule through charge transfer with the metal surface. Since studies of molecules and atoms chemisorbed on metal surfaces are of prime importance, it becomes apparent that the availability of increased photon flux would open the door for qualitatively new PSID studies.

C. BIOLOGY

An important problem in biology is the understanding of the internal structure of living biological cells. Such cells are composed of water, proteins, carbohydrates, lipids and nucleic acids and have a typical size of 0.5 - 5 μm. In order to determine internal cell structures down to 50-100 A in size a microscopy technique is needed which does not only provide the desired resolution but also does not damage or destroy the cell during the measurement period. The radiation used for imaging should thus have a wavelength < 50 A in order to avoid limitation of the resolution by diffraction and it should have a suitable cross-section for interaction with the carbon, nitrogen and oxygen atoms of the cell.

In the past electron microscopy has been the technique of choice because of its high spacial resolution. However, electrons interact strongly with matter and the resulting short scattering lengths required the samples to be thin (< 0.1 μm). Typically, biological cells had to be dehydrated and sectioned before they could be studied under vacuum in an electron microscope. From a cross-section point of view soft X-rays in the range 10-100 A are the ideal radiation for the study of biological cells, as shown in Figure 11. Their scattering lengths for C and O lie between

0.1 - 5 μm and are tuneable by more than an order of magnitude by changing the photon energy across the C or O K edge. It is both the level of reactivity and the tuneability of reactivity of soft X-rays which is the basis for their potential use for microscopy.

The level of reactivity directly determines the radiation damage in the cell. Sayre et al.[37] have investigated this problem in detail and calculated the feature size which is visible with statistical significance for soft X-ray and electron irradiation of a wet biological cell, provided that the dosage remains below a level (10^4 J/g) where severe structural damage will occur. They find the resolution to be limited to ~1000 A for electron and ~100 A for soft X-ray radiation. While electron microscopy is capable of atomic size resolution for thin, dry and structurally stable samples radiation damage problems greatly spoil the effective resolution for the thicker, wet and fragile biological cells. Furthermore, electron microscopy is usually carried out in vacuum and has therefore a serious compatibility problem with the wet and living state of cells.

a) Contact Microscopy

Soft x-ray microscopy can be carried out in several ways. The prominent technique used so far is contact microscopy.[15] Here the specimen is placed in contact with a photosensitive resist and an image of the sample is recorded in a transmission geometry using a parallel x-ray beam. Using $h\nu$ = 290 eV radiation and a PMMA resist a spatial resolution of 50 A can be obtained. Higher energy x-rays spoil the resolution because of the generation of secondary electrons with longer scattering lengths in the resist. For example, at $h\nu$ = 1550 eV the obtainable resolution deteriorates to about 350 A. With present bending magnet sources coupled to a

monochromator with a few eV resolution, typical exposure times are of the order of 1 min. In order to record stop-motion pictures of changes in the cell in response to certain stimuli, one would like to reduce the exposure time to about a msec. This becomes possible by directly using the first harmonic of an undulator as shown in Fig. 1 and discussed in Section 2B. Soft x-ray radiation of a few eV resolution and a flux of > 10^{16} photons/sec could be obtained.

There are three limitations with the contact technique which call for the development of alternate imaging methods. The low detective quantum efficiency of x-ray resists (~ 10%) causes 90% of the illuminating radiation to be wasted for imaging although it contributes to radiation damage in the cell. For thick cells, the resolution is not limited by the resist but by Fresnel diffraction features which may lead to effective resolutions as large as 500-1000 Å. The contact technique gives little or no three-dimensional information. These shortcomings may be overcome in the future by use of point projection microscopy or holography with soft x-rays.

b) Zone Plate Scanning Microscopy

Rather than recording a picture of the whole cell and relying on a photoresist for spatial resolution scanning microscopy looks at one spot of the sample at one time. As shown in Fig. 12a a severely demagnified image of a monochromatic "source" is created by a zone plate condenser. Typically the "source" consists of a pinhole illuminated by a soft x-ray monochromator. The radiation transmitted through a small area of the sample which is determined by the zone plate focus is recorded by a proportional counter (100% efficiency). The whole picture is assembled by scan-

ning the sample with piezoelectric drives. Scanning microscopy reduces radiation damage because all photons which traverse the sample are used for image formation. At present the resolution is limited by the quality of the zone plates to about 600 A. The scanning technique has produced pictures of about 2000 A resolution with an exposure time of an hour or so.[38] With improved optics capable of imaging to spot sizes close to 100 A radiation sources with a small emittance are needed in order to avoid large losses in photon flux as discussed in Section 2. For soft x-ray scanning microscopy undulators will offer gains of the order of 10^5 in usable photon flux over bending magnet sources.

c) Holography

The desire to obtain complete three-dimensional images of cells has prompted the development of soft x-ray holography. A simple experimental scheme, due in principle to Gabor, is shown in Fig. 12b. A zone plate is used as a monochromator to create a secondary monochromatic source for the holographic imaging process. This source of size d_2 coherently illuminates the sample and a detector (e.g. a screen coated with a photoresist or a photographic film) within an opening angle θ_2. The waves scattered from and those transmitted through the sample interfere to give fringes whose intensity distribution is recorded. The recorded intensity distribution, i.e. the hologram, may be magnified with an electron microscope and an image of the sample reconstructed by computer. Alternately, a laser can be used instead of the soft x-ray beam to decode the original hologram and create an image of the original sample (cell).

The development of soft x-ray holography has so far been impeded by the lack of suitable soft x-ray sources. As stated above the illuminat-

ing radiation needs to be coherent. This requires that the lateral coherence condition $d_2\Theta_2 < \lambda$ (Fig. 12b) is satisfied. Furthermore, the radiation needs to have a large longitudinal coherence length $l = \lambda^2/\Delta\lambda$, i.e. a high degree of monochromaticity ($\lambda/\Delta\lambda \gtrsim 10^3$). Both requirements call for a source with a small emittance or large spectral brilliance. Just as visible light holography blossomed with the invention of the laser soft x-ray holography will reveal its power probably not before the availability of undulators.

4. Conclusions

Next generation electron storage rings with undulator insertion devices were shown to benefit all VUV experiments by at least a factor of 20 in total photon flux over presently available bending magnet sources. For experiments requiring either high energy or spatial resolution or low energy resolution gains up to five orders of magnitude in specific photon flux can be achieved. Examples of experiments in different scientific areas were presented which indicate that in many cases improvement factors of 10^2-10^3 in specific photon flux are sufficient to open the door for qualitatively new science. These new scientific opportunities exist in basic science disciplines such as physics, chemistry, and biology as well as in more applied fields such as chemical engineering (e.g. studies of surface catalytic processes), electrical engineering (e.g. studies of solid-solid interfaces) or materials science (e.g. studies of the electronic and crystallographic structure of amorphous materials).

Only a few selected VUV techniques and their applications have been discussed here. One can imagine many more studies which will become feasible with the availability of undulator sources. Application of the

VUV imaging concepts used for microscopy will enable microprobe analysis (spot size ~100 Å) of materials and surfaces by means of photoemission, SEXAFS and PSID. The creation of small images with highly monochromatic radiation will also greatly benefit ARPES studies because the uncertainty in the photoelectron collection angle (i.e. wavevector) is reduced. Spin polarized ARPES studies of magnetic materials and their surfaces will become as routine as present spin unresolved ARPES studies. Here the undulator flux will compensate for the low efficiency of Mott detectors used in such investigations. SEXAFS studies of C, N, O atoms and their molecules are presently limited by photon flux and/or signal-to-background problems. With the increased flux from an undulator (possibly without additional monochromatization, see Section 2B) such studies could even be carried out by fluorescence detection which does not suffer from interference problems with photoemission peaks as does Auger detection. Finally, excited state spectroscopics of gases and solids will become possible where a laser or a second undulator beam is used for pumping. Such studies are presently difficult because of the low duty cycle of lasers as compared to the continuous-wave nature of synchrotron radiation. All in all it appears that a quantum jump in VUV science lies within our reach with the utilization of undulators on suitably designed electron storage rings.

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TABLE 1

ENHANCEMENT IN PHOTON FLUX FOR UNDULATOR OVER BENDING MAGNET SOURCES FOR DIFFERENT ENERGY RESOLUTIONS

RESOLUTION ΔE = 0.1 EV

λ(Å)	$h\nu$ (eV)	TGM Acceptance For Bend. Mag. (mrad)[a]	Photon Flux Ratio Undulator/Bend. Mag.
50	250	3	2×10^2
12	1030	1	2×10^3

RESOLUTION ΔE = 1.0 eV

λ(Å)	$h\nu$ (eV)	TGM Acceptance For Bend. Mag. (mrad)[a]	Photon Flux Ratio Undulator/Bend. Mag.
50	250	18	30
12	1030	22	60

[a]TGM accepts all of undulator radiation

TABLE 2

ESCA SPECTROSCOPY WITH Al $K\alpha$, BENDING MAGNET AND UNDULATOR RADIATION

Source	Power or Ring Current	Photon Energy	Spot Size on Sample (mm)	Energy Resolution (eV)	Photons / sec
ESCA	1 kW	1486.6	2x4	0.2	10^{10}
Bending Magnet	500 mA	300-600 (variable)	< 1x1	0.1	$5x10^{10}$
Undulator	500 mA	300-600 (variable)	< 1x1	0.1	10^{13}

REFERENCES

1. J. A. R. Samson, Techniques of Vacuum Ultraviolet Spectroscopy (Wiley, New York, 1967).

2. For reviews see: Synchrotron Radiation: Techniques and Applications, C. Kunz, Ed. (Springer, Berlin-New York, 1979); Synchrotron Radiation Research, H. Winick and S. Doniach, Eds. (Plenum Press, New York-London, 1980); Handbook on Synchrotron Radiaton, E. E. Koch, Ed. (North-Holland, 1983).

3. I. Lindau, private communication, April 1984.

4. See Proceedings of Conferences on Synchrotron Radiation Instrumentation: Nuclear Instruments and Methods 152 (1978); 172 (1980); 195 (1982).

5. Photoemission in Solids I and II, Topics in Applied Physics, Vols. 26 and 27, M. Cardona and L. Ley, Eds., Springer, Berlin, 1979; I. Lindau and W. E. Spicer in Synchrotron Radiation Research, H. Winick and S. Doniach, Eds., (Plenum Press, New York-London, 1980) p. 159.

6. E. E. Koch and B. F. Sonntag in Synchrotron Radiation: Techniques and Applications, C. Kunz, Ed. (Springer, Berlin-New York 1979) p. 269.

7. E. W. Plummer and W. Eberhardt, Adv. Chem. Phys. 49, 533 (1982); F. Himpsel, Adv. Phys. 32, 1 (1983).

8. S. D. Kevan, D. H. Rosenblatt, D. Denley, B.-C. Lu and D. A. Shirley, Phys. Rev. Lett. 41, 1565 (1978); C. H. Li, and S. Y. Tong, Phys. Rev. Lett. 43, 526 (1979); J. J. Barton, C. C. Bahr, Z. Hussain, S. W. Robey, J. G. Tobin, L. E. Klebanoff and D. A. Shirley, Phys. Rev. Lett. 51, 272 (1983).

9. For a review of SEXAFS spectroscopy see: J. Stöhr in Emission and Scattering Techniques, Ed. P. Day (Reidel, Dordrecht, 1981); J. Stöhr, R. Jaeger, S. Brennan, Surf. Sci. 117, 503 (1982).

10. J. Stöhr and R. Jaeger, Phys. Rev. B26, 4111 (1982).

11. For a review see: M. L. Knotek in Proceedings of the First International Workshop on Desorption Induced by Electronic Transitions - DIET 1, Williamsburg, VA (May 1982). Springer Series in Chemical Physics Vol. 24 (Springer-Verlag, Berlin, 1983) p. 139.

12. W. Eberhardt, T. K. Sham, R. Carr, S. Kummacher, M. Strongin, S. L. Weng and D. Wesner, Phys. Rev. Lett. 50, 1038 (1983).

13. R. Jaeger, J. Feldhaus, J. Haase, J. Stöhr, Z. Hussain, D. Menzel and D. Norman, Phys. Rev. Letters 45, 1870 (1980).

14. A. R. Neureuther in Synchrotron Radiation Research, H. Winick and S. Doniach, Eds. (Plenum Press, New York-London 1980), p. 223.

15. J. Kirz and D. Sayre in Ref. 14, p. 277; E. Spiller in Handbook on Synchrotron Radiation, E. E. Koch, Ed. (North-Holland, 1983), p. 1091.

16. J. E. Spencer and H. Winick in Ref. 14, p. 663.

17. L. Blumberg, J. Bittner, J. Galayda, R. Heese, S. Krinsky, J. Schuchman and A. Van Steenbergen, IEEE Trans. Nucl. Sci. NS-26, 3842 (1979).

18. Report of the ALS/SSRL Users Workshop, May 9-11, 1983, Lawrence Berkeley Laboratory Publication 5095.

19. C. T. Chen, E. W. Plummer and M. R. Howells (to be published).

20. E. W. Plummer (private communication).

21. K. Siegbahn et al., Nova Acta R. Soc. Sci. Ups. Ser. IV 20, 224 (1967).

22. S. M. Goldberg, C. S. Fadley and S. Kono, J. Electron Spectrosc. 21, 285 (1981).

23. C. J. Sparks, Jr. in Ref. 14, p. 459.

24. M. O. Krause in Ref. 14, p. 101.

25. D. H. Levy, L. Wharton and R. E. Smalley in Chemical and Biochemical Applications of Lasers, Edit. C. B. Moore Vol. II (Academic press, New York 1977) p.1.

26. J. B. Hopkins, P. R. R. Langridge-Smith, M. D. Morse and R. E. Smalley, J. Chem. Phys. 78, 1627 (1983).

27. E. A. Rohlfing, D. M. Cox, R. Petkovic-Luton and A. Kaldor (to be published).

28. D. Trevor (private communication).

29. Tran Minh Duc, C. Guillot, Y. Lassailly, J. Lecante, Y. Jugnet and J. C. Vedrine, Phys. Rev. Lett. 43, 789 (1979).

30. S. D. Kevan, R. F. Davis, D. H. Rosenblatt, J. G. Tobin, M. G. Mason, D. A. Shirley, C. H. Li and S. Y. Tong, Phys. Rev. Lett. 46, 1629 (1981).

31. For a review see: Proceedings of the First International Conference on EXAFS and XANES. Frascati, Italy 1982, Springer Series in Chemical Physics Vol. 27 (Springer-Verlag, Berlin 1983).

32. J. Stöhr, J. L. Gland, W. Eberhardt, D. Outka, R. J. Madix, F. Sette, R. J. Koestner and U. Döbler, Phys. Rev. Lett., 51, 2414 (1983).

33. J. Stöhr, J. L. Gland, E. B. Kollin, R. J. Koestner, A. L. Johnson, E. L. Muetterties and F. Sette (to be published).

34. M. L. Knotek and P. J. Feibelman, Phys. Rev. Lett. 40, 964 (1978); P. J. Feibelman and M. L. Kotek, Phys. Rev. B18, 6531 (1978).

35. M. L. Knotek, V. O. Jones and V. Rehn, Phys. Rev. Lett. 43, 300 (1979).

36. R. Jaeger, J. Stöhr and T. Kendelewicz, Surface Science, 134, 547 (1983).

37. D. Sayre, J. Kirz, R. Feder, D. M. Kim and E. Spiller, Ultramicroscopy 2, 337 (1977)

38. For recent results in microscopy see: Proceedings of SPIE, Science with Soft X-rays, Vol. 447 pp. 157-204.

39. M. R. Howells, Possibilities for X-ray Holography Using Synchrotron Radiation Brookhaven National Laboratory Report BNL-33994.

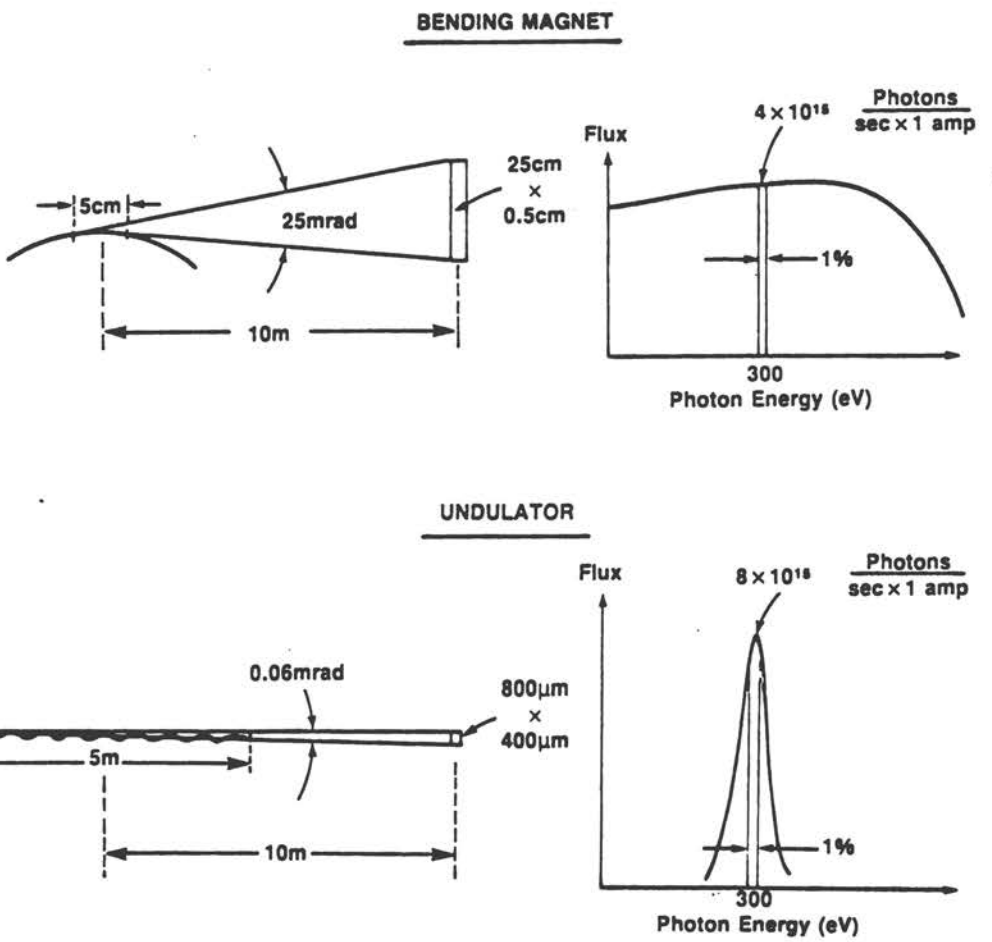

BENDING MAGNET
5cm
25mrad
25cm
×
0.5cm
10m
Flux
4×10¹⁵
Photons
sec×1 amp
1%
300
Photon Energy (eV)
UNDULATOR
0.06mrad
800μm
×
400μm
5m
10m
Flux
8×10¹⁵
Photons
sec×1 amp
1%
300
Photon Energy (eV)

Figure 1

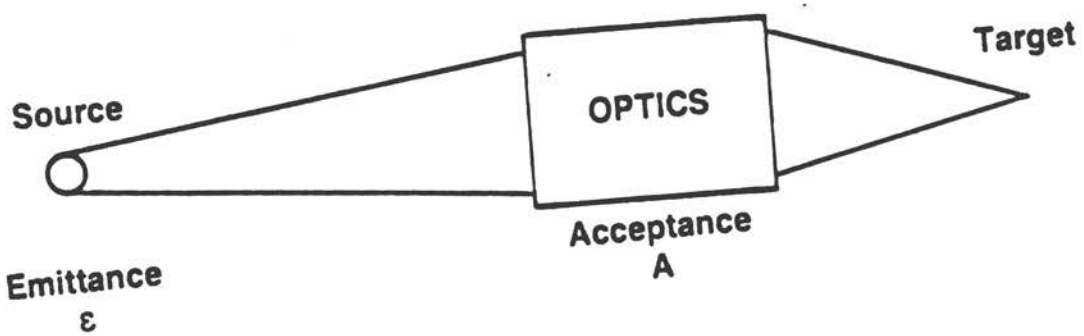


Figure 2

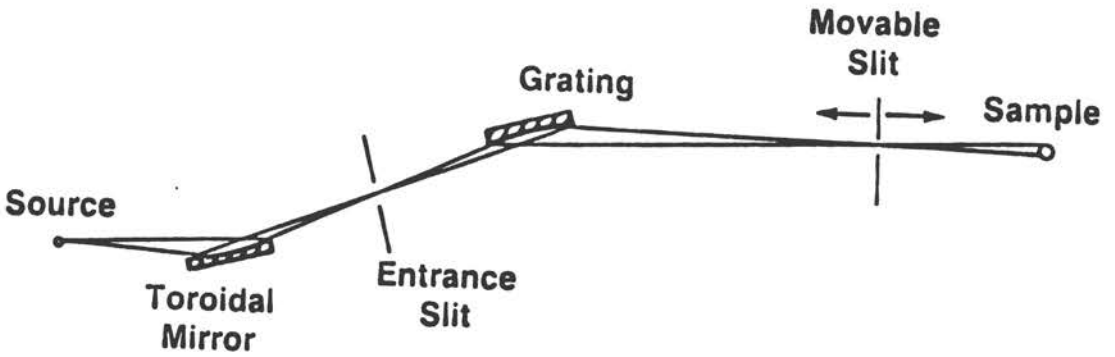

Movable
Slit
Grating
Sample
Source
Entrance
Slit
Toroidal
Mirror

Figure 3

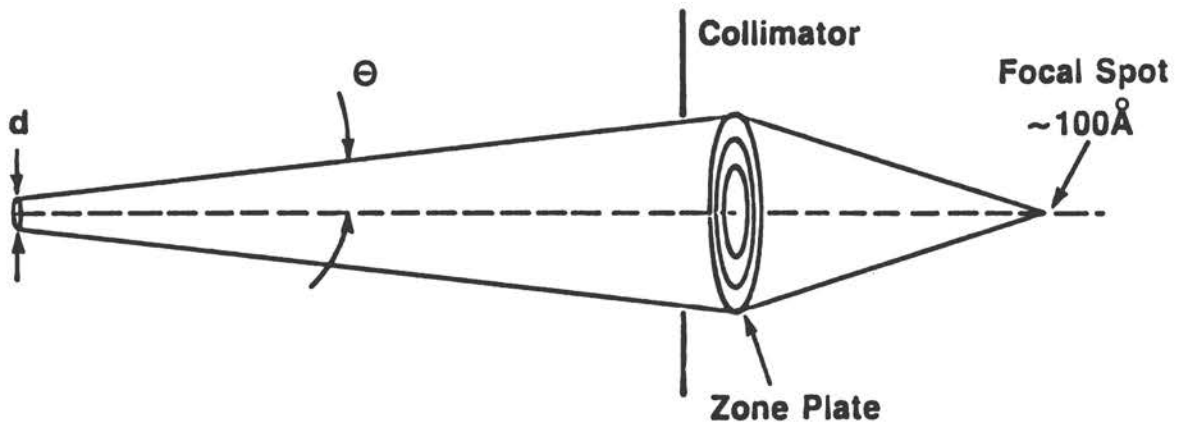


Figure 4

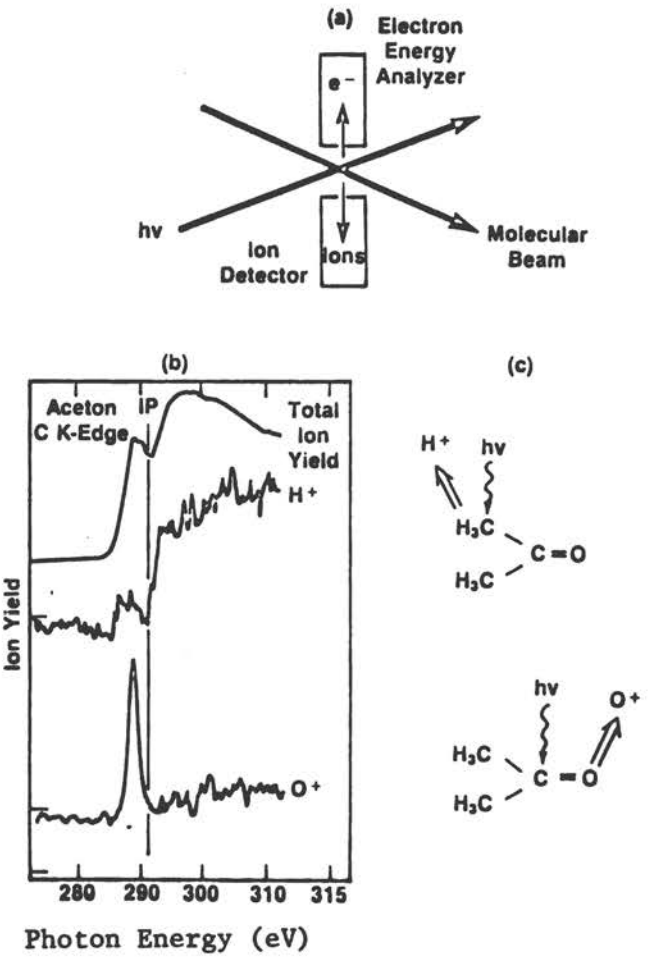

(a)
Electron
Energy
Analyzer
e⁻
hv
Ion
Detector
Ions
Molecular
Beam
(b)
Aceton
C K-Edge
IP
Total
Ion
Yield
H⁺
O⁺
Ion Yield
280
290
300
310
315
Photon Energy (eV)
(c)
H⁺
hv
H₃C
C=O
H₃C
hv
O⁺
H₃C
C=O
H₃C

Figure 5

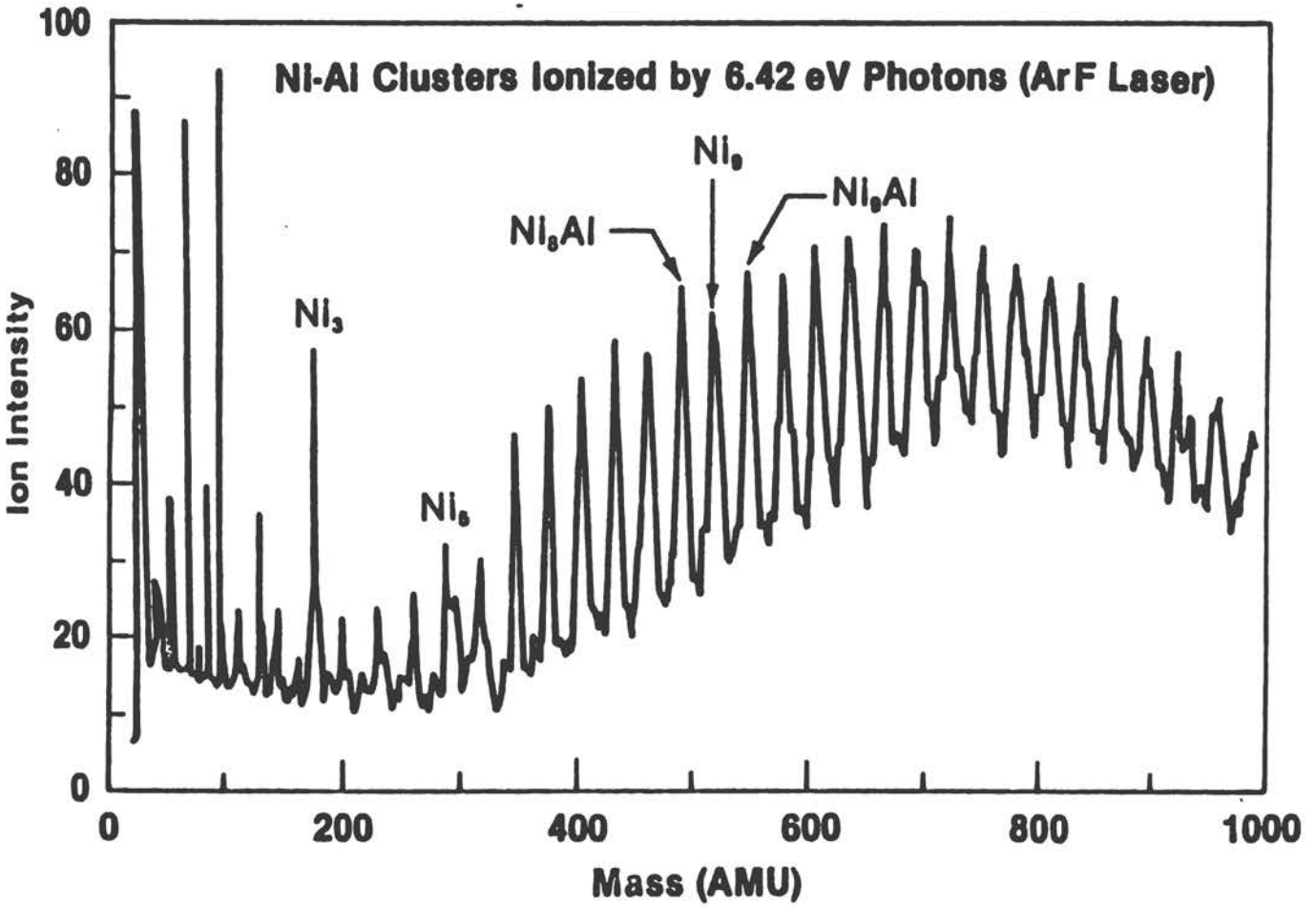

Ni-Al Clusters Ionized by 6.42 eV Photons (ArF Laser)
Ion Intensity
Mass (AMU)
0
20
40
60
80
100
0
200
400
600
800
1000
Ni3
Ni5
Ni8Al
Ni9
Ni9Al

Figure 6

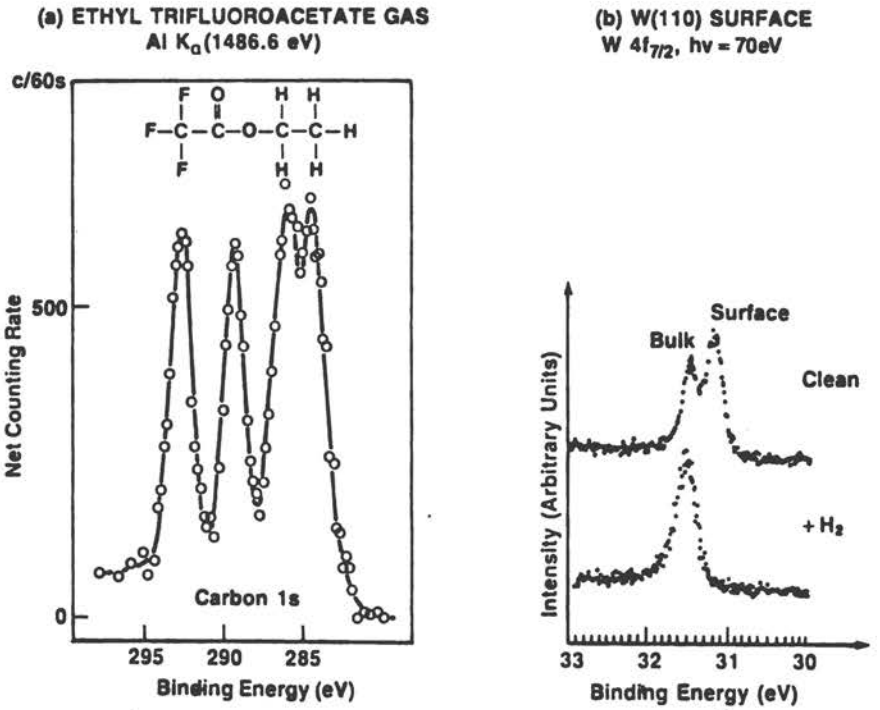

(a) ETHYL TRIFLUOROACETATE GAS
Al K_α(1486.6 eV)
c/60s
Net Counting Rate
500
0
Carbon 1s
295
290
285
Binding Energy (eV)
(b) W(110) SURFACE
W $4f_{7/2}$, hv = 70eV
Surface
Bulk
Clean
+ H_2
Intensity (Arbitrary Units)
33
32
31
30
Binding Energy (eV)

Figure 7

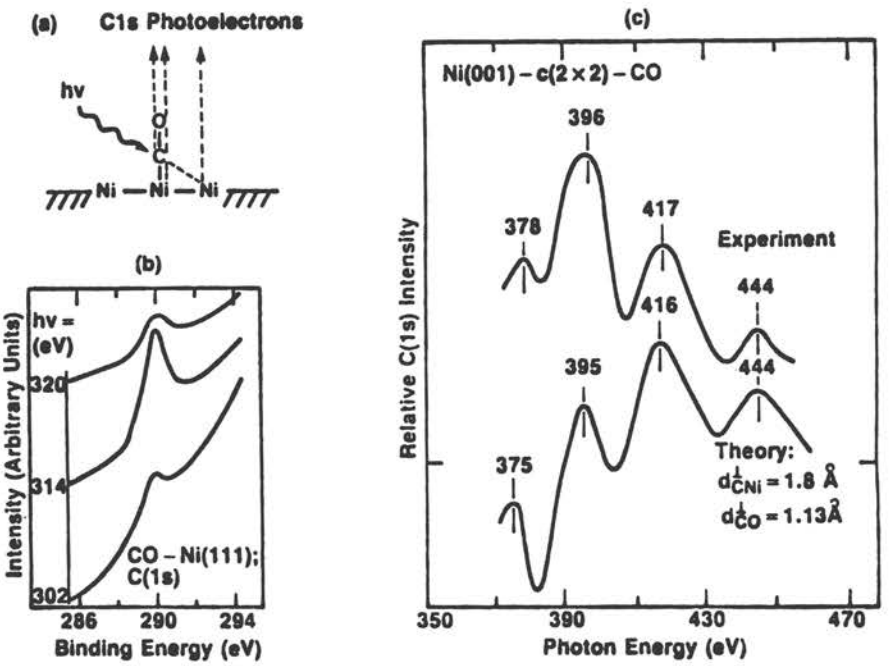

(a) C1s Photoelectrons
hv
O
C
Ni — Ni — Ni
(b)
hv = (eV)
320
314
302
CO – Ni(111); C(1s)
Intensity (Arbitrary Units)
286
290
294
Binding Energy (eV)
(c)
Ni(001) – c(2 × 2) – CO
396
378
417
Experiment
444
416
395
444
375
Theory:
$d^{\perp}_{CNi}$ = 1.8 Å
$d^{\perp}_{CO}$ = 1.13Å
Relative C(1s) Intensity
350
390
430
470
Photon Energy (eV)

Figure 8

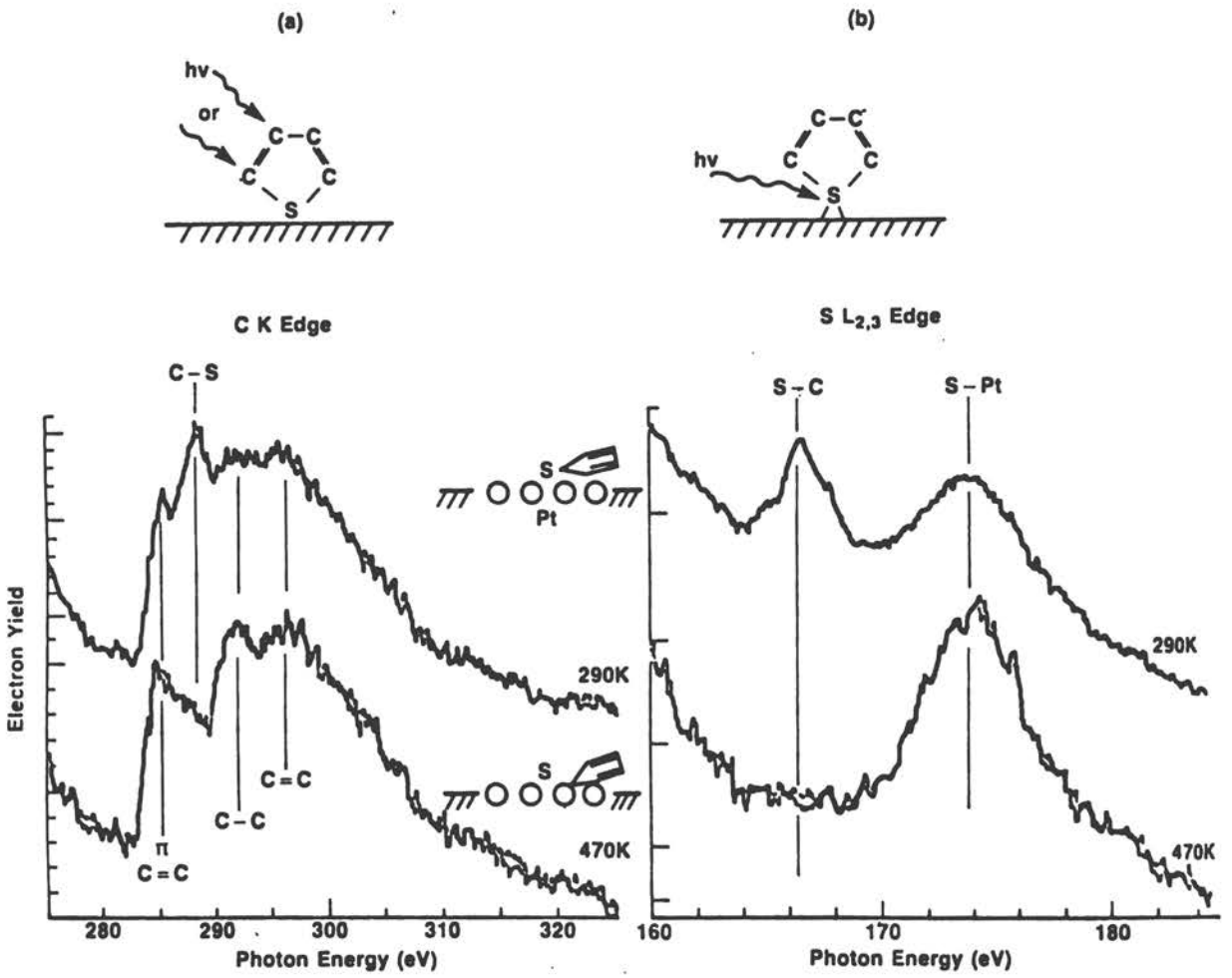
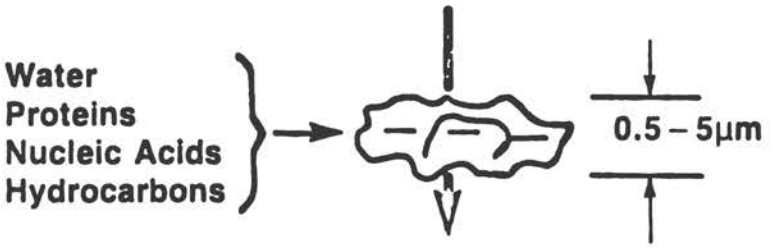

(a)
(b)
hv
or
C–C
C
C
S
hv
C–C
C
C
S
C K Edge
S $L_{2,3}$ Edge
C–S
S–C
S–Pt
S
Pt
290K
S
C=C
C–C
π
C=C
470K
Electron Yield
280
290
300
310
320
160
170
180
Photon Energy (eV)
Photon Energy (eV)

Figure 9

(a)
H+ Yield
NH3 Multilayer
Submonolayer
NH3/Ni(110)
×60
H+ Yield (Arbitrary Units)
390
400
410
420
430
Photon Energy (eV)
(b)
H+
hv
H H H
N
NH3 Solid
H+
hv
H H H
N
Ni

Figure 10


Water
Proteins
Nucleic Acids
Hydrocarbons
0.5 – 5μm

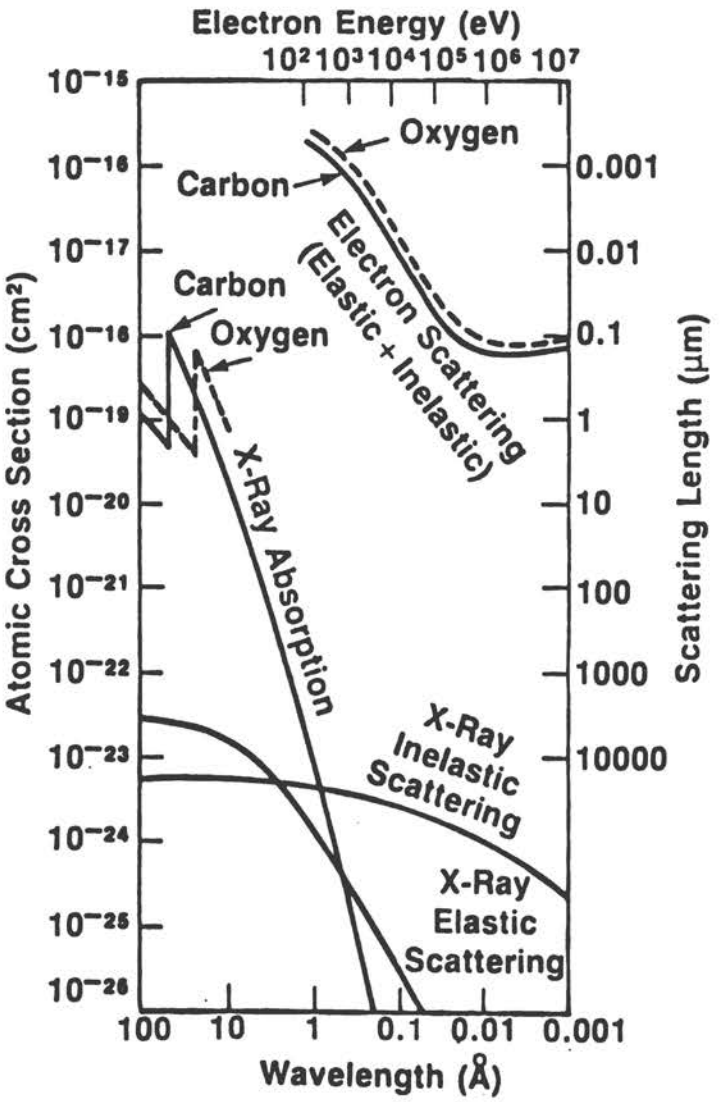

Electron Energy (eV)
10² 10³ 10⁴ 10⁵ 10⁶ 10⁷
Oxygen
Carbon
Electron Scattering (Elastic + Inelastic)
Carbon
Oxygen
X-Ray Absorption
X-Ray Inelastic Scattering
X-Ray Elastic Scattering
Atomic Cross Section (cm²)
Scattering Length (μm)
Wavelength (Å)
Range of Interest

Figure 11

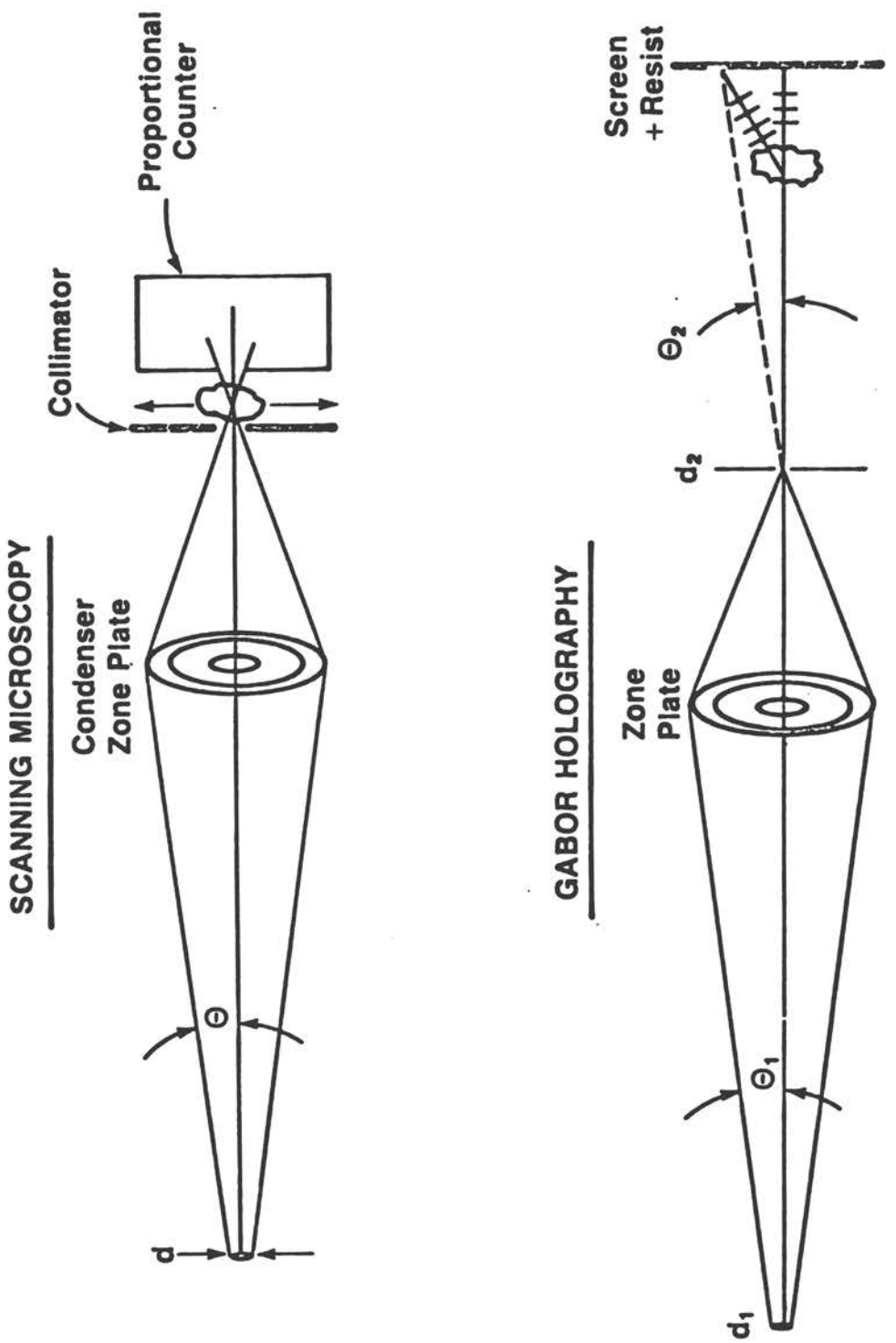

SCANNING MICROSCOPY
Condenser Zone Plate
Collimator
Proportional Counter
Θ
d
GABOR HOLOGRAPHY
Zone Plate
Screen + Resist
Θ2
d2
Θ1
d1

Figure 12

X-RAY MICROPROBE CHARACTERIZATION OF MATERIALS:

THE CASE FOR UNDULATORS ON ADVANCED STORAGE RINGS*

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Presentation to the

MAJOR MATERIALS FACILITIES COMMITTEE
NATIONAL RESEARCH COUNCIL
Washington, D.C.

March 17, 1984

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X-ray microprobe characterization of materials: the case for undulators on advanced storage rings

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ABSTRACT

The unique properties of X rays offer many advantages over electrons and other charged particles for the microcharacterization of materials. X rays are more efficient in exciting characteristic X-ray fluorescence and produce higher fluorescent signals to backgrounds than obtained with electrons. Detectable limits for X rays are a few parts per billion and are 10^{-3} to 10^{-5} less than for electrons. Energy deposition in the sample by X rays is 10^{-3} to 10^{-4} less than for electrons for the same detectable concentration. High-brightness storage rings, especially in the 6 GeV class with undulators, will be approximately 10^{3} brighter in the X-ray energy range from 5 keV to 35 keV than existing storage rings and provide for X-ray microprobes that are as bright as the most advanced electron probes. Such X-ray microprobes will produce unprecedented low levels of detection in diffraction, EXAFS, Auger, and photoelectron spectroscopies for both chemical characterization and elemental identification. These major improvements in microcharacterization capabilities will have wide-ranging ramifications not only in materials science but also in physics, chemistry, geochemistry, biology, and medicine.

I. INTRODUCTION

Efforts to obtain micro-diffraction and micro-elemental analysis to understand the properties of matter have been made since the early part of this century when the first X-ray probes were constructed. Conferences have been held on the design and application of X-ray microprobe sources.[1] In the early 1950s there was an upsurge in interest in microanalytical methods. Microprobes with electrons to bombard the sample quickly become the instrument of choice for microcharacterization. Electrons could easily be focused to spot sizes less than 1 μm-diam with enormous intensities compared to X-ray sources. Though X-ray excitations give a much better signal to background, their generation required electron bombardment of a metal target with X rays emitted into 4π srad which then had to be gathered and focused to a small spot with inefficient X-ray optics. With the commercial availability of high-intensity and high-resolution electron microprobes, the unique properties of photons could not overcome the lack of intensity from their weak sources. Interest in X rays as an excitation source for microprobe analysis faded, leaving electrons as the dominant microprobe source. It is a conservative estimate that 1200 to 2500 electron probes currently are being used for microcharacterization of matter in the United States. This represents an investment of $1 billion or more in instrumentation alone. The wide usage of analytical microprobes is well documented in

the several yearly conferences and journals of the electron microscopy and microprobe societies and attests to the great emphasis being placed by the scientific community on the need for microstructural characterization of matter.

With the advent of electron storage rings, an intense source of X rays has become available. The energy spectrum in the hard X-ray region is 10^4 to 10^5 times more brilliant than our conventional X-ray sources (2 kw to 60 kw dissipated by electrons impinging on metal targets). In fact, with magnetic devices especially suited for extracting the radiation from proposed new high-brightness storage rings, the brightness in units of photons or particles s^{-1} mm^{-2} $mrad^{-2}$ is 2×10^{19} and equivalent to that for the most advanced electron probes having field-emission electron guns.[2] To achieve this brightness for the energy range from 2 keV to 35 keV requires undulators on low-emittance electron storage rings in the 6 GeV energy range. This energy range covers the electron energy levels of the K- and/or L-shells for all the atoms and is most useful for fluorescent and diffraction analysis. Present X-ray storage rings (NSLS at Brookhaven; SPEAR at SSRL, Stanford; CESAR at CHESS, Cornell) are 10^{-3} to 10^{-4} less bright in this energy range.

The improved brightness of a 6 GeV ring with undulators offers major advantages over present storage rings. Scientists will be able to study the chemical composition, geometrical arrangements of the atoms, and electronic structure at unprecedented low levels of concentration. The chemical identity of the elemental composition of matter is a prerequisite to their synthesis, and knowledge of the geometrical arrangement and chemical bonding of the atoms is fundamental to understanding the basic physical and chemical behavior of materials. Much of our progress in the design of materials has come by trial and error. But the science of materials has advanced rapidly in recent years and microcharacterization techniques have made a major contribution providing both chemical identity and geometrical information about the atoms. Yet modern technology is making increasing demands on materials for better performance in terms of their electrical characteristics and under the most adverse environments of high temperature, corrosive atmosphere, and intense radiation fields. More stringent requirements are being placed on the control of manufacturing methods including tightening restrictions on impurity levels, on structure and compositional variations, on presence of minor phases, and on controlling interfaces.[3-5] The behavior of grain boundaries and other interfaces can determine if a material is ductile and has toughness or is brittle and unreliable for use in structural applications. Minor amounts of second phases can improve the strength of materials or make them unfit for service. Segregation of trace elements to interfaces and second phases can have dramatic effects on the properties of materials. Synergestic effects among trace elements is observed but poorly understood. Concentrations are often below present detectable limits for nondestructive analysis and improved microcharacterization methods are needed. The construction of X-ray microprobes on new high-brightness storage rings will produce unique microcharacterization capabilities unmatched by any other method.

As electron microprobes have clearly dominated the field of microcharacterization, the merits of the use of X rays for excitation of the sample will be compared to electrons. A few of the many possible applications are cited where

microcharacterization is important to advancing our understanding of materials properties. For more extensive information the reader should refer to the electron microscopy and microprobe literature.

II. DETECTION LIMITS WITH X RAYS VERSUS ELECTRONS

A standard definition of the minimum detectable mass fraction[6] based on Poisson counting statistics for 95% confidence in detection is

$$\text{Minimum Detectable Mass Fraction (MDMF)} = 3.29\, C_Z (N_b)^{1/2}/N_S \ , \qquad (1)$$

where C_Z is the mass fraction of element Z, N_b the background counts, and N_S the counts in the signal. To evaluate Eq. (1), we need to know the fluorescent cross sections to calculate the number of events in the signal and to evaluate the background. An extensive literature review on this subject provides the information for the evaluation.[7] The relevant data are presented in Figs. 1–3. As shown in Figs. 1 and 2, the number of characteristic fluorescent events is typically 10 to 200 times larger for X-ray excitation than for the same number of electrons. As shown in Fig. 3, the fluorescent signal to background is approximately 10^4 times larger for X-ray excitation than for electron excitation. This extremely favorable property of X rays derives from the fact that about 90% or more of the incident X-ray energy is dissipated by ionization of the inner shells. In contrast, only 0.1% of the energy dissipated by electrons gives rise to the fluorescent radiation of interest. Much of their energy is consumed by interactions with the least-bound outer-shell electrons. The deceleration of the incident electrons in the target produces Bremsstrahlung radiation which is responsible for most of the background beneath the fluorescent signals of interest.

We find that 10^{-3} fewer X rays than electrons are required for the same MDMF. In terms of energy deposited, electron energies from 20 keV to 100 keV usually exceed by three to ten times the ionization energy of the bound electron. X-ray energies can be chosen to lie just above the ionization energy (2 keV to 33 keV). As 10^3 more electrons with energies from three to ten times those of X rays are required for the same MDMF, the energy deposited by electrons is 3×10^3 to 10^4 times that deposited by X rays in thick targets. For thin targets most of the incident electron energy is transmitted, but even less incident X-ray energy is absorbed. In air-dried blood cells and 8 μm-thick tissue sections[8] exposed to synchrotron radiation and charged particles, X-ray fluences 10^2 to 10^3 times greater were required to produce similar damage. X-radiation damage to the samples may be orders of magnitude less than the comparison made on the basis of energy deposition alone. Thus with X-ray excitation we have the important choice of being able to either lower the detectable limits for the same fluences or to reduce the radiation damage and heat deposited in the sample for the same MDMF. Since heating and radiation damage of organic samples is of primary concern in modern electron probes, X rays offer major improvements.

III. X-RAY INTENSITIES FROM UNDULATORS ON HIGH-BRIGHTNESS STORAGE RINGS

With the proposed X-ray intensities from undulators on high-brightness storage rings (see other sections of this document and SSRL Report 83/01 and NSLS Report, Planned Evolution of NSLS, October 1983), fluxes are predicted to be on the order of 2.7×10^{15} X rays s^{-1} in an energy bandwidth, $\Delta E/E$, of 0.1%. Projections of an electron source size in the storage ring of $2\sigma_x = 0.8$ mm and $2\sigma_y = 0.2$ mm and divergences of 0.01 mrad in both the horizontal and vertical planes for undulators produce a brightness of 2×10^{19} X rays s^{-1} mm^{-2} $mrad^{-2}$. Considerations of the X-ray-focusing optics[7,9,10] have shown that demagnifications of 100:1 are clearly feasible with about 50% reflection efficiencies and that demagnifications approaching 1000:1 may become possible. Because of the small divergence of undulator radiation, X-ray optics can intercept the entire emittance and both focus and monochromate with high efficiency. We base our arguments for the intensities obtainable for an X-ray microprobe on a modest demagnification of 100:1. A demagnification of 100:1 results in a probe size of 2×8 μm^2, and further reduction is achieved by pinholes in heavy metal foils. The predicted intensities are given in Table I. Comparisons are made with those from the brightest storage ring now in commissioning and the most intense electron microprobe sources. A gain of 1.4×10^4 in intensity per eV is obtained over present low-emittance rings. In addition, undulators in comparison to superconducting wigglers peak the energy in narrow bandwidths reducing the heat load on X-ray optics. At 10 eV energy bandwidths the brightness from undulators will match that available from the most advanced electron probes. Though undulators peak the intensity at harmonic energy intervals, energies ranging from 2 keV to 40 keV are available in either the first or second harmonic. When only discrete X-ray energies are selectable from undulators, then 2, 4, 10, 18, and 35 keV or similar energies are acceptable for most microprobes fluorescent and diffraction analysis.[7] For fluorescent excitation, energy spreads of $\Delta E/E = 1$ are acceptable.[7] For diffraction analysis of the compounds present, a $\Delta E/E = 10^{-2}$ to 10^{-3} is required. For microprobe EXAFS analysis and photoelectron spectroscopy, $\Delta E/E$ should be 10^{-4} to 10^{-5}. These energy resolutions can be achieved with presently available nearly perfect crystals, and the microprobe energy resolution tailored to meet the experimental needs of a variety of applications.

IV. SPATIAL RESOLUTION

Inherently, X-ray excitation for microprobe analysis offers the highest spatial resolution in thick samples of any radiation because the low-scattering cross sections of X rays limit the lateral spreading of the probe. Though electron field-emission sources are much smaller (approaching 10 Å-diam) and are focused to diameters of atomic dimensions, lateral spreading of the electrons in matter produce interaction regions of about 1 μm-diam in thick samples.[11] Electron-probe analysis of ferrous materials having specimen thicknesses of 1000 Å to 2000 Å produce an interaction region of approximately 500 Å-diam even though the incident probe diameter is much less. Diffraction limits may keep the useful X-ray probe diameter to 500 Å and greater.[10] An X-ray microprobe with a beam diameter of 500 Å to 1 μm would compete favorably with the spatial resolution of electron microprobes in a great majority of the samples of

interest. For extremely thin particles and films (< 1000 Å), the electron microprobe has spacial resolutions ranging from a few angstrom to a few hundred angstroms. Although 500 Å-diam appears feasible for an X-ray microprobe, it is not a fundamental limit. In a 500 Å-diam probe, the diffraction-limited divergence angle is 5 mrad for 12 keV X rays but only 0.2 mrad for 100 keV electrons. This places a limit of 10 μm to the depth of beam penetration in the sample before divergence of the X-ray beam in the sample exceeds the intended probe size.

V. DETECTION LIMITS FOR AN X-RAY MICROPROBE BASED ON A 6 GeV RING WITH UNDULATORS

A. Fluorescent Elemental Analysis

The minimum detectable mass fraction is calculated with Eq. (1) using the X-ray intensities given in Table I, the fluorescent cross section and yields of Figs. 1 and 2, and the signal to backgrounds from Fig. 3. We assume an analyzing crystal intercepting 1 cm^2 of fluorescent radiation 10 cm from the sample for a solid angle of 10^{-3}. The number of fluorescent counts in the signal is:

$$\frac{\text{Signal Counts (Ns)}}{\text{Sec } 10^{-6}\ gg^{-1}} = 0.1\ (\text{Thick-target yield}) \times 10^{14}\ \left(\frac{\text{Incident Photons}}{\text{Sec } \mu m^2}\right)$$

$$\times\ 10^{-3}(\text{Solid Angle}) \times 10^{-6}\ (\text{Mass Fraction of } 10^{-6}\ gg^{-1}):$$

$$\frac{N_S}{\text{Sec } 10^{-6} gg^{-1}} = 10^4\ \frac{\text{Counts}}{\text{Sec } 10^{-6} gg^{-1}}\ \text{from a 1 } \mu m^2 \text{ spot.}$$

With a signal to background of 10:1 at 10^{-6} gg^{-1} and a homogeneous distribution of the element, the MDMF is 10.5×10^{-9} gg^{-1} s^{-1} which is 2×10^{-4} times the MDMF for the best electron probes with wavelength dispersive optics. An increase to 100 secs counting time would lower the MDMF to 1.5×10^{-9} gg^{-1}.

As the detection of elements at interfaces is important to many materials problems, we calculate the detectable levels for a planer distribution of elements. Assume that one monolayer of an impurity element replaces one 2 Å-wide atomic plane. For an X-ray probe diameter of 1 μm^2, 5000 atomic planes end-on would be irradiated by the beam. Since one of the atomic planes out of 5000 consists of impurity atoms, the concentration of the impurity is 2×10^{-4} gg^{-1} in the volume irradiated by the probe. (This assumes that none of the impurity exists outside the boundary.) Since the MDMF is 10.5×10^{-9} gg^{-1} s^{-1}, then the detection of 5×10^{-5} of a monolayer s^{-1} of impurity is feasible. However, in

most materials we expect some of the impurity to be distributed in the matrix. Typical elemental concentrations of 2×10^{-3} to 10^{-4} gg^{-1} are used to affect grain-boundary behavior. Plotted in Fig. 4 are the calculated profiles of X-ray-probe scans for an iron sample containing 0.1 wt % titanium uniformly distributed in the matrix and with one monolayer of titanium in the grain boundary. The shape and size of the microprobe beam can be defined by pinhole apertures to better match the geometry of the interface to improve the contrast and lower the detectable limit. For this case of titanium in iron where 0.1 wt % of the same impurity is in the matrix, the minimum detectable impurity with the plane of the grain boundary parallel to the direction of the probe (end on) is 5×10^{-3} of a monolayer for both the 1 μm^2 and 500 A^2 probes. As predicted by Eq. (1) a decrease in the probe diameter does not change the detectable limits for a line distribution since the signal decreases linearly and the background decreases as the square of the probe size. If the region next to the boundary is denuded of the impurity, then the smaller probe size has the advantage of better providing the spatial resolution to determine that information. The rectangular-shaped probe has a detectable limit of 6×10^{-4} of a monolayer in the presence of 0.1 wt % in the matrix. Typical experience with advanced analytical electron probes is that one monolayer of impurity at a boundary is at the detection limit.

For impurity atoms and particles or second phases on surfaces and exposed interfaces the characteristic fluorescence or diffracted radiation is not absorbed by the matrix and even lower detection limits are possible. The number of signal counts is

$$\frac{N_S \text{ (Signal counts)}}{\text{Sec atom}} = \frac{I_0 \sigma}{4\pi R^2} , \qquad (2)$$

where I_0 is the incident intensity, and σ is the fluorescent cross section. I_0 is taken from Table I and a typical value for σ from Fig. 1. With the signal to background taken from Fig. 3 (a conservative estimate for surface impurities), the definition of the MDMF predicts that with a probe area of μm^2, in a time of one second, and with 95% confidence, the following can be detected:

2.7×10^{-4} monolayer, 5×10^3 atoms, and 40 A-diam particle.

For a 500 A^2 probe, in a time of one second, the following are typical detection limits:

5.4×10^{-3} monolayer, 250 atoms, and 15 A-diam particle.

The assumption is made here that the particle is smaller in diameter than the probe so that reducing the probe diameter lowers the background by the square of the reduced diameter while the signal remains constant. Small probe size is a major advantage in the detection of particles smaller than the probe diameter. For an isolated particle on a very thin substrate, where the background contribution to the signal is less, even lower limits of detection can be achieved. For electron probes, the minimum detectable mass of iron in a molecule of

ferritin has been reported to be 10^{-19} g in 100 secs counting time, or 11,000 iron atoms per second at a probe current of 1.0 nA in a 60 nm-diam probe.[12] The iron K-edge fluorescent cross section for 10 keV X rays is (see Fig. 1) at least 50 times larger than for 20 keV to 100 keV electrons. So even if we ignore the better signal to background for X-ray excitation, the MDMF with X rays is less than 1/50 of that for the same electron flux. A comparison of the fluorescent analysis capabilities of X-ray and electron microprobes is given in Table II.

B. Diffraction Analysis

X rays also have some advantages over electrons when used for diffraction. Diffraction measurements provide important information such as the crystal structure, compound identification, and how the geometrical arrangements of the atoms deviate from perfect periodicity. For the same number of 10 keV X rays or electrons impinging on a metal sample, the X rays are approximately 200 times more likely than electrons to undergo a useful elastic-scattering event. Electrons are most likely to lose energy by straggling energy-loss processes adding to the unwanted background unless removed by energy-analysis spectrometers. Electrons are also more likely to undergo multiple-scattering events which complicate the interpretation of the measured diffraction pattern.[13] X-ray microprobes permit the use of thicker samples reducing the problem of defect migration to interfaces and strain relief which can be a problem in thin samples.

With the criteria expressed in Eq. 1, the MDMF by diffraction with a μm^2 X-ray probe in one second is:

10^{-2} of a monolayer, 1.6×10^3 atoms in a particle, and 28 A-diam particle.

This is a conservative estimate as an experiment with less flux for the favorable case of a monolayer of lead deposited on the surface of a copper single crystal predicts a minimum detectable coverage of approximately 10^{-3} of a monolayer from the observed 5×10^4 signal counts s^{-1} with a signal to background of 500:1.[14] For amorphous materials, the diffuse scattering from only six monolayers of matter could be measured with a 1 μm-diam probe. Recent X-ray diffuse-scattering measurements from thin amorphous layers convinced the authors to predict that analysis of 100 A films is feasible even at intensities 10^{-3} of those proposed for the microprobe.[15]

Among the most prominent applications of synchrotron radiation in the X-ray-energy region is the measurement of the extended X-ray absorption fine structure (EXAFS).[16] Such measurements permit the determination of the average number of near-neighboring atoms and average bond distances about a central atom whose absorption edge is scanned by changing the X-ray energy. The ability to determine the chemical environment of a particular element at low concentrations has resulted in major contributions to our understanding of the role of minor elements in matter.[17] The projected 3×10^{10} photons s^{-1} $(eV)^{-1}$ for a 500 A-diam probe would extend the ability to make EXAFS measurements on extremely small quantities of matter and with high-spatial resolution.

A summary of the fluorescent and diffraction detectable limits of an X-ray microprobe is given in Table III.

VI. DEPTH PROFILING

The total reflection of X rays offers a means for measuring both elemental composition and phases as a function of depth from the surface. By varying the penetration depth of X rays with small glancing angles, sensitivity is increased for surface and near-surface information. Shown in Fig. 5 is the angular variation in penetration length of 17.4 keV X rays for a germanium surface.[18] For angles below about 2 mrad, only the first 25 Å contributes to the fluorescent and diffraction signal. As the grazing-incidence angle increases, the signal comes from deeper beneath the surface approaching the usual absorption penetration above 6 mrad. The development of this nondestructive X-ray-profiling technique using the highly collimated radiation from undulators would extend the advantages of X-ray fluorescent and diffraction analysis to the characterization of surfaces, overlayers, and interfaces at unprecedented low levels of detection.

VII. HEATING OF THE SAMPLE

The question arises whether excessive heating of the samples will occur from the energy in the X-ray probe. Intensities used in the detection limit calculation ranged from 10^{14} μm^{-2} to 2.5×10^{11} $(500\ Å)^2$ X rays s^{-1} and are comparable to those available in electron probes. Shown in Fig. 6 is the calculated maximum temperature rise of thin samples at the point of the beam impingement neglecting radiative heat loss.[19] A sample is thin when the absorption for the incident radiation is linearly proportional to the sample thickness. The sample is assumed to be in good thermal contact around its edge. Specimen thermal conductivities, k, and X-ray linear-absorption coefficients, μ, were chosen to span the range from good to poor thermal conductors. At the highest projected X-ray microprobe flux of 10^{14} X rays s^{-1}, good thermal conductors with low absorption coefficients would not get excessively hot. At fluxes of 10^{12} X ray s^{-1} contained in a 0.1 μm-diam probe, most samples would not be overheated. For infinitely thick samples (total absorption of the X-ray beam), the temperature rise would be from two to ten times less than given in Fig. 6. Thus, all the projected flux from undulators on low-emittance rings is useful. When appropriate, flux can be traded for improved spatial resolution. Electron microprobes deposit more energy in a smaller sample volume nearer to the surface than a similar number of X rays. Since only 10^{-3} to 10^{-4} as many X rays as electrons are required for the same MDMF, heating can be made less of a problem for X-ray microprobes.

VIII. THE NEED FOR X-RAY MICROPROBE CHARACTERIZATION OF MATERIALS

Segregation of elements and nonuniform distribution of phases in materials are the rule rather than the exception. Common interfaces in materials to which segregation occurs are surfaces, grain and precipitate boundaries, dislocations,

and surfaces formed by defects such as vacancy and interstitial configurations. Intentionally added trace elements and unintentional impurities play a major role in the physical and chemical properties of matter. Besides their effect on electrical properties, minor elements can have a major effect on both surface and mechanical properties because of their bias for segregation.[5] Segregation may extend outwardly for distances of microns from the interface or be confined to single-atomic dimensions. Microprobe characterization of segregation in materials is important to understanding their properties.

The amount of actual quantitative data on segregation of elements is rather limited; many of the observations are inferred from property changes with controlled additions of minor elements. Electron microprobes with elemental detection limits above 50×10^{-6} gg^{-1} are not sensitive enough to detect the distribution of a majority of minor elements affecting materials properties. Electron microanalysis is done mainly to identify precipitates and to study phase separation when elemental concentration differences have developed enough for detection. Much of the quantitative data on segregation to interfaces has been directed toward understanding the remarkable effect it may have on grain-boundary cohesion. Auger electron spectroscopy (AES) using electron excitation to create the signal has provided the bulk of the data from fractured surfaces. AES is a truly surface-sensitive technique detecting only the first one or two atomic layers at coverages to 0.01 of a monolayer. Because of the poor signal to background, AES is not sensitive to low concentrations. Sensitivity to the first two atomic layers precludes its use for studying interface segregation with the nominal 500 A-diam beam end-on to the boundary. Thus fracturing in vacuum is necessary to expose the surface and preclude absorbed gases. The technique is limited to materials that can be fractured along the grain boundaries. X-ray fluorescent radiation from the K-shells of all but the lightest elements will penetrate several thousand angstroms so that detection of the grain boundary impurities can be measured with the probing beam end-on to the boundary without fracturing the specimen. The profile of the impurity distribution is inferred by deconvolution of the beam profile from the measured profile. It is very difficult with AES to be sure if the impurities are in the form of precipitates or in solution in the matrix. An X-ray microprobe could identify the two forms since diffraction analysis would identify phases and fluorescence the elements. As the chemical bonding of the segregant can change when exposed at a surface, the ability to detect impurities at an intact interface using an X-ray microprobe in the EXAFS, electron, or soft X-ray spectroscopy modes would provide information not now available.

A review of all the many obvious applications where X-ray microprobes would produce needed information for new developments in the science and technology of materials would be an enormous task. Even an order of magnitude improvement in performance over existing microprobes is sufficient justification for their funding. Gains in sensitivities of 10^3 plus the additional advantages of X rays as a probe would make it difficult to predict all the many unseen advantages. Advantages of an X-ray microprobe to a few of the large generic areas of materials science are illustrated by specific examples.

A. Crack Growth and Fracture

The catastrophic and unpredictable failure of structural components by crack initiation and propagation requires that they be greatly overdesigned compared with what is necessary to withstand the applied loads. As the basic mechanism of cracking is not well understood, expensive solutions are used: high strength is traded off for crack-resistant ductility requiring thicker members to insure reliable performance. Observations of crack initiation and propagation in thin metal foils under simple tension with transmission electron microscopy reveal the dislocation distributions associated with the plastic deformation ahead of the crack tip (Fig. 7).[20] The crack tip (at the end of the arrow) radiates dislocations in the forward direction to accommodate the high-stress levels around the crack. Quantitative information important to an understanding of the strain distributions is lost because of the necessity of using thin foils which permits buckling that relieves the elastic strain. Samples more consistent with practical situations and thick enough to preserve the elastic strain could be studied with an X-ray microprobe in diffraction gaining new information about strain distributions to test current theories of fracture.[21] In addition, the role played by impurities in fracture could be studied at concentrations orders of magnitude less than presently possible.

B. Ductile Alloys

Ordered alloys can have desirable high-temperature properties,[22] but lack of ductility greatly restricts their application. An example of such an ordered alloy lacking ductility is Ni_3Al which has superior high-temperature strength exceeding that for type 316 stainless steel and Hastelloy-X. The addition of small amounts of boron and manganese can change the cohesive energy of the grain boundaries producing a ductile material. Shown in Fig. 8, upper left, are the separated grains that resulted from hot-rolling the brittle Ni_3Al. In Fig. 8, upper right, the same material is made ductile enough to deep-draw to a 25 mm-diam cup at room temperature after minor alloying additions. The curve in the lower part of Fig. 8 shows the dramatic change in the tensile elongation with the addition of boron. Auger electron spectroscopy was used to show that boron is segregated to the grain boundaries, but the chemical form of the boron could not be determined.[23] An X-ray microprobe with orders of magnitude better signal to noise would provide both diffraction and elemental analysis producing information on chemical bonding at interfaces without having to fracture the surfaces.

C. Creep

A mode of deformation of crystalline materials held at high temperatures under low stresses is grain-boundary creep. An example of the failure of a Ni-20 wt % Cr-alloy by this process is shown in Fig. 9. Grain-boundary creep followed by crack initiation and propagation leads to rupture of the sample. Use of interface-active solutes is a means of changing the rate of this diffusion-controlled creep. The addition of 0.11 wt % Zr to a Ni-Cr alloy is shown in Fig. 10 to have a major effect on improving the creep-rupture performance by extending the service life and reducing the elongation while increasing

the load-carrying capacity.[24] X-Ray microprobe measurements of the elemental segregation to the grain boundaries, grain boundary diffusivity, and the strain and deformation present at the boundaries would provide new information towards understanding and controlling this phenomenon.

D. Ceramics

The brittleness of ceramic materials prevents their desirable high-temperature strength, wear, and corrosion resistance from being widely used in structural applications. Design criteria are uncertain since crack initiation and propagation are poorly understood. Fracturing occurs over a wide range of stresses and is influenced by poorly understood impurities at interfaces. Sintering ceramics to high density improves their resistance to fracturing apparently by reducing the voids which act to initiate cracks along the grain boundaries.[25] Among the methods used to achieve high-sintering densities and to increase toughness are the additions of small amounts of other elements which segregate to grain boundaries. An example of the effect of magnesium on the sintered density of alumina is the development by the General Electric Company of optically translucent alumina (Lucalox) for use in high-pressure sodium lamps. Though several studies have shown that the magnesium segregates to the grain boundaries, from the standpoint of the chemistry that occurs at the boundary, the effect is poorly understood.[26] Second phase additions are also used to control grain boundary fracture in the development of tougher ceramics. More ductile metals or ceramics placed in the grain boundaries will absorb some of the energy by plastic deformation. An example in zirconia-toughened alumina is shown in Fig. 11. The darker particles in this transmission electron micrograph are zirconia which undergo a phase transformation under stress absorbing energy from the crack. Thus more stress is required to propagate the crack. X-ray microprobe measurement of the strain distributions in the grains adjacent to the crack, of second phases by diffraction, and of the elemental segregation by fluorescence would provide new information on which to base our understanding for improved crack-resistant ceramics.

E. Diffusion

The rate of diffusion of elements is important whenever dissimilar materials are in contact. Diffusion controls the characteristics of mass transport which includes the rate at which chemical equilibrium is reached, the rate of growth and dissolution of precipitates, corrosion rates, and rates of transformation. Since most materials consist of more than one element, knowledge of the lattice and short-circuiting paths of diffusion is key information to the design of new materials. Diffusion rates are necessary to understand the thermodynamics of phase equilibria, the kinetics of transformations, and in particular the way materials undergo radiation damage such as from ion implantation and fusion or fission reactors. An X-ray microprobe detecting concentrations at 10^{-9} gg^{-1} levels with fractional μm resolutions would be extremely useful for obtaining diffusion information. In short-circuit diffusion where data are difficult to obtain, radioactive tracers are often used. An example is shown in Fig. 12 where radioactive Ni63 is used to obtain an autoradiographic image of nickel diffusion into a copper grain boundary.[27]

Densitometer measurements of the exposed film were made with a 6.3 × 6.3 μm^2 slit. An X-ray microprobe would have the elemental sensitivity to directly determine quantitatively the concentration gradients for the diffusion of unlike elements.

Preferential corrosion along grain boundaries is common in stainless steels, and nickel-, chromium-, and aluminum-base alloys in aqueous environments. Trace element segregation to the boundaries is associated with a sensitization mechanism that may have a large effect on intergranular corrosion. A lack of chemical information about the boundary leaves the process poorly understood.

F. Electronics

The science and technology of designing and fabricating high-performance and reliable integrated circuits and microchips are dependent in a large measure on the control of certain impurities and trace-element additions which are generally below the detectable limits of electron probes. Miniaturization in integrated-circuit technology and increasing circuit densities on microchips with spacing of 1 μm or less have pushed the requirements for chemical, structural, and elemental information to levels below what can presently be detected in such small dimensions. A silicon chip on an electronic circuit board is shown in Fig. 13. Literally millions of electrical contacts are made and reliability depends on each performing satisfactorily. The failure of micrometer-sized connections and circuits occurs from aging mechanisms such as grain growth, interdiffusion, surface crystallization, and crack propagation. An accelerated understanding of this degradation requires microcharacterization at levels below those presently obtainable. Because of the part per billion detection capabilities with submicron resolutions, X-ray probes will have wide application in the electronics industry.

G. Radiation Effects

Structural materials are subjected to high doses of energetic radiation in existing fission and planned fusion reactors. Important changes in their physical properties include swelling, creep, and embrittlement. Another form of irradiation is ion implantation to control surface and near-surface properties. Common to both processes are the large number of point defects produced by direct displacement of the atoms in the material and the alterations of the composition by transmutations or implantation of different elements. The high flux of vacancies and interstitials leads to enhanced diffusion which may induce segregation and precipitation at interfaces or void formation by vacancy collection. To improve radiation resistance, efforts are made to promote the removal of vacancies and interstitials by recombination or to prevent the agglomeration of like defects.[28] Shown in Fig. 14(a) are the voids generated by irradiation of an unmodified stainless steel leading to large swelling of the alloy. The additions of 0.2 wt % titanium to the steel dramatically reduces the swelling as shown in Fig. 14(b). Grain boundaries, dislocations, precipitates, and substitutional elements can act as sinks for the point defects and/or promote their recombination. Electron microprobe and transmission electron microscopy are

extensively used for microcharacterization of radiation damage and much remains to be done to understand this complex phenomenon. An X-ray microprobe will bring needed new information to this materials problem with 10^{-3} or lower elemental detection limits, diffraction information about strain and precipitation, and with chemical bonding insights obtained through EXAFS and other spectroscopies.

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REFERENCES

[1]Cosslett, V. E., A. Engström, and H. H. Pattee, Jr., eds. 1957. X-Ray Microscopy and Microradiography, New York: Academic Press, Inc.

[2]Zaluzec, N. J. 1979. Quantitative x-ray microanalysis: instrumental consideration and applications to materials science. Chapter 4, pp. 121–167 in Introduction to Analytical Electron Microscopy, J. J. Hern, J. I. Goldstein, and D. C. Joy, eds. New York: Plenum Press.

[3]Kriege, O. H. and J. Y. Marks 1976. Nonuniform distribution (both micro and macro) of trace elements in high-temperature alloys. Pp. 1017–1022 in National Bureau of Standards Special Publication 422, Accuracy in Trace Analysis: Sampling, Sample Handling, Analysis, Vol. II, P. D. LaFleur, ed. Washington, D.C.: U. S. Government Printing Office.

[4]Davis, C. M. 1976. Trace element analysis of nickel and nickel-base alloys — a review of current methods. Pp. 1005–1016 in National Bureau of Standards Special Publication 422, Accuracy in Trace Analysis: Sampling, Sample Handling, Analysis, Vol. II, P. D. LaFleur, ed. Washington, D.C.: U. S. Government Printing Office.

[5]Hondros, E. D. and M. P. Seah 1977. Segregation to Interfaces. International Metals Review 22:262–301.

[6]Currie, L. A. 1968. Limits for qualitative detections and quantitative determination. Anal. Chem. 40:586–593.

[7]Sparks, C. J., Jr. 1980. X-ray fluorescence microprobe for chemical analysis. Chapter 14, pp. 459–512 in Synchrotron Radiation Research, H. Winick and S. Doniach, eds. New York: Plenum Press.

[8]Slatkin, D. N., A. L. Hanson, K. W. Jones, H. W. Kramer, and J. B. Warren 1984. Damage to air-dried human blood cells and tissue sections by synchrotron radiation. Brookhaven National Laboratory Report BNL-34555.

[9]Howells, M. R. and J. B. Hastings 1983. Design considerations for an x-ray microprobe. Nucl. Instr. and Meth. 208:379–386.

[10]Ice, G. E. and C. J. Sparks, Jr. 1984. Focusing optics for a synchrotron x-radiation microprobe. Nucl. Instr. and Meth. In press.

[11]Goldstein, J. I. 1979. Principles of thin film x-ray microanalysis. Chapter 3, pp. 83–120 in Introduction to Analytical Electron Microscopy, J. J. Hern, J. I. Goldstein, and D. C. Joy, eds. New York: Plenum Press.

[12]Shuman, H. and A. P. Somlyo 1976. Electron probe x-ray analysis of single ferritin molecules. Proc. Nat. Acad. Sci. USA 73(4):1193–1195.

[13]Cowley, J. W. 1975. Diffraction Physics, New York: American Elsevier.

[14]Marra, W. C., P. H. Fuoss, and P. E. Eisenberger 1982. X-ray diffraction studies: melting of Pb monolayers on Cu(110) surfaces. Phys. Rev. Lett. 49(16):1169–1172.

REFERENCES (cont.)

[15]Fischer-Colbrie, A., P. H. Fuoss, M. Marcus, and A. Bienenstock 1983. X-ray scattering study on thin amorphous films. Pp. VII–140,141 in SSRL Report 83/01, K. Cantwell, ed.

[16]Winick, H. and S. Doniach, eds. 1980. Chapters 10–13 in Synchrotron Radiation Research, New York: Plenum Press.

[17]Bianconi, A., L. Incoccia, and S. Stupcich, eds. 1983. Proceedings of Second International Conference on EXAFS and Near-Edge Structure, New York: Springer-Verlag.

[18]Becker, R. S., J. A. Golovchenko, and J. R. Patel 1983. X-ray evanescent-wave absorption and emission. Phys. Rev. Lett. 50(3):153–156.

[19]Hobbs, L. W. 1979. Radiation effects in analysis of inorganic specimens by TEM. Chapter 17, pp. 437–480 in Introduction to Analytical Electron Microscopy, J. J. Hern, J. I. Goldstein, and D. C. Joy, eds. New York: Plenum Press.

[20]Kobayaski, S. and S. M. Ohr 1981. In situ observations of the formation of plastic zone ahead of a crack tip in copper. Scripta Metallurgica 15:343–348.

[21]Ohr, S. M. and S.-J. Chang 1982. Dislocation-free zone model of fracture: comparison with experiments. J. Appl. Phys. 53(8):5645–5651.

[22]Stoloff, N. S. and R. G. Davies 1966. The mechanical properties of ordered alloys, Vol. 13 in Progress in Metal Science, B. Chalmers and W. Hume-Rothery, eds., New York: Pergamon Press.

[23]Liu, C. T., C. L. White, C. C. Koch, and E. H. Lee 1983(7). Preparation of ductile nickel aluminides for high temperature use. Pp. 32–41 in Proceedings of the Symposium on High Temperature Materials Chemistry-II, Z. A. Munir and D. Cubicciotti, eds. Pennington, N. J.: The Electrochemical Society, Inc.

[24]Schneibel, J. H., C. L. White, and M. H. Yoo 1984. On the improvement of creep strength and ductility of Ni-20% Cr by small zirconium additions. Submitted for publication to Metall. Trans.

[25]Rice, R. W. 1977. Microstructural dependence of mechanical behavior of ceramics. Pp. 199–381 in Treatise on Materials Science and Technology, Vol. II, Properties and Microstructure, New York: Academic Press.

[26]Taylor, R. I., J. P. Coad, and A. E. Hughes 1976. Grain-boundary segregation in MgO-doped Al_2O_3. J. Am. Ceram. Soc. 59(7,8):374–375.

[27]Renouf, T. J. 1970. The measurement of grain boundary diffusion by the method of autoradiography. Phil. Mag. 22(176):359–375.

[28]Mansur, L. K. and E. E. Bloom 1982. Radiation effects in reactor structure alloys. J. of Metals 34(10):23–31.

TABLE I. Comparison of X-ray microprobe intensities from 6 GeV ring.

	14 keV X-rays 2.5 GeV, 500 mA wiggler	14 keV X-rays 6 GeV, 200 mA undulator	100 keV e^- Electron microprobe field emission[a]
Brightness Photons or $e^-/s\ mm^2\ mrad^2$	10^{16}[b]	2×10^{19}[b,c]	3×10^{19}
Intensity P or e^-/Area sec	$\frac{5 \times 10^{12}}{10\ \mu m^2\ s\ 280\ eV}$	$\frac{2 \times 10^{15}}{10\ \mu m^2\ s\ 10\ eV}$	
	$\frac{5 \times 10^{11}}{\mu m^2\ s\ 280\ eV}$	$\frac{1 \times 10^{14}}{\mu m^2\ s\ 10\ eV}$	$\frac{6 \times 10^{13}}{\mu m^2\ s\ eV}$[d]
	$\frac{1 \times 10^{9}}{500\ A^2\ s\ 280\ eV}$	$\frac{3 \times 10^{11}}{500\ A^2\ s\ 10\ eV}$	$\frac{6 \times 10^{11}}{500\ A\ s\ eV}$
			$\frac{6 \times 10^{9}}{30\ A^2\ s\ eV}$
			$\frac{10^{7}}{4\ A^2\ s\ eV}$

[a] Zaluzec, N. J. 1979. Quantitative x-ray microanalysis: instrumental considerations and applications to materials science. Chapter 4, pp. 121–67 in Introduction to Analytical Electron Microscopy, J. J. Hern, J. I. Goldstein, and D. C. Joy, eds. New York: Plenum Press.

[b] National Synchrotron Light Source, Planned Evolution of NSLS, October 1983.

[c] Stanford Synchrotron Radiation Laboratory, SSRL Report 83/01.

[d] LaB_6 electron source.

TABLE II. Comparison of the characteristics of the proposed X-ray microprobe with those of the most advanced electron microprobes for fluorescent chemical analysis.

Characteristics		X rays	Electrons
Minimum detectable mass fraction s^{-1} for 1 μm-diam probe		0.01 ppm	50 ppm
Minimum detectable mass s^{-1} for 500 A probe		250 atoms	10,000 atoms
Minimum spatial resolution (samples > 1 μm thick)		~500 A	10^3 to 10^4 A
Minimum spatial resolution (samples 100 A to 2000 A thick)		~500 A	10 to 500 A
Number of electrons and X rays for the same MDMF		1	10^3
Number of energy units deposited in thick targets for same MDMF		1	10^3 to 10^4
Operating atmosphere		air, gas water, vapors	vacuum
Relative signal to background (contrast)		10^4	1
Accuracy for quantitative analysis	similar standards	~1%	~10%
	pure element standards	~5%	>10%
Relative fluorescent cross section		10 to 200	1
Relative thick-target fluorescent yields		10 to 150	1
Charge collection on electrically insulating samples		negligible	must be coated with conducting film

TABLE III. Detection limits for an X-ray microprobe based on radiation from an undulator on a 6 GeV low emittance storage ring.

Distributions of the elements	Probe size	Detection limits by fluorescent analysis	Detection limits by diffraction analysis
Homogeneous	1 μm-diam	10^{-8} gg^{-1} s^{-1}	$<10^{-4}$ gg^{-1} s^{-1}
Embedded planer interfaces	1 μm- to 500 A-diam	5×10^{-5} monolayers s^{-1} 5×10^{-3} monolayers s^{-1} in presence of 0.1 gg^{-1}	< monolayer
Surface atoms or particles	1 μm-diam	2.7×10^{-4} monolayers s^{-1} 5×10^{3} atoms s^{-1} 40 A-diam particle s^{-1}	Crystalline 10^{-2} monolayers s^{-1} 1.6×10^{3} atoms s^{-1} 28 A-diam particle s^{-1} Amorphous 6 monolayers s^{-1}
	500 A-diam	5.4×10^{-3} monolayers s^{-1} 250 atoms s^{-1} 15 A-diam particle s^{-1}	

FIGURE CAPTIONS

Fig. 1 Fluorescence cross sections for the elements when excited by X rays, protons ($^1H^+$), and electrons (e) of varying energies (after Sparks[7]).

Fig. 2 Thick-target fluorescence yields of pure elements for X rays, protons, and electrons of varying energies (after Sparks[7]).

Fig. 3 Comparison of the fluorescent signal-to-background ratio for various excitation radiations at a concentration of 10^{-6} gg^{-1} for an X-ray fluorescent radiation detection system with an energy resolution of the natural linewidth (after Sparks[7]).

Fig. 4 Calculated fluorescent intensity profile for an X-ray microprobe scan over a grain boundary containing a monolayer of titanium when the iron matrix contains 0.1 wt % titanium.

Fig. 5 Penetration depth of 17.4 keV X rays into germanium varies as a function of grazing incidence angle, α, to provide for nondestructive profiling of chemical information (after Becker et al[18]).

Fig. 6 Temperature rise from a 1 μm-diam X-ray beam impinging on a thin 10 mm-diam sample with side cooling. k/μ is the thermal conductivity in W/m•K divided by the X-ray linear absorption coefficient in m^{-1}. The k/μ values for various elements and materials are shown.

Fig. 7 Transmission electron micrograph of a shear crack with the dislocation network forming the plastic zone ahead of the crack (after Kobayaski and Ohr[20]).

Fig. 8 Brittle materials such as Ni_3Al shown with its grains separated in the upper left can be made ductile as illustrated by the cup (25 mm-diam) deep-drawn at room temperature. The lower curve shows the dramatic effect of adding boron to improve the ductility. Little is known about the chemical effect boron has on increasing the cohesion of the grain boundaries (courtesy of C. T. Liu, Oak Ridge National Laboratory).

Fig. 9 Failure of a Ni-20 wt % Cr alloy at 800°C by grain boundary fracture (courtesy of J. H. Schneibel, Oak Ridge National Laboratory).

Fig. 10 Segregation of minor concentrations of elements can effect the mechanical properties of materials through grain boundary modifications (after J. H. Schneibel et al[24]).

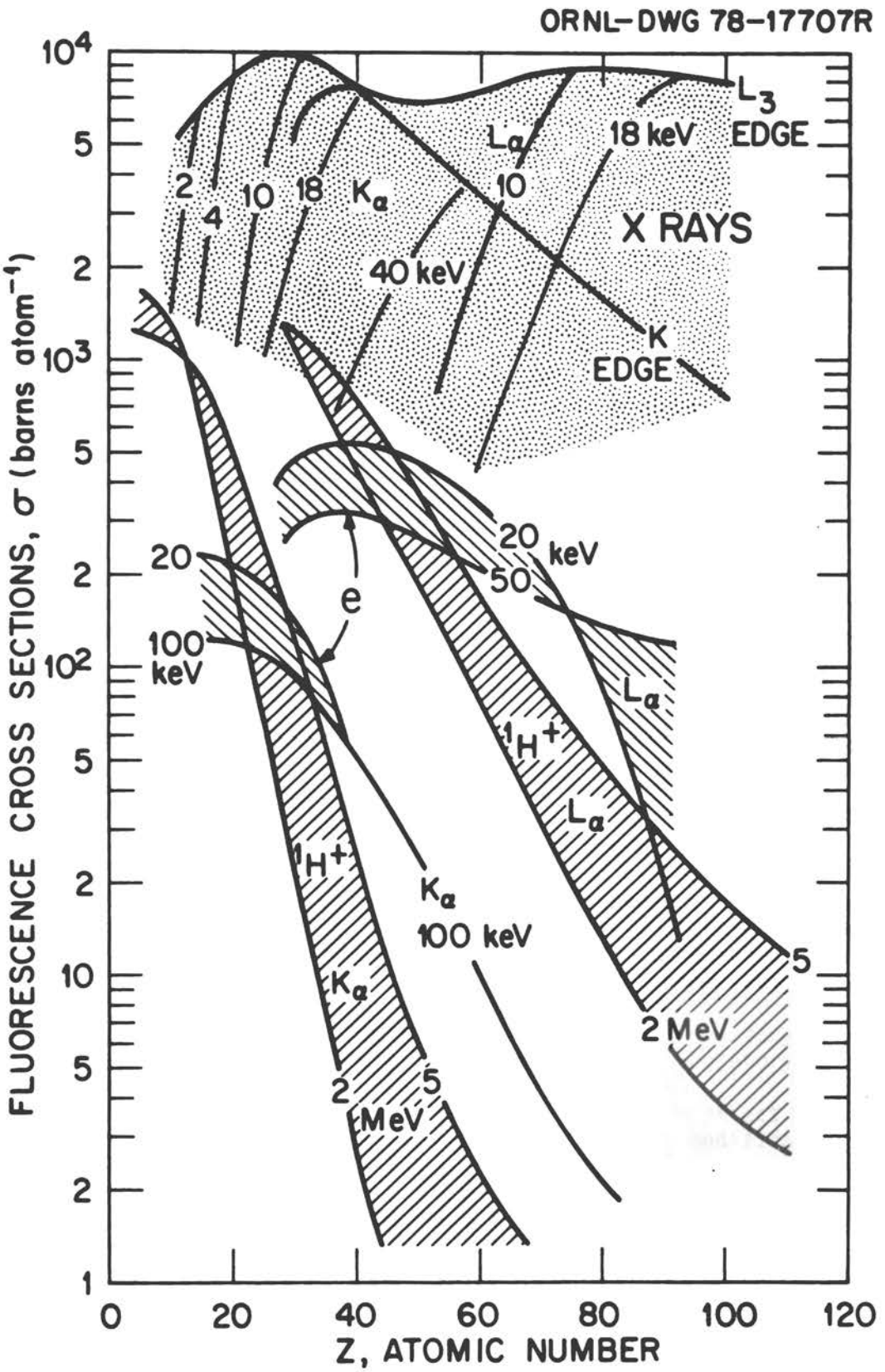
Fig. 11 Grain boundary cracking in ceramics is a major limitation to their application as structural members. Additions of 20 vol % ZrO_2 (the darker particles in this transmission electron micrograph) to Al_2O_3 improves the resistance to cracking (courtesy of P. F. Becher, Oak Ridge National Laboratory).

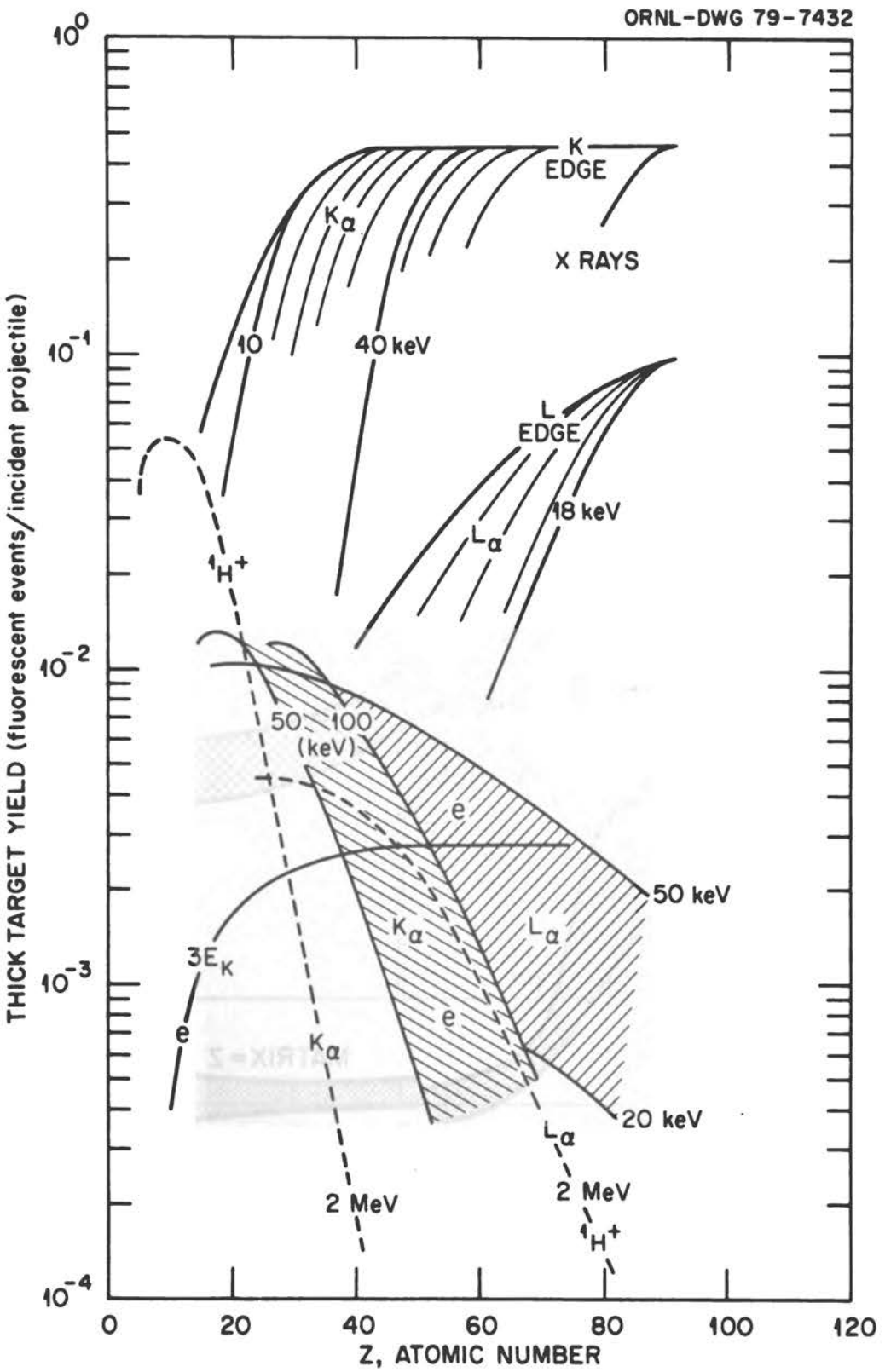
FIGURE CAPTIONS (cont.)

Fig. 12 An autoradiographic image of Ni_{63} tracer diffusion into a copper grain boundary. Diffusion along the boundary occurres at a faster rate than through the grain (after T. J. Renouf[27]).

Fig. 13 Advancements in minaturization and reliability of electron circuit boards and silicon microchips as shown here require nondestructive microcharacterization at submicron resolutions and below the detectable limits of electron microprobes.

Fig. 14 (a) Stainless steel of composition Fe-13 wt % Cr-15 wt % Ni irradiated with 4 meV Ni^{++}_{ions} to a dose of 70 displacements per atom at 675°C. The formation of many voids caused the alloy to swell. (b) Same composition and irradiation as in (a) except for 0.2 wt % Ti addition; the swelling was reduced dramatically (courtesy of Eal Lee, Oak Ridge National Laboratory).


ORNL-DWG 78-17707R
FLUORESCENCE CROSS SECTIONS, σ (barns atom⁻¹)
Z, ATOMIC NUMBER
X RAYS
L3 EDGE
K EDGE
18 keV
40 keV
2
4
10
18
Kα
Lα
20 keV
50
100 keV
20
100 keV
e
1H+
2 MeV
5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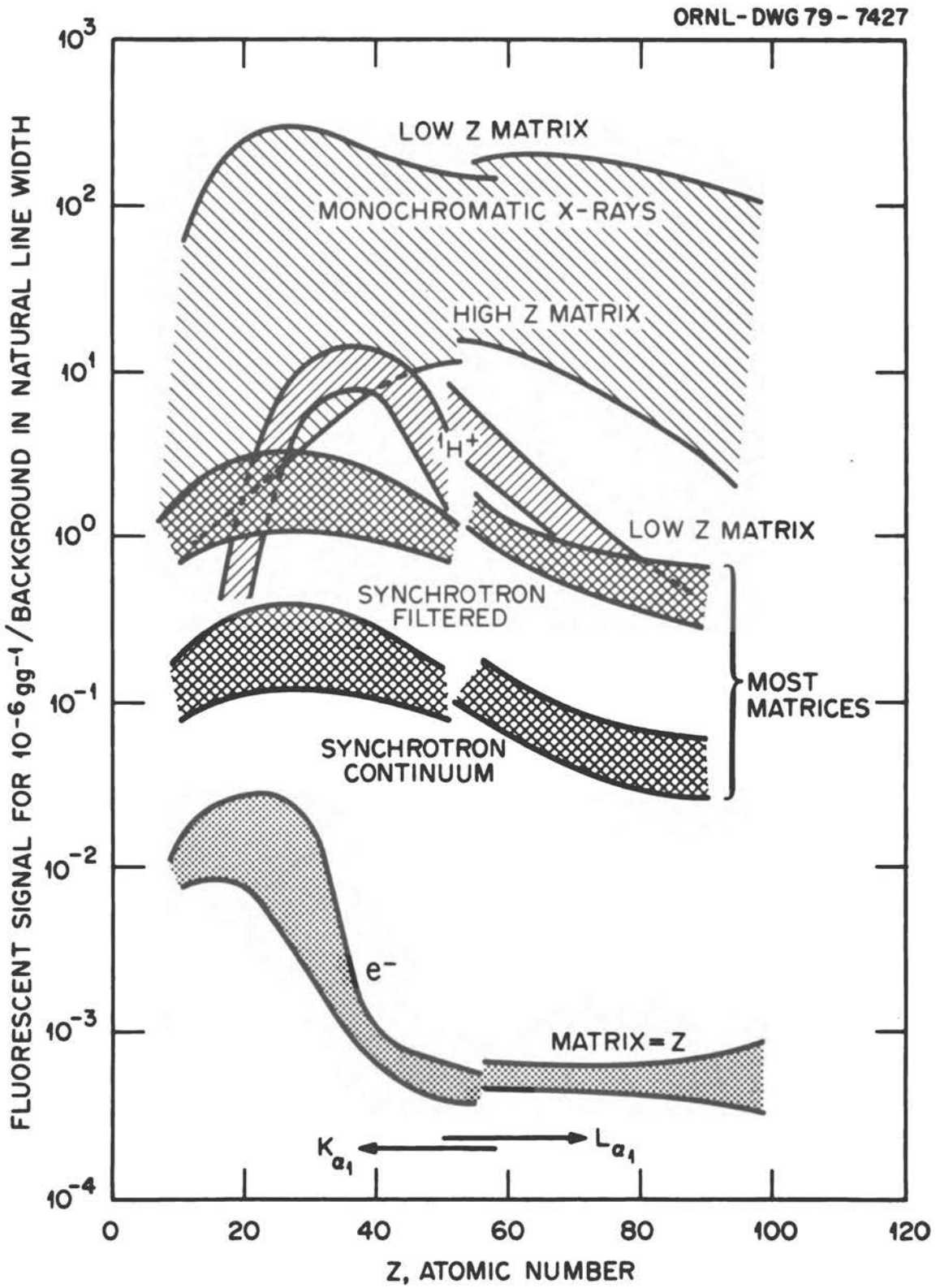
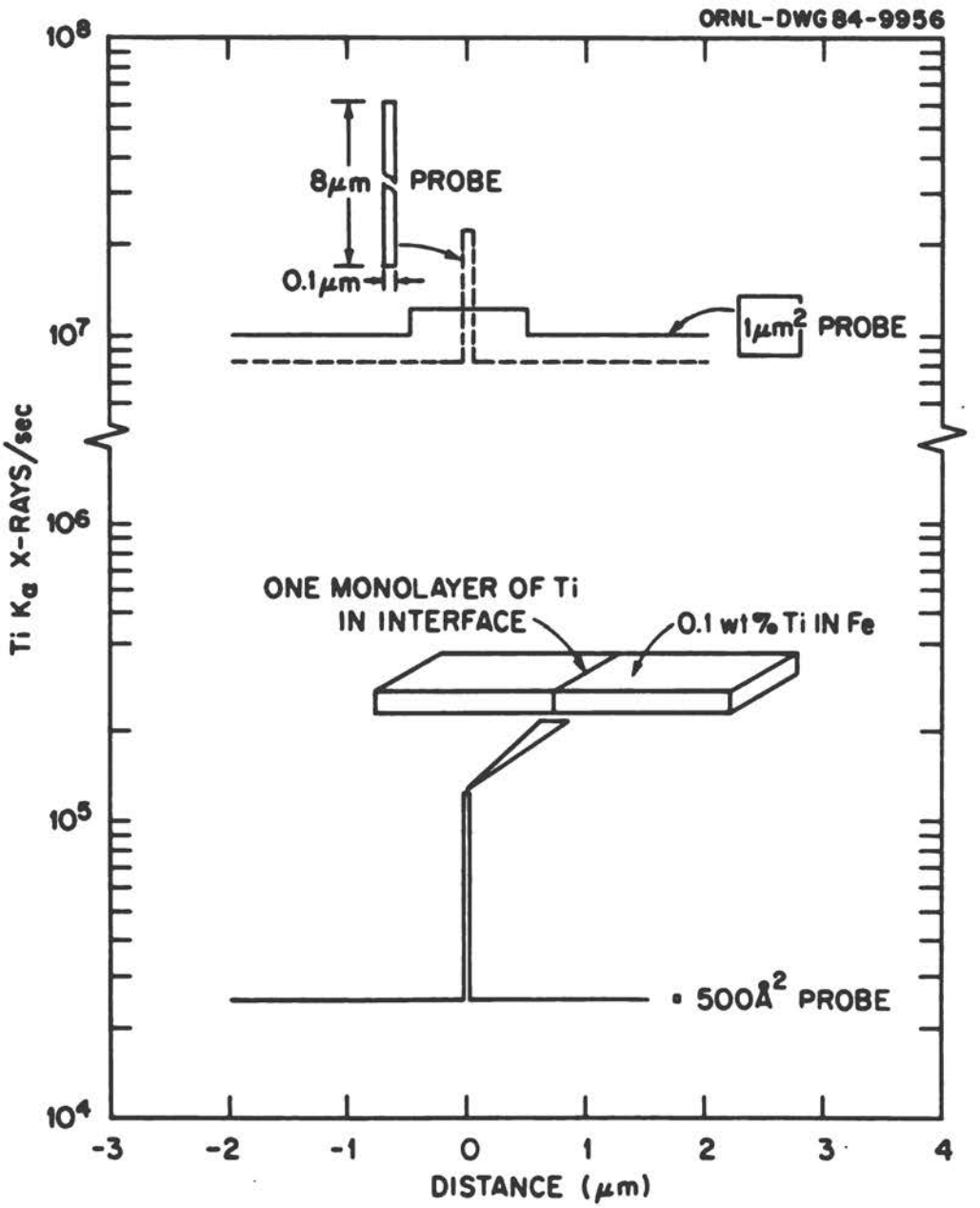
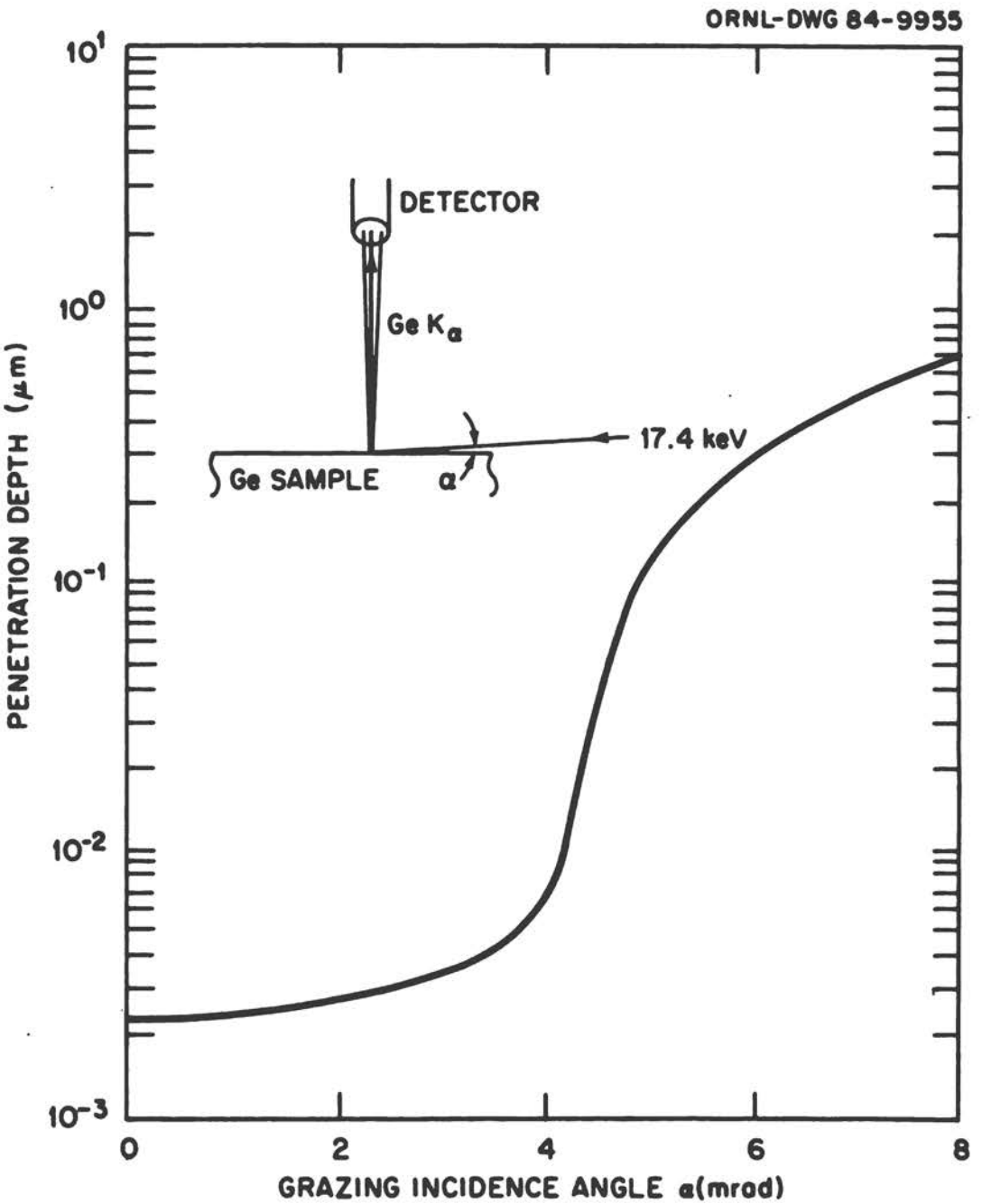
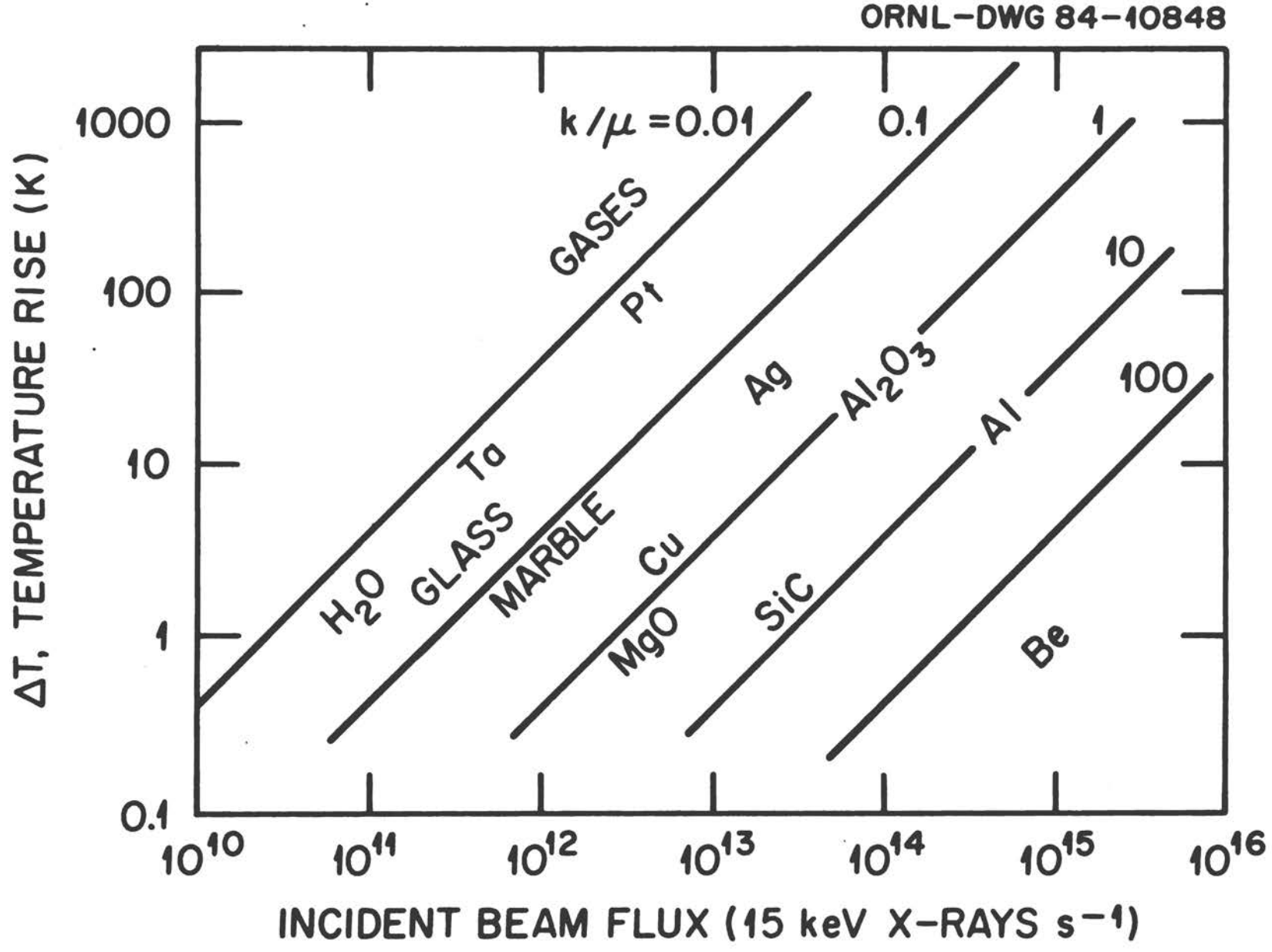
THICK TARGET YIELD (fluorescent events/incident projectile)
Z, ATOMIC NUMBER
K EDGE
X RAYS
K_α
10
40 keV
L EDGE
18 keV
L_α
$^1H^+$
50
100
(keV)
e
50 keV
K_α
L_α
$3E_K$
e
K_α
e
20 keV
L_α
2 MeV
2 MeV
$^1H^+$


ORNL-DWG 79-7427
FLUORESCENT SIGNAL FOR 10^{-6} gg^{-1}/BACKGROUND IN NATURAL LINE WIDTH
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
LOW Z MATRIX
MONOCHROMATIC X-RAYS
HIGH Z MATRIX
$^1H^+$
LOW Z MATRIX
SYNCHROTRON FILTERED
MOST MATRICES
SYNCHROTRON CONTINUUM
e^-
MATRIX = Z
K_{α_1}
L_{α_1}
0
20
40
60
80
100
120
Z, ATOMIC NUMBER

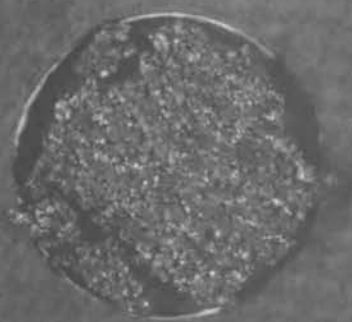

ORNL-DWG 84-9956
8μm PROBE
0.1μm
1μm² PROBE
ONE MONOLAYER OF Ti
IN INTERFACE
0.1 wt% Ti IN Fe
• 500Å² PROBE
Ti Kα X-RAYS/sec
DISTANCE (μm)
10⁸
10⁷
10⁶
10⁵
10⁴
-3
-2
-1
0
1
2
3
4


ORNL-DWG 84-9955
DETECTOR
Ge K_α
17.4 keV
Ge SAMPLE
α
PENETRATION DEPTH (μm)
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
0
2
4
6
8
GRAZING INCIDENCE ANGLE α(mrad)


ORNL-DWG 84-10848
ΔT, TEMPERATURE RISE (K)
1000
100
10
1
0.1
k/μ = 0.01
0.1
1
10
100
GASES
Pt
Ta
Ag
Al_2O_3
H_2O
GLASS
MARBLE
Cu
Al
MgO
SiC
Be
10^{10}
10^{11}
10^{12}
10^{13}
10^{14}
10^{15}
10^{16}
INCIDENT BEAM FLUX (15 keV X-RAYS s^{-1})


g=[1̄1̄1]
(123)
2 µm

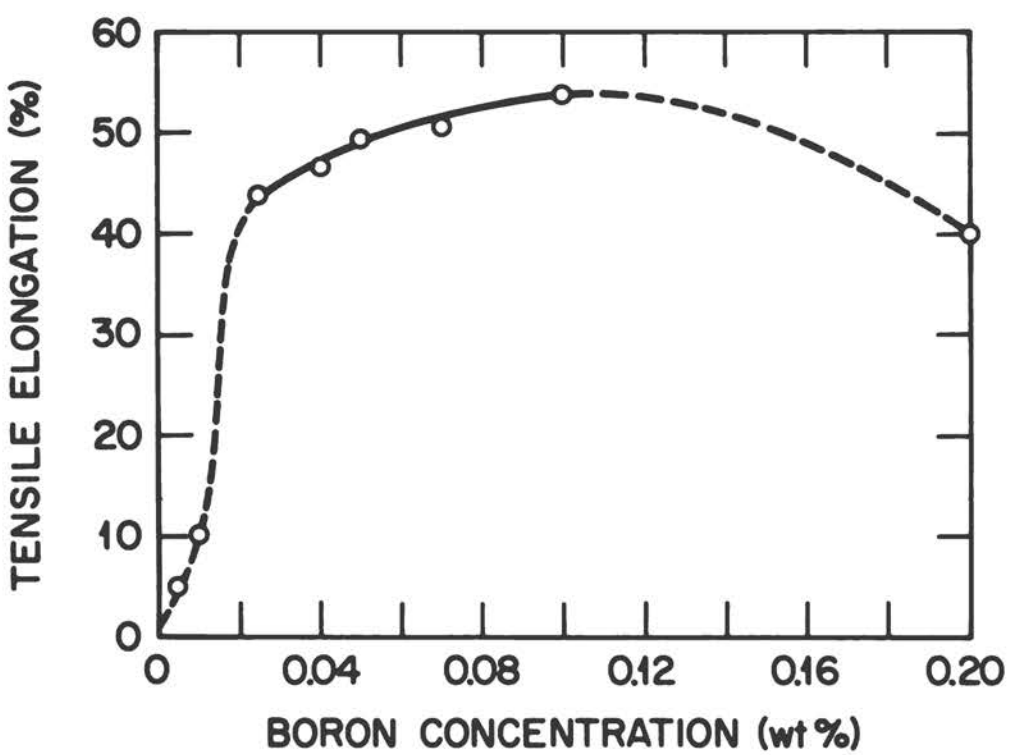
NICKEL ALUMINIDES BASED ON Ni_3Al CAN BE MADE DUCTILE BY MICROALLOYING



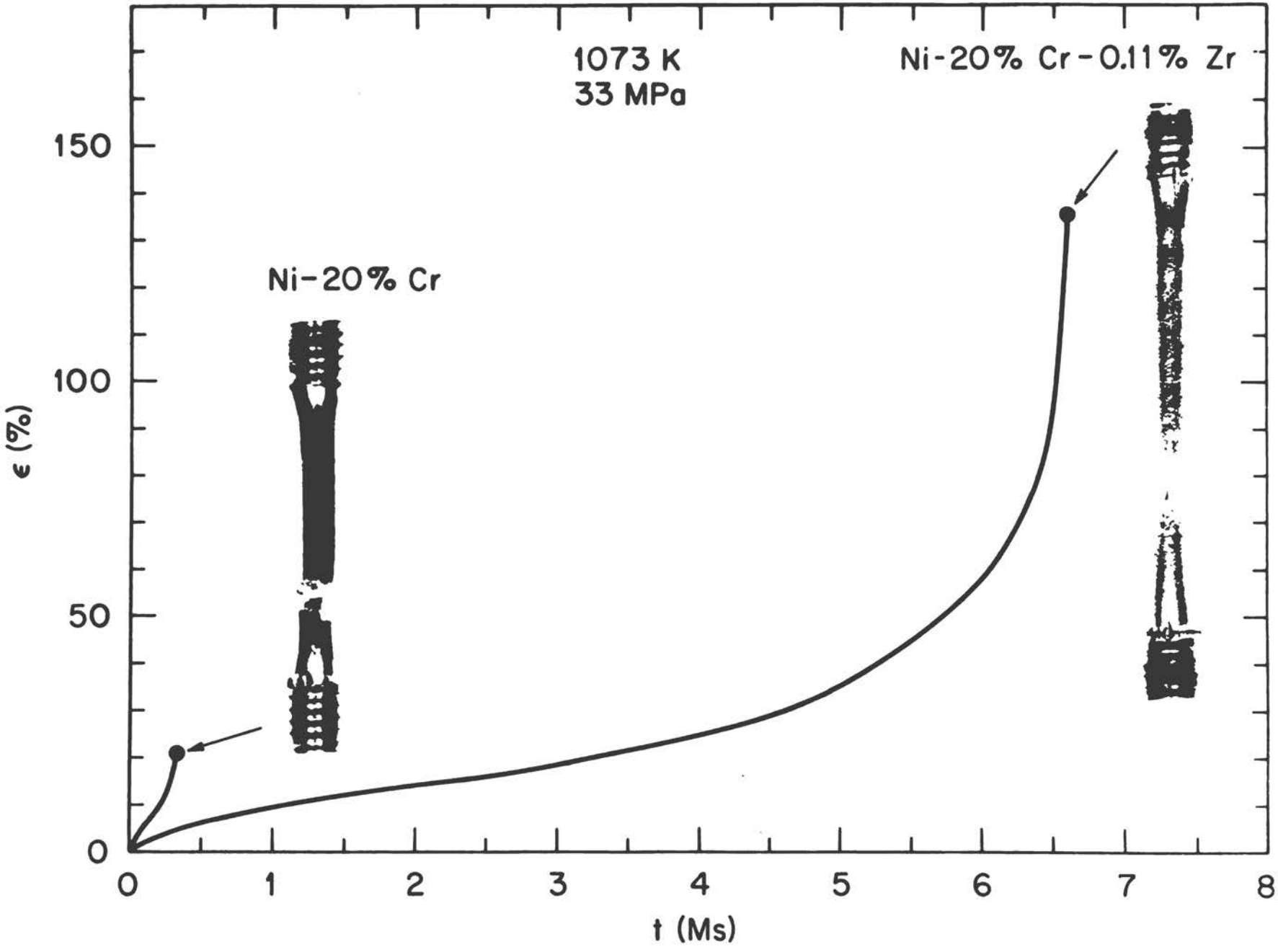
UNMODIFIED
Ni_3Al

Ni_3Al DOPED
WITH B AND Mn

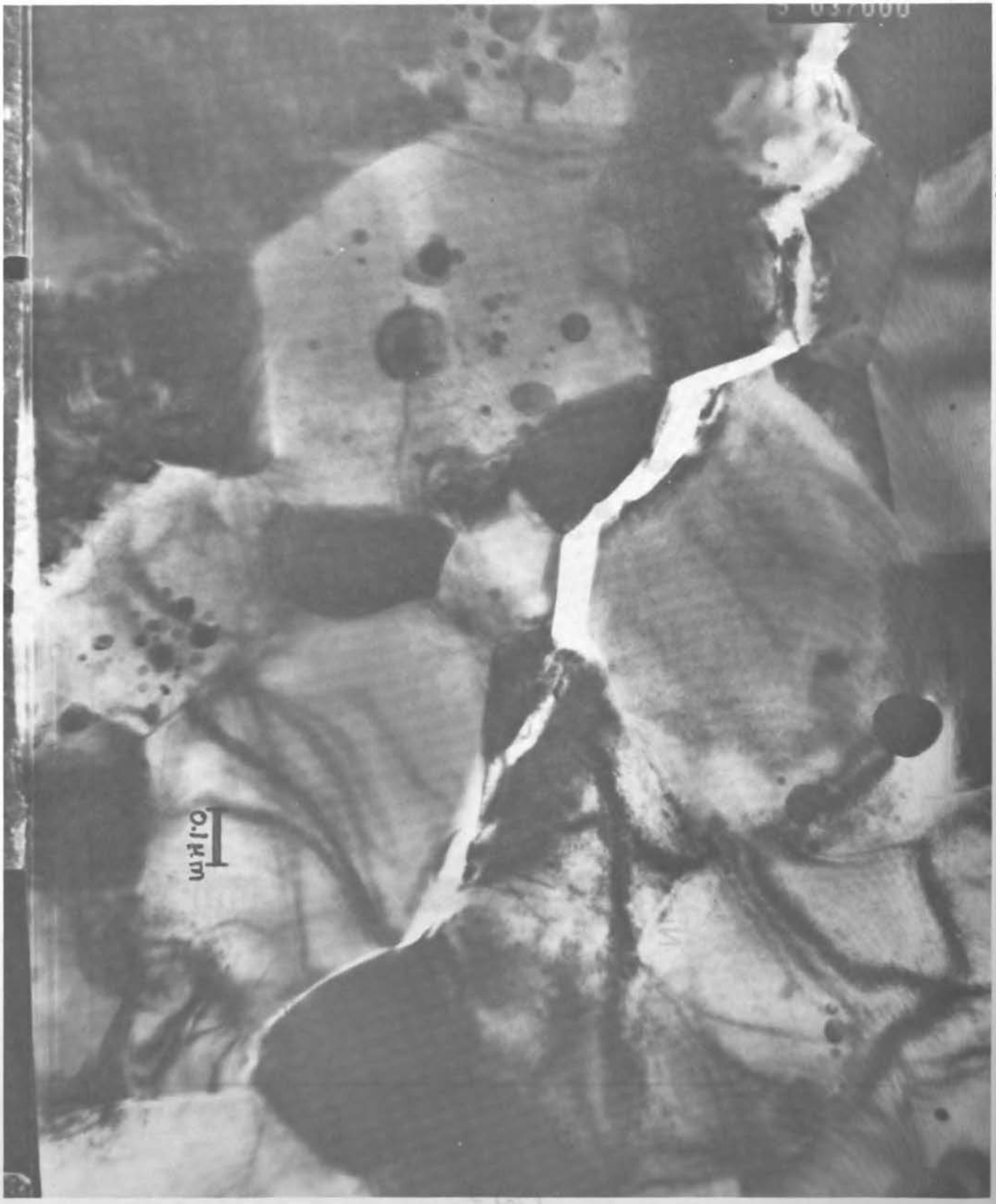
- THE ALUMINIDES ARE MUCH STRONGER THAN STAINLESS STEELS AND SUPERALLOYS AT ELEVATED TEMPERATURES



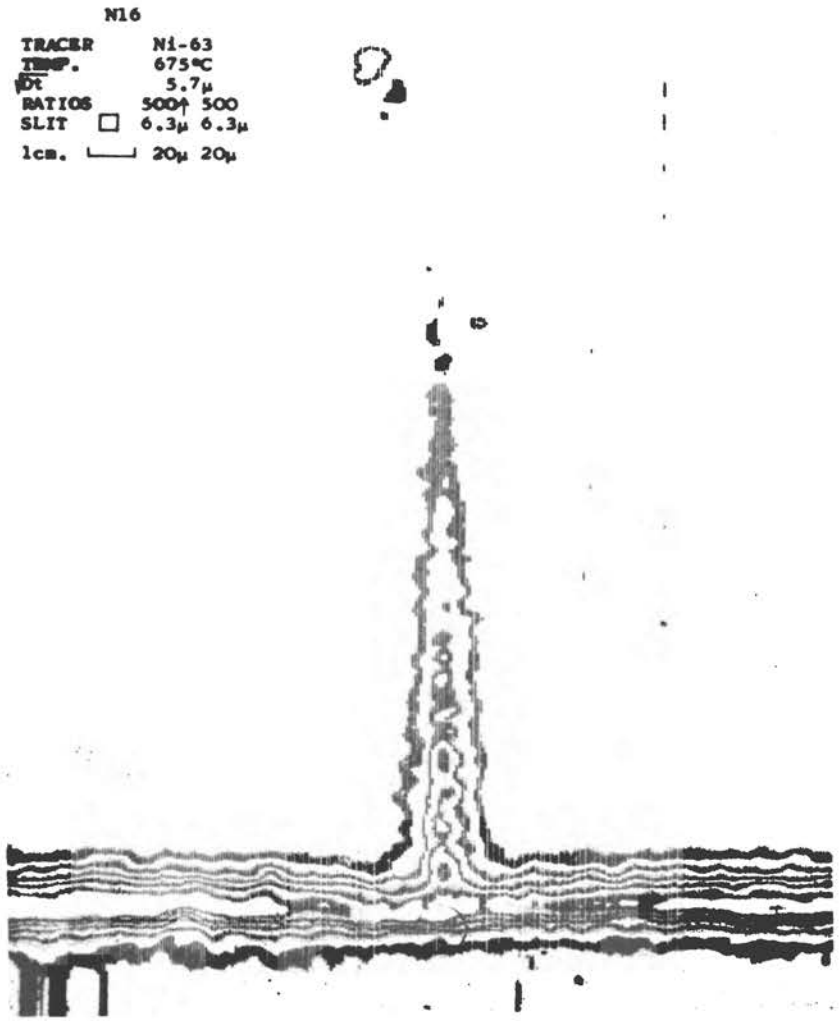

100 µm
200X


1073 K
33 MPa
Ni-20% Cr-0.11% Zr
Ni-20% Cr
150
100
50
0
ε (%)
0
1
2
3
4
5
6
7
8
t (Ms)

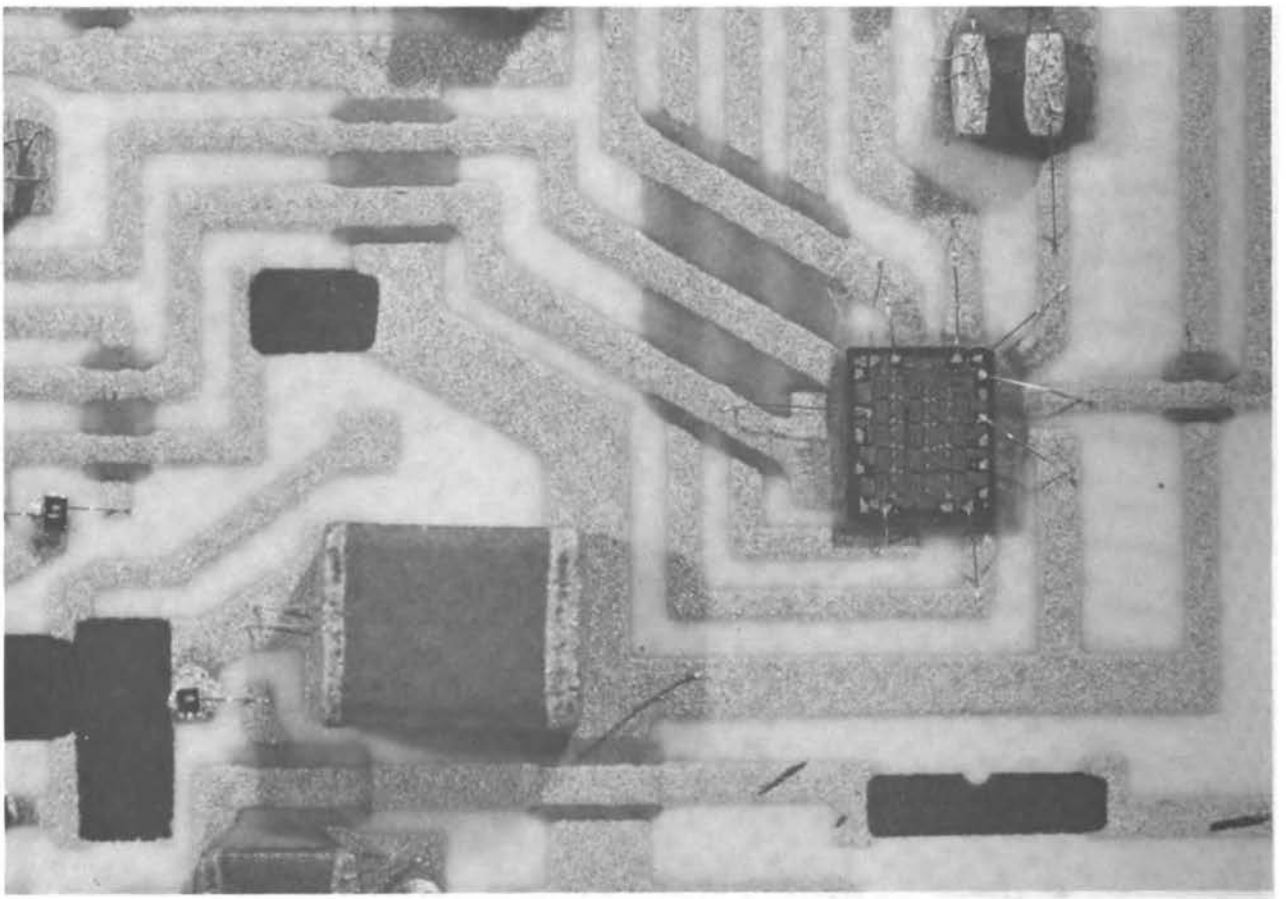
Mag = (2.5×37,000)

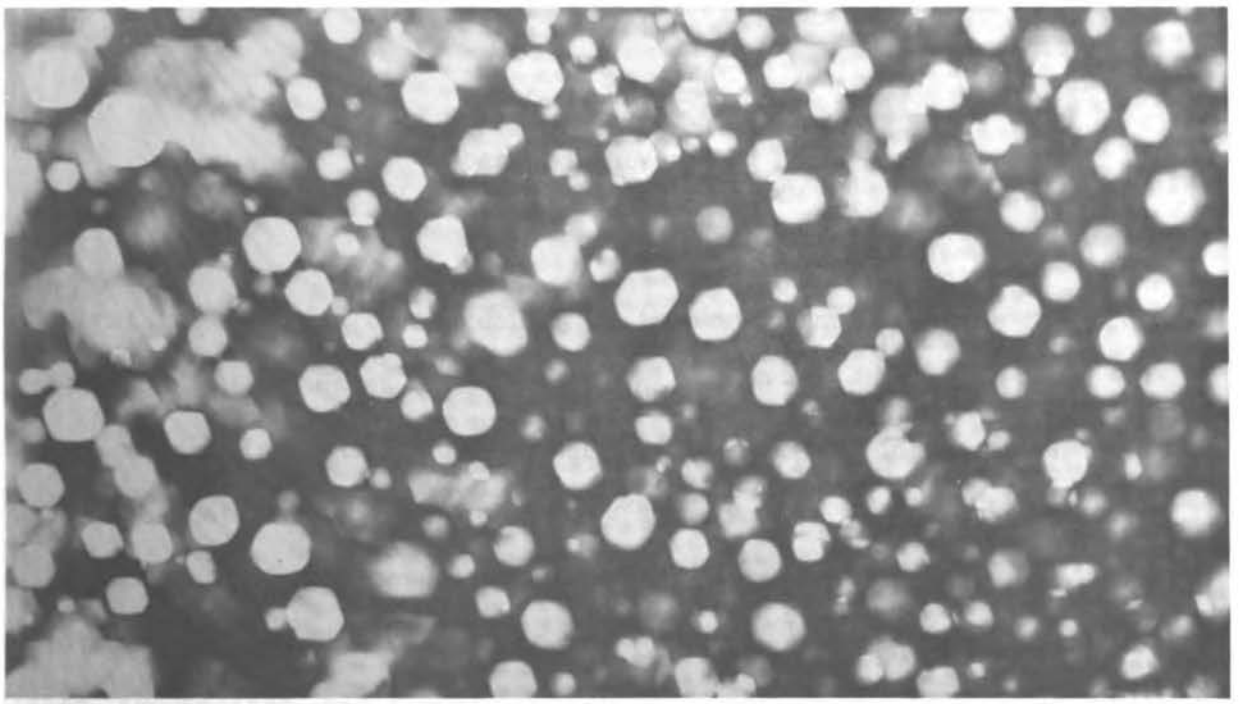


@ 139K7

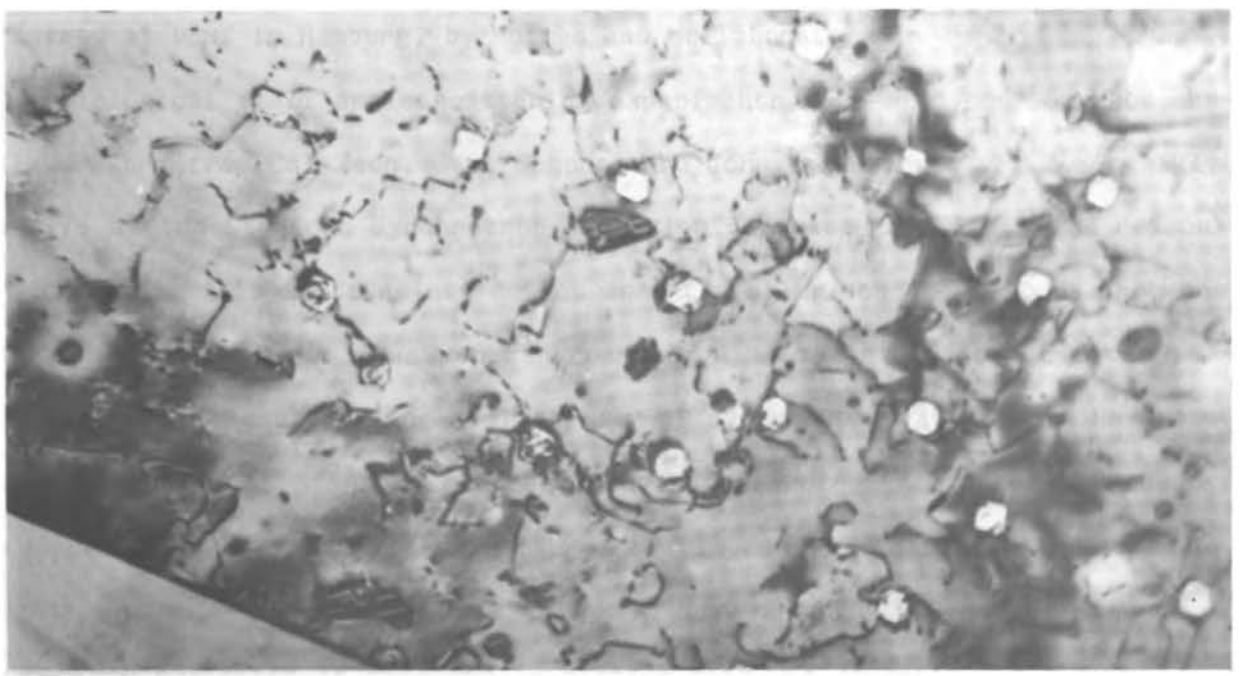

N16
TRACER Ni-63
TEMP. 675°C
Δt 5.7μ
RATIOS 500↑ 500
SLIT □ 6.3μ 6.3μ
1cm. 20μ 20μ

(*a*)





a.



b.

SYNCHROTRON RADIATION RESEARCH IN BIOLOGY AND MEDICINE

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Stanford, California 94305

First let me begin by addressing my thanks to the Committee for giving me the opportunity to present some of my own thoughts, and those that I have derived from talking with my colleagues, about synchrotron radiation research on materials that are derived from living systems.

I thought it might be useful, just for historical perspective, to say a few things about the development of this field. The earliest experiments applying synchrotron radiation to biological systems were small angle diffraction studies of muscle contraction. Actually, these were not done using an electron-storage ring, but rather a synchrotron. The experiments were performed at DESY in Hamburg, by Holmes and collaborators in 1972 [1].

Biological small angle scattering experiments were also done by Webb and collaborators from Cal Tech, Stan Sampson and John Baldeschwieler, during 1974 and 1975 at the Stanford Synchrotron Radiation Laboratory (SSRL). The reason for mentioning this is to relate to you an interesting statement about what one San Francisco Chronicle news reporter perceived as the evolution to occur in this field as a result of the availability of synchrotron radiation. He wrote that the studies at Stanford had resulted in synchrotron radiation providing the means to take "x-ray motion pictures of tiny living things." And if that was not enough, for those of you that may have trouble understanding how synchrotron radiation is produced, a storage ring was described as a source of x-ray light coming from "electrons whizzing around inside of a large copper

doughnut."

Now, having reduced all of storage-ring technology and biology synchrotron experiments to those two simple things, I would like to consider structural information that can be obtained on biomolecules from studies of their interaction with electromagnetic radiation.

The basic paradigm that faces all chemists, physicists, and biologists interested in structure and function is the question of precisely how structure relates to function. In other words, if we can understand something about the structure of a biological material, we might have some hope of understanding how it functions.

Clearly, one can ask that the structure-function question on a very large scale (or anatomical level): How does your heart function? What impairs its function? You can ask the question on an intermediate-size scale: How are our cells organized? How are their organelles arranged? How do they function? We can progress down to the atomic scale and ask: How does an enzyme function? How do the atoms move that allow that enzyme to carry out a catalytic reaction?

I would like to outline the scale and the types of techniques that I would like to discuss to address structural questions on these different scales. I will not talk about all of these techniques in detail; rather, I will highlight four specific examples. An example on the gross anatomical level would be that of **digital radiographic imaging** (angiography is another word which is used for this technique). X-ray images of organs are recorded at a resolution of the order of a quarter to a half of a millimeter. One can learn things about the anatomy of the organs that may impair this function. You will hear later about the technique of digital subtracting angiography using synchrotron radiation [2].

You have already heard a fair amount about x-ray microscopy. In biology,

the interest is that one could study, at a resolution of a few hundred angstroms, organelles within cells. You heard about distribution of ions within various structures; hopefully one would be able to learn something about these questions at the level of cellular organization. I will not have anything more to say about microscopy, because that has been covered by others.

Small-angle x-ray scattering (SAXS) is an area which gives us an intermediate level of atomic-structure resolution. SAXS will tell us about the shape of a molecule and provide information about how that shape changes in solution as a function of a biological stimulus or biological reaction, not at a one angstrom resolution level but at a 10 to 20-angstrom level [3]. If we have a protein, SAXS studies can tell us whether it perhaps is a sphere or whether it is a cigar-shaped object, and how that shape may change when it interacts with other proteins or when it interacts with other effector-type molecules.

Protein crystallography is a technique which, at least in concept, is familiar to a large number of people. It is the technique which has provided virtually all the information that we have about the detailed atomic arrangement of atoms in crystals of macromolecules at resolutions of the order to 2 to 6 angstroms. There are a few cases where protein crystallographic resolution is better than 2 angstroms, but they are quite rare. Resolution is primarily limited by the ability of protein crystals to diffract, which is related to their internal order or to the size of specimens available to obtain high angle enough diffraction data. Synchrotron radiation is extending the range of problems that can be studied using this technique.

I will also discuss **extended x-ray absorption fine structure (EXAFS) spectroscopy.** EXAFS provides the ability to look at a specific metal site in a complex molecule and give very accurate information about the local geometrical

arrangement at that site [4]. Here, the resolution is better than 1 angstrom. In fact, in favorable though not all cases, one can get distances to an accuracy on the order of plus or minus .01, but commonly more like .02, of an angstrom.

Synchrotron radiation has played, or will play, an important role in each of these preceding structural methodologies. What I really think the future new generation of storage rings, and the brilliance which they will provide, offers is possibility for the evolution of what are primarily now static techniques into dynamic ones. In particular, time-resolved x-ray experiments in the crystallography regime have been proposed and a few have been attempted. I would not at this time say that they have yielded any really qualitatively new information, and I will come back and comment a bit about those later.

However, we are beginning to see x-ray techniques in the small-angle scattering regime begin to yield important and new information about mechanisms in biological reactions or processes in the millisecond to sub-millisecond time range.

Time-resolved EXAFS, that is, taking the EXAFS spectroscopy and using it in a time-resolved fashion, also offers hope for obtaining millisecond to sub-millisecond information. These are indicative that even faster studies are possible. We can now envision the dynamic study of biologically relevant processes involving metal ions.

Finally, there are also experiments using the pulsed time structure of the synchrotron source. These are fluorescence measurements which can be made on materials in the microsecond to nanosecond -- and even, in some of the newer proposed sources, sub-nanosecond to picosecond time regime. However, this is not a field with which I am involved and I would not do it justice to attempt to cover it.

Let me first turn to the topic of protein crystallography. Information about the detailed structural arrangement of atoms in macromolecules is now available for more than 100 protein structures. The information has come from x-ray diffraction studies of single crystals of these materials which have been purified from the organism and crystallized.

Let us consider the role of synchrotron radiation in protein x-ray crystallography. First, let me emphasize that, as a technique using conventional sources, crystallography has indeed provided virtually all the information that we have on the atomic level about the structure of proteins and nucleic acids. These structures included metalloenzymes, standard enzymes, and a variety of nucleic acid containing materials. These structures were solved using conventional x-ray sources, no synchrotrons were involved whatsoever.

You may ask, then, the question: Why synchrotron radiation? In particular, there are several things that can be said. One is that the classical phase problem, that is, determining the phase of the scattered x-ray beam, is one which is solved in the laboratory by a technique called multiple isomorphous replacement. There are now clear indications (though I would say not really yet well demonstrated), that one can solve this problem by recording the diffraction data at multiple wavelengths [5].

There are now several laboratories working actively on multiple wavelength phasing. I do not want to discuss this technique further now, because I do not think that it is an area which is going to benefit in a dramatic way, at least at the moment, from a new generation of brighter sources. It is an area in its infancy, one in which we have sufficient flux right now to deal with the problems. It is, however, an important area of

application of protein crystallography using synchrotron radiation.

What is also interesting is that the high intensity of synchrotron radiation provides the ability to collect data much more rapidly on protein crystals. For reasons that relate to the rate of biological damage per unit time of irradiation, it turns out that one can frequently get, as has been well demonstrated, more data per crystal than one can with a conventional source [6]. In part, this is because one can achieve a very high flux with a much more monochromatic beam. The damage processes have a time-dependence which, to some degree, often appears independent of dose. It has been clearly shown by many examples that there is an advantage to collecting data faster with a more intense source.

Figure 1 is a diffraction photograph which was provided by Dr. Jack Johnson of Purdue which illustrates in a quite beautiful sense the kind of diffraction photograph one obtains from a protein crystal. This diffraction pattern is actually from a virus crystal. There are some 20,000 individual Bragg reflections in this this pattern. It required the order of three hours to record using synchrotron radiation. A similar picture, to much lower resolution, required something like 60 hours to obtain using a standard rotating anode x-ray tube. Thus, one sees that the increase in flux from the synchrotron gives rise to the ability to record data much more rapidly and to higher resolution than was possible using even the best available rotating-anode sources.

This is not necessarily true for all crystals, but it is particularly true for crystals with large unit cells and crystals which have been seen to be susceptible to radiation damage effects.

Obtaining diffraction data to higher resolution provides another distinct advantage. Dr. Max Perutz of MRC Cambridge put it quite well. He said that he

spent (off and on) something like 15 years of his life, or thereabouts, trying to collect high-resolution data on crystals of deoxyhemoglobin. He went to the synchrotron facility at LURE and in one day collected a much higher resolution data set on deoxyhemoglobin than he had ever been able to obtain before. The refinement from this data set provided detailed structural information on a molecular level that was very important in further defining the role of the geometry at the Fe site in cooperativity.

The protein crystallographers are now saturating three beam lines on European and facilities will probably soon do the same in the U.S. Now the question is: What does it buy you and what is the future capacity? It is clearly an important question in the U.S. We have a large body of crystallographers who are beginning to use this source; indeed, some have been traveling to Europe for some time to use sources there.

Higher brilliance should allow one to do diffraction experiments on much smaller crystals. Not many experiments have been done in this regard with proteins, but calculations based on extrapolations of known cases suggest that this will be the case.

What does "much smaller" mean? Calculations by Helliwell [7] suggest that one might be able to go down into the 20- to 50-micron size range for diffraction studies of protein crystals. Now, one typically requires crystals on the order of 300 to 700 microns on a side. There are still, however, technical problems to be solved in handling such small crystals and reducing the background scatter from the surrounding support. High intensity synchrotron radiation is a particular advantage if one is dealing with samples which cannot be grown into large crystals. This is quite a common problem for many proteins, especially those that are membrane bound.

Let us next consider **small-angle x-ray scattering.** SAXS is a method

which yields lower resolution information, such as overall shapes of molecules. One is usually dealing (in most experiments to date) with isolated materials that have been purified.

The important point to be made is that with intense synchrotron sources, and in particular the next generation of synchrotron sources, SAXS becomes well suited to following changes in structure as a function of time. For example, if one wants to look at a biological assembly process such as how some larger supermolecular structure assembles from subunits, then dynamic SAXS offers a way of doing this. Another example would be to study how a biological structure, such as a muscle, changes in structure as a it contracts.

There are several examples of dynamic SAXS studies but I will not cover all of them. There is a lot of work done on dynamic studies of muscle contraction, where the time resolution is of the order of 10 milliseconds. There is more recent work on tubulin assembly done by a group of workers in Europe. I will not consider these examples.

I would like to discuss a more recent example, which is that of the study of how chromatin is organized and reorganizes upon binding small metal ions. This is work (currently in press) by Bordas and collaborators [8], and I think it illustrates the type of study that one can do using dynamic small-angle x-ray scattering.

The study involves the condensation of a material called chromatin. Chromatin is basically a packaged form of DNA involving proteins called histones. The interesting question is how this forms a structure which can relax and unrelax, in which the relaxation is mediated by cations.

Bordas and collaborators have used stop-flow methods to initiate chromatin condensation by mixing together the components and following the process using SAXS as a function of time. Without describing the experimental

details, they have learned that the uncondensed form of chromatin looks sort of like a helical rope in a superhelical state (the pitch is 320 angstroms). When they induce condensation by cations, this results in a helical rotation followed by a change in pitch. You could describe it sort of like the helical equivalent of an accordion motion. This motion is quite clearly reflected as changes as a function of time in the SAXS pattern. The experiment needs brilliance because of the small sample size. One is initiating the event by mixing in a mixing chamber. The time domain limitation is on the order of 50-milliseconds because of the mixing times at the volumes currently required for the experiment. This is an experiment which would dramatically benefit from increased brightness in both the time domain you can study and in the sort of physical constraints of mixing volumes. This is a biologically important example in which one has addressed the way in which DNA becomes accessible in this condensation reaction.

I will just mention briefly one other SAXS application. A similar type of application would be to gap junctions. These are pores which connect cells. Gap junctions have channels which open and close and allow communication to occur by passage of small molecules and ions between cells. It is thought that the opening and closing of channels occurs by a tilt of helical rods. This is an ideal problem that could be studied by dynamic SAXS.

You have heard about the reflection diffraction experiments. This is an area which has a lot of promise for studies of biological systems. It is an area which is in its infancy, and one which will again benefit because of the small scattering cross-sections from greatly enhanced brilliance in new generation synchrotron sources. I would just like to mention work of one particular group, this is H. McConnell at Stanford, together with M. Seul, in a collaboration with Peter Eisenberger. They have actually looked in the

reflection-diffraction geometry, at scattering from phospholipid arrays [9]. They are interested in understanding the nature of the phase transitions and the presence of various intermediate phases in order-disorder transitions in these phospholipids. The work that they have done is on monolayers in which they have functionalized a silicon substrate and bound to a monolayer of lipid. They observe diffraction peak counts using the 8-pole wiggler at SSRL on the order of 1000 counts per second for the best samples. More typically, they see 10 to 20 counts per second. These are experiments that would dramatically benefit from the enhanced brightness of an x-ray undulator. McConnell and collaborators have actually observed changes in the diffraction peaks as a function of passing through a phase transition of the lipid bilayer. The idea is to understand the physics of melting of the phospholipid bilayers by diffraction experiments.

Looking to the future, the idea that one would like to follow is to try to apply this technique not just to phospholipids, but to study materials which have been bound to these ordered arrays of phospholipids. One such example is shown in Figure 2 which is from an electron micrograph taken by J. Reidler, working in R. Kornberg's lab. One sees a very nice ordered patch of immunoglobulin molecules (IgG's), which have been put down onto an ordered understructure of derivatized molecules which bind to those immunoglobulins. This is a small patch, a few microns square. These ordered domains have actually now been obtained in somewhat larger patches, and there is hope that one could get them up to perhaps a 20 to 30 micron size. If one could do surface diffraction from these domains, one would have some hope of being able to understand the structure of the macromolecules forming the arrays.

I would like to discuss two more applications of synchrotron radiation. One of those is **x-ray absorption spectroscopy (XAS)**. This is a method which

has been revolutionized by the availability of synchrotron radiation.

Prior to synchrotron radiation sources, almost anything that was studied using x-ray absorption spectroscopy required high concentrations. One simply could not look at dilute samples. With the advent of synchrotron radiation, XAS has become used in many fields to provide local electronic and geometrical structural information about a selected absorbing atom.

XAS is a technique which does not require crystalline samples, although one can apply it to single crystals. Studies have now been done on quite a number of dilute biological systems and they benefit, in particular, from both flux and brilliance. Brilliance is important because the volumes with which one has to deal are quite small (because the samples are often hard to obtain) and, in many cases, the concentrations very low. Higher numbers of photons are needed to achieve sufficient statistics on dilute samples. Thus, the combination means that one needs both brilliance and flux.

What will happen, I believe, is again an evolution toward dynamic studies. However, let me discuss an example of the kind of information one can get from these studies using an application which actually is particularly close to my own research. These are EXAFS spectra taken of biological materials which have the ability to fix dinitrogen. The protein nitrogenase carries out this enzymetic function and has two components. The larger component contains molybdenum and iron metals. The x-ray absorption spectrum at the molybdenum K edge has provided significant information about the Mo site in nitrogenase. Analysis of EXAFS data allowed us to propose two alternate models for the molybdenum environment of this enzyme [10], which were completely unknown at that time, shown in Figure 3. It can be seen that one is a cube-like structure, while the other is an extended flat structure. What has evolved since these studies has been intensive chemical studies in many labs to

synthesize model complexes. In parallel, there have been many studies of the protein in various of its physiologically active states. Recently, Steve Cramer at Exxon has taken the EXAFS work one step farther. He has studied single crystals of nitrogenase. The detailed structure is not yet known (that is, the orientation of the atoms is not known). He has recorded the EXAFS spectra of the crystals as a function of orientation. The synchrotron radiation is plane-polarized, and then the polarization dependence of the molybdenum-iron-sulfur complex in this structure, as you change angle with the polarization vector and look at the absorption, would be very different for the two types of proposed structures. These results, without going into detail, indicate that the extended type of structure is not present in the nitrogenase enzyme; it must be something of the more spherical cube type.

Thus, using polarized XAS spectra from single crystals has allowed one to obtain additional information about geometric structure. Again, brilliance is important in the single crystal application because the single crystals are hard to grown large and the data rates are very low. Higher brilliance for use with small crystals is very important.

Finally, in terms of the EXAFS, let me just mention that there is some hope of doing time-resolved studies. For example, molecules such as myoglobin have been studied already, where the dynamic change in the EXAFS spectrum as a function of photodissociation of CO from CO-myoglobin has been followed. These studies are beginning to look promising but need to further evolve before fundamental new information is obtained. The feasibility of time resolved XAS studies has been demonstrated. Again, with increased brilliance, one would be able to carry out these experiments on more dilute biological systems in faster time domains.

In summary, for x-ray absorption spectroscopy experiments, brilliance,

flux, and total capacity are all important. Let me note, just in passing, that approximately 25 percent of the proposals at SSRL relate to biological studies and this has remained constant with time. SSRL, for example, is still a factor of approximately two overscribed for beam time.

The last area of synchrotron radiation research that I would like to describe is one medical application. There are potentially other medical applications, but given that I am not an expert in the field I will not speculate. I am also not an expert in noninvasive angiography, so I would attribute all of the information I will present to Ed Rubenstein, Barry Hughes, and Bob Hofstetter of Stanford, who have been carrying out these experiments at SSRL.

On the anatomical level, synchrotron radiation again offers us something important in terms of a resource. The idea is to visualize blood vessels and heart chambers by x-ray absorption imaging, particularly blood vessels in the arterial bed surrounding the heart. In the conventional angiography procedure, this is done by inserting a catheter into the arm or leg, advancing it to a location near the heart. The procedure is costly (requiring hospitalization) and carries very high risk. Using synchrotron radiation, one can record the absorption spectrum above and below the K absorption edge of an injected x-ray opaque material, (typically one containing iodine which has an absorption edge at about 33 Kev).

A couple of statistics are interesting: about 1/2 million of the conventional angiographic procedures, using standard x-ray sources, are performed in the U.S. at the cost of $1.5 to $2 billion a year. The synchrotron method involves using lower levels of an iodinated contrast agent, but greatly enhancing the sensitivity by doing the above-and-below edge difference method. The increased sensitivity allows intraveneous injection

rather than the high risk catheratization procedure.

In the actual experiment, the synchrotron beam is monochromatized by a fast-switching channel-cut monochromator (one in which the wavelengths can change above and below the iodine edge quite rapidly). The image is recorded by a one-dimensional position sensitive detector. In the current geometry, the object is moved up or down to create the full image.

Figure 4 shows one of the earlier images that had been obtained. This is from the heart of a dog, in which the arterial beds had been visualized by an iodine injection into a central vein. In this case one can clearly see the aorta around the ventricle of the heart.

It is the hope that one would be able to use this non-invasive procedure for patients in probable need of surgery, who would otherwise have to be subjected to the conventional high-risk diagnostic procedure. One can, in principle, use this procedure to follow postoperative progress without further risk of injury to the patient. Also, one could use it to screen people who were normally thought to be healthy to look for signs of coronary-artery disease. The last point I might make is that this is a method which, I do not believe, will not benefit from brilliance, but one which benefits from flux. But there is potentially a large demand and capacity, certainly, in the medical research applications area.

With that fairly rapid overview, I hope I have provided some perception of the nature of the fields in biological-related sciences that can benefit and do benefit from synchrotron radiation research.

References

1. Holmes, K. C., R. T. Tregear, and F. Barrington Leigh. 1980. Interpretation of the small angle x-ray diffraction from insect flight muscle in rigor. Proc. R. Soc. London Ser B. 207:1.

2. Hughes, E. B., H. D. Zeman, L. E. Campbell, R. Hofstadter, J. Meyer-Berlchoot, J. N. Otis, J. Rolfe, J. P. Stone, S. Wilson, E. Rubenstein, D. C. Harrison, R. S. Kernoff, A. C. Thompson and G. S. Brown. 1983. The application of synchrotron radiation to non-invasive angiography. Nucl. Instr. and Meth. in Phys. Res., 208:665.

3. Stuhrmann, H. B. 1981. Anomalous Small Angle Scattering. Quart. Rev. of Biophys. 14:433.

4. Cramer, S. P. and K. O. Hodgson. 1979. X-ray absorption spectroscopy: a new structural method and its applications to bioinorganic chemistry. In Progress in Inorg. Chem., S. F. Lippard, ed. New York: John Wiley and Sons.

5. Phillips, J. C. and K. O. Hodgson. 1980. The use of anomalous scattering effects to phase diffraction patterns from macromolecules. Acta cryst. A36:856.

6. Greenhough, T. J. and J. R. Helliwell. 1983. Prog. Biophys. and Mol. Biol. 41:67.

7. Helliwell, J. R. and R. Fourme. 1983. The ESRP as a facility for protein crystallography in Proceedings of the SSRL New Rings Workshop. SSRL report 83/02.

8. Perez, Grau L., J. Bordas and M.H.J. Koch. 1984. Chromatin superstructure: Synchrotron radiation x-ray scattering on solutions and gels. Nucleic Acid Research. 12:2987.

9. Seul, M., P. Eisenberger and H. M. McConnel. 1983. X-ray Diffraction by Phospholipid Monolayers on Single Crystal Silicon Substrates. Proc. Natl. Acad. Sci. USA. 80:5795.

10. Cramer, S. P., K. O. Hodgson, W. O. Gillum, and L. E. Mortenson. 1978. The molybdenum site of nitrogenase-preliminary structural evidence from x-ray absorption spectroscopy. J. Amer. Chem. Soc. 100:3398.

Figure Captions

Figure 1. X-ray diffraction photograph of cowpea mosaic virus recorded using synchrotron radiation at LURE in Orsay, France. The photograph, containing about 29,000 reflections, was recorded in only 3 hours and 20 minutes and extends to 4.3 A resolution. A poorer photograph, extending only to 7A resolution required 60 hours to record on a 6 x 20 rotating anode x-ray tube. The high intrinsic collimation of the synchrotron radiation gives rise to resolution of the peaks arising from diffraction of the crystal with the largest unit cell dimension of 1041A. This photograph was provided by Dr. Jack Tshasai of Purdue University.

Figure 2. Electron micrograph of an ordered array of IgG immunoglobulin molecules attached to a hapten functionalized substrate. The hexagonal order is evident in the domains of a few microns square in size. Surface reflection-diffraction experiments from similar (but larger) domains should provide detailed structural information on the antibody molecules and how they interact. This photograph was provided by Dr. J. Reidler and R. Kornberg at Stanford.

Figure 3. Two models proposed for the molybdenum site of the nitrogenase enzyme system. The models were derived from EXAFS studies and represent the first details known about the structure of the site. Work is in progress (see text) to further define the exact nature of Mo-Fe-S site and understand its role in the catalytic conversion of

dinitrogen to ammonia.

Figure 4. Images of the central arterial circulation of an anesthetized dog recorded with synchrotron radiation. A small bolus of iodine-containing contrast agent was injected into a central vein and the top image recorded 8 seconds later, the middle-image 10 seconds later and the lower image 12 seconds later. The globular object in the upper left is the left ventricle, the toroidal object sweeping to the right and then downward to the left is the arch of the aorta, from which arise the large central arteries that supply the upper extremities and the head. Spatial resolution was 0.5 mm.

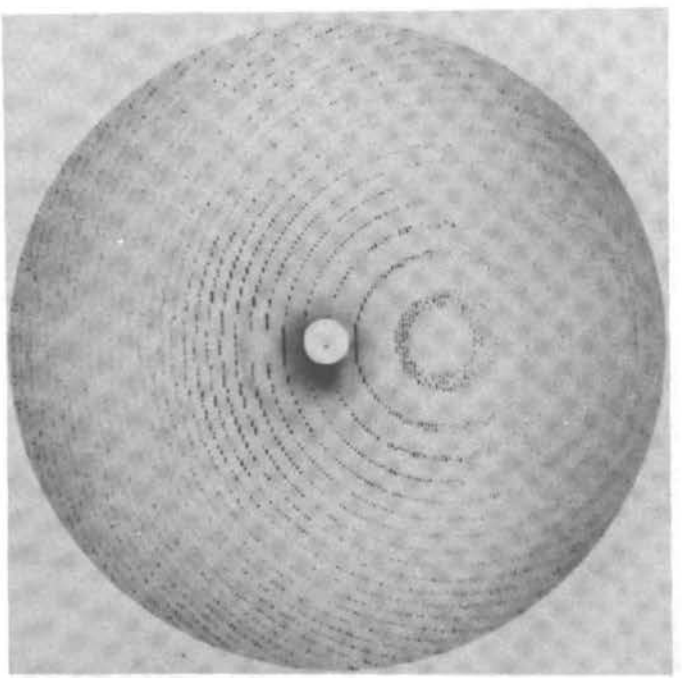


Figure 1

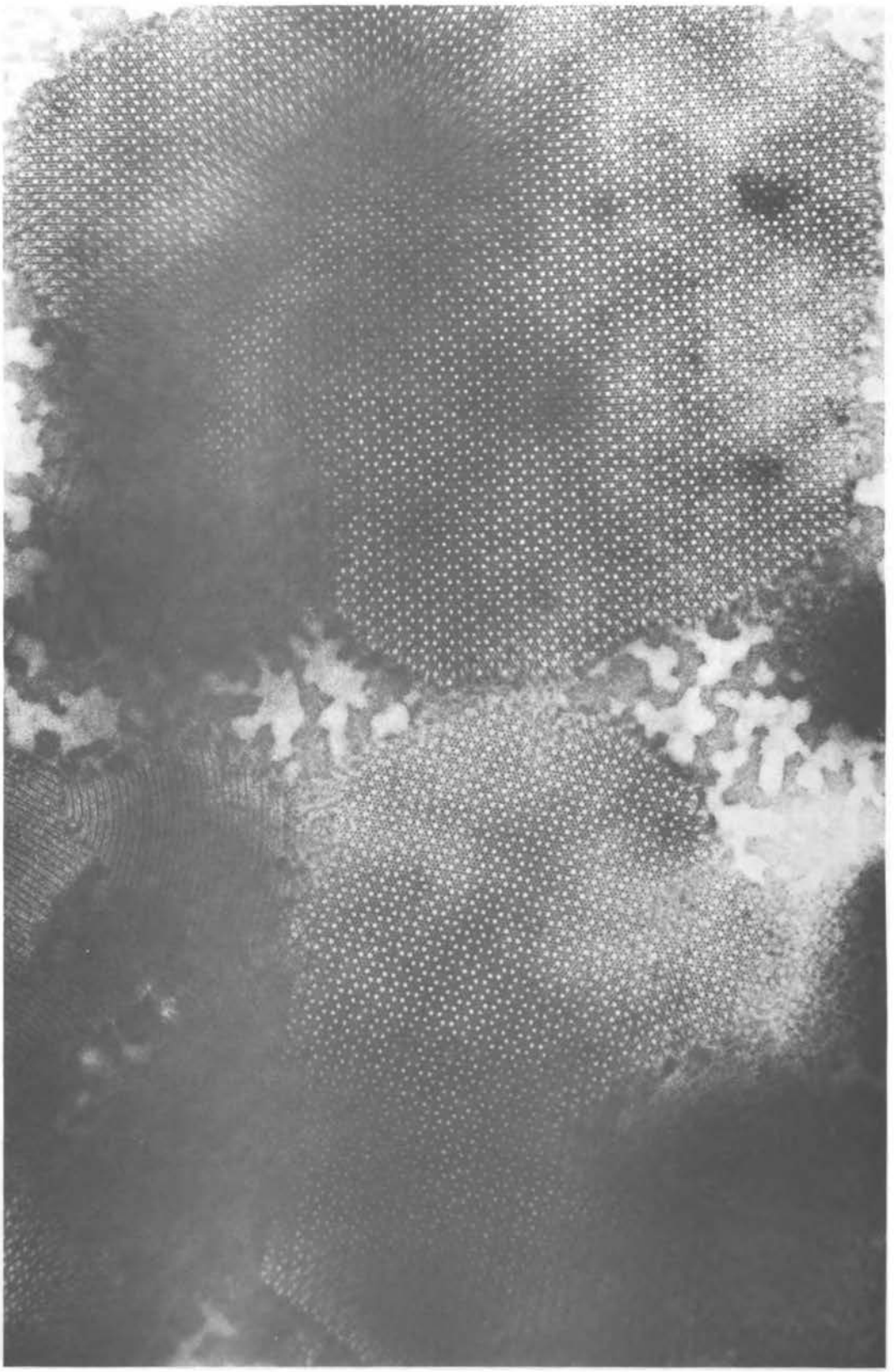
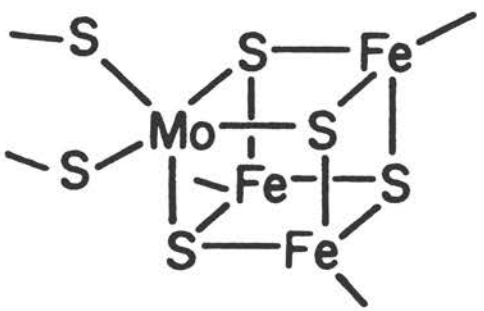


Figure 2



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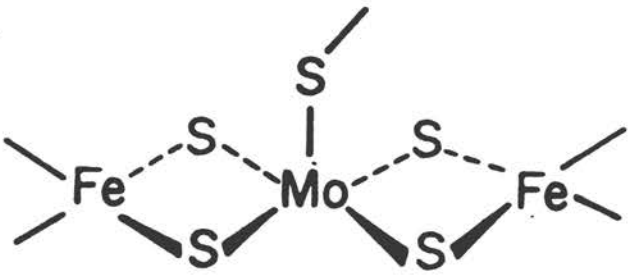

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Figure 3

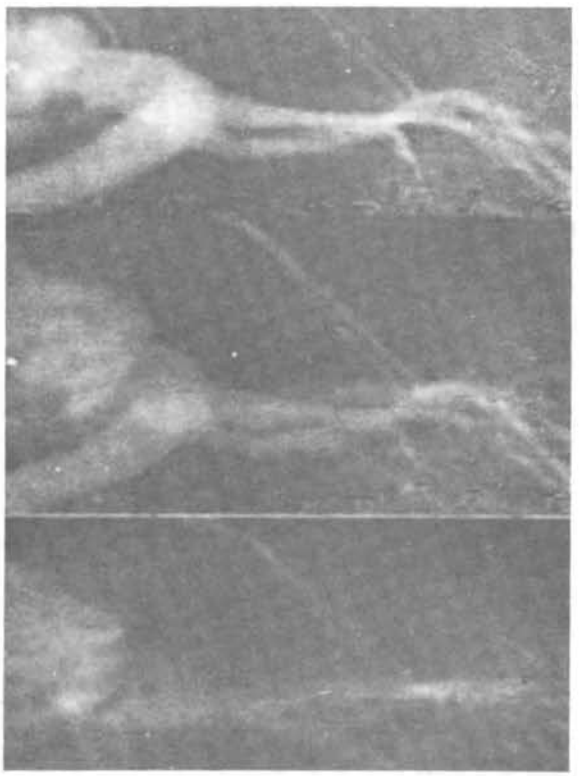


Figure 4

PHYSICS

PRESENTATION OF J. AXE

DR. AXE: Neutron scatterers spend a lot of time in energy-momentum space (some people would say too long) so I want to begin by showing you how energy-momentum space looks to a neutron scatter. (See Fig. 1) The neutrons probe different regions of this space, depending upon their energy. Low energy neutrons probe a small region with relatively high resolution; higher energy thermal neutrons can probe a correspondingly larger region and, finally, epithermal neutrons can cover a much larger region, but with correspondingly less resolution. There are two principal ways that neutrons interact with matter. The first is through nuclear interaction, by which we can determine the motion of atoms. This motion can range all the way from very slow diffusion of, say, micromolecules up to a very energetic recoil of atoms produced by epithermal neutrons. In-between there are various kinds of vibrations, all of which are of interest. The neutron also has a magnetic moment and that gives us information about magnetic fluctuations and their energy scale also varies from very slow critical scattering all the way up to very energetic itinerant spin waves or atomic multiplet splittings and this brings us to the following conclusion:

> The range of interactions that are of interest in condensed-matter physics varies over some eight orders of magnitude in energy and it is clear that we need epithermal, thermal and cold neutrons in order to adequately probe them.

I. RECENT ACCOMPLISHMENTS:

In Table I, I have listed some major technical and scientific accomplishments of neutron scattering in condensed matter physics in the last decade. I will have more to say about many of these topics later but I want to concentrate here on two of the technical advances. The first is the use of cold sources and neutron guides; cold sources to increase the flux of low-energy neutrons, the neutron guides to increase the number of instruments in order to better utilize them. This is a technique that is used to maximum advantage in reactors only in the 1970s, whereas the high-flux reactors in the United States were built in the sixties. So we have not yet taken advantage of the economies that this offers. The second thing that I want to call your attention to is that the development of high-energy resolution spectrometers took place entirely in Western Europe and, as yet, they have not made their way into the United States. These are the two principal technical areas that the proposals for reactor upgrades would hope to rectify.

A. Critical Phenomena

Now let's talk about some specific experiments. I think it could be argued that the major conceptual accomplishment of the last decade in physics was the widespread use of scaling arguments to solve intractable problems. In condensed-matter physics, the central problem in this area has always been how to understand phase transformations. For many years, the theoretical testing grounds for studying phase transformations have been magnets. This goes back at least to Onsager's famous solution to the Ising model. What I have shown in Fig. 2 is a bit of what is now ancient history in the critical phenomena game. It shows how well the sub-lattice magnetization of a real quasi-two-dimensional magnetic system obeys the solution of Onsager's abstract model for magnetic phenomena.[1] This is an early example that set the stage for many other beautiful neutron-scattering studies that continue even to this day to test and sometimes to guide the theories of critical phenomena. Note also that sublattice magnetization is something that really only could be measured with neutrons.

B. Low-Dimensional Magnetism

It is not only critical phenomena in which low-dimensional systems are sometimes of special interest, and that is because it is often possible to solve complicated many-body problems in one dimension that are simply intractable in three dimensions. For example, unlike a ferromagnet, an anti-ferromagnet has a complicated ground state because of quantum mechanical effects, and the quantum mechanical effects become more important the smaller the angular momentum of the spin involved. Because spin waves represent fluctuations about that ground state, these quantum mechanical complications show up in the spin waves as well.

Shown in Fig. 3 are neutron-scattering results for two one-dimensional anti-ferromagnets. One of them, which contains manganese (S=5/2) which obeys essentially a classical description of the spin waves. The other, CPC, contains copper (S=1/2) in which this quantum effect is large. These measurements[2] showed, for the first time, that the prediction by Des Cloizeaux and Pearson[3] that the energy of a spin wave for quantum system was different from that of a classical system by the ratio of $\pi/2$ is rather exactly obeyed.

C. Charge Density Waves & Phonon Instabilities

Neutrons are good for studying spin fluctuations; everyone agrees about that. But since they are neutral, therefore, they are very poor for studying charge fluctuations. Right? Well, not necessarily. If the frequency of the charge fluctuation is lower than that of the phonon frequencies, then the charge fluctuation drives the nuclei which, after all, are charged, and you can see the original charge fluctuation through anomalies in the phonons.

There is a very nice example of this which occurs in quasi-one-dimensional metals. It had been predicted for many years that a uniform, one-dimensional electron gas should be unstable against the formation of a

charge density wave, the so-called Peierls' instability. This instability was first seen as a very spectacular frequency anomaly in the longitudinal acoustic phonons in this material, KCP.[4] (Fig. 4).

There are really two key ideas illustrated here. One is that structural phase transformations can result in instabilities in the phonons; that is, from phonons whose frequency goes to zero. The other idea is that the period of the charge-density wave, which is determined by the Fermi surface, is not necessarily related to the underlying periodicity of the lattice, and that gives rise to an incommensurate charge-density wave, which has various interesting and unusual properties. Both of these topics, soft phonons and incommensurate systems, are currently prominent in condensed-matter physics.

D. Hydrogen in Metals

Another important topic in recent years has been the study of hydrogen in metals. I want to give a single example. One of the big surprises of this field was that palladium became a superconductor when one added hydrogen. This implied a coupling of the superconducting electrons to very high-energy hydrogen vibrational modes. Equally puzzling was the inverse isotope effect; that is, Tc, rather than decreasing when the H was replaced by D, increased.

There are a variety of proposals to understand this collection of queer properties and one of them was that the hydrogen single-particle potential was different than that for deuterium. Fig. 5 shows some data taken with epithermal neutrons (at a reactor in this case, rather than a spallation source), in which both the fundamental hydrogen vibrational mode and the split overtone mode are clearly seen. Similar studies performed on the deuteride showed that their was very little difference between the H and D potentials, but that both were very anharmonic.[5] This suggests that a rival theory which stresses the role of anharmonicity is a more promising one by which to understand PdH_x.

E. Superconductivity and Magnetism

Another major achievement in superconductivity in the last few years has been the discovery of materials in which superconductivity and magnetism co-exist. This was once believed to be impossible. The fact that some kind of magnetic ordering is occurring in these new materials was strongly suspected from various macroscopic measurements, but the exact nature of this magnetic order (ferromagnetic, anti-ferromagnetic, or whatever) could only be determined by neutron-scattering studies. Fig. 6 shows some neutron powder-diffraction measurements on $TbMo_6S_8$ above and below the magnetic-transition temperature.[6] The prominent new peaks are the result of this new magnetic order that has occurred. By studying the positions and intensities of these peaks, one can determine exactly the magnetic structure, which in this case is antiferromagnetic. At low temperatures $TbMo_6S_8$ is simultaneously superconducting. (The situation for ferromagnets (e.g. $HoMo_6S_8$) is more complex. In this case the onset of

ferromagnetic order destroys superconductivity, but there is an intermediate phase in which superconductivity coexists with a qualitatively new form of modulated magnetic order, which has been discovered in small angle neutron scattering studies.)

Returning to Fig. 6 for a moment, notice that the nuclear and magnetic peaks are of about the same intensity. If one were to study this effect with x-rays, since the x-ray magnetic scattering cross-section is down by about a factor of 10^6 relative to charge scattering in principle, one would also see these magnetic peaks, but they would be down by a factor of 10^6 from the other peaks and hidden in background. What I think this means is that while it is clearly important to establish the x-ray magnetic scattering cross-section and probably in particular situations which Dr. Moncton has talked about earlier, it may be useful; but for routine scattering studies of magnetic phenomena, I think it is clear that neutrons are going to continue to be the probe of choice.

Notice also the temperatures in Fig. 6. These measurements involved the use of a He^3-He^4 dilution refrigerator, which brings up another strong point for neutrons: they are so weakly interacting with matter that they can easily penetrate into special sample environments (low temperatures, high pressures, and so on.)

F. Summary

I want to just quickly summarize some thoughts up to this point.

1. In many cases, the excitement that is involved centers around the material rather than the technique. I have chosen one- and two-dimensional magnets or metals or bizarre superconductors, and so on. Other people in the audience undoubtedly would have picked a different subset of materials, but I think the lesson is still there. Often the techniques are standard, the physics of the materials is new.

2. The moral, as far as I can see, is that as long as new materials are going to be synthesized, we have to have a strong conventional neutron-scattering program to characterize them. However, as we will hear in more detail later we are falling behind Western Europe in instrumenting even these conventional reactor sources.

II. NEW OPPORTUNITIES:

I want to spend the rest of the time looking at some examples of new opportunities that are afforded in three areas: spallation sources; existing reactor instrument upgrades; and, finally, higher intensity sources.

A. Spin-Echo Techniques

A key instrument which is responsible for the last two decades of

energy on scale in Fig. 1 has been the neutron spin-echo spectrometer. Since it works on an entirely different principle than a conventional spectrometer, I want to spend a few minutes explaining that to you. Referring to Fig. 7, imagine that one starts with a white beam of neutrons that is vertically polarized and then flips the polarization by $\pi/2$ so that it is now out of the plane of the figure; there are various devices that will do that. If you now apply a magnetic field vertically, then the moment will begin to precess around this field. But since each neutron has a different velocity, each will spend a different amount of time in the field, precess a different amount and, therefore, by the time this initially well polarized beam comes out of the magnet, it is going to be completely depolarized.

Imagine further, for simplicity, that the sample elastically scatters this beam, changing only its direction. Now after the scattering event apply exactly the same field, but in a reverse direction. (I depart briefly from the situation shown in Fig. 7, but be patient.) The neutrons, although they are initially unpolarized will have their histories reverse, so to speak, as they precess through the reversed fields. By the time they come out, they are going to be back in phase, with their polarizations all pointing out of the screen, and then the final $\pi/2$-flipper will flip them back up and one can measure this recovered polarization by a suitable detector. In fact, for technical reasons, it turns out to be easier, rather than to reverse the magnetic field at the back end, to reverse the spin of the neutrons, which explains the additional π-flipper behind the sample. But the result is just the same as I have just described.

For inelastic scattering, the details are a little bit harder to follow, but the essential idea is, once again, that you can use a polarized white beam and that beam polarization is again lost and recovered. That is the neutron spin-echo principle.[7] The net result is that while a conventional spectrometer requires incident energies that are comparable with the energy resolution that you wish to maintain in the scattering event, in the neutron spin-echo case that condition is relaxed (by sometimes as much as a factor of 10^5) with corresponding gains in the amount of intensity that you have under those conditions.

I am sure that the later speakers are going to have examples of neutron spin-echo results. I want to show you just one that is of interest in condensed-matter physics. This involves studying the critical dynamics of ferromagnetism in iron.[8] The open circles in Fig. 8a are the results of conventional neutron-scattering measurements of the width of the critical scattering in iron. The closed circles represent new data taken in the higher resolution regime open to neutron spin echo. What these data apparently show is the breakdown of dynamical scaling ($\Gamma_{q \propto} q^2$) in the hydrodynamic regime -- this is something that was not before suspected.

B. Other Uses of Polarized Neutrons

Constructing new instruments is one way to open up fresh opportunities, and a very important one. But there are also some areas where I believe that there can be important new advances using existing instruments through modest (say ~5x) increases in flux. The first

example is in the use of polarized neutrons. They are routine now in elastic diffraction experiments, but the use of polarized neutrons in inelastic studies has always been and continues to be very severely limited by intensity. Fig. 9 shows some indication of how useful polarized neutrons are in the study of magnetic excitations.[9] In iron, at low temperatures (in the ordered magnetic state), it is not difficult to find "windows" where one can cleanly separate the magnetic scattering, the magnon peaks, from the non-magnetic scattering, the longitudinal and the transverse phonons (Fig. 8a). However, above the transformation temperature, in the so-called "paramagnetic" regime, the magnetic scattering is more diffuse and in order to get reliable data, it is almost mandatory to use polarized neutrons. Fig. 8b shows how the use of polarized neutrons to separate out the spin-flip scattering, which contains the magnetic excitation, from the non-spin-flip scattering, which is non-magnetic, clarifies the data.

C. Dynamics of Atoms on Surfaces

Dr. Moncton mentioned in an earlier talk the use of x-rays to study the structures of monolayer films adsorbed on graphite. Although much of the pioneering structural work, in fact, was done with neutrons, I think he is correct in pointing out that the better momentum resolution of synchrotron x-rays is going to make them the tool of choice for future studies of this kind. However, I believe that neutrons, with a modest increase in flux, do have a future in studying the dynamics of adsorbed films. In Fig. 9 are shown some recent data representing inelastic scattering of deuterated ethylene on graphite.[10] Here a phase transformation occurs as a function of monolayer coverage -- I do not have time to go into the details. But you can see that this structural change is mirrored in changes in the structure of the phonon spectrum, and these are understood in some detail. When I look at these data, it reminds me of data taken in the late fifties and early sixties on bulk phonons, before the existence of the current generation of high-performance reactors. In that case, a factor of 5-10 in neutron flux ushered in a qualitatively new era, in which the phonon-dispersion curves, rather than rather crude phonon densities-of-status, could be measured. I can well imagine that another factor of five could do that for surface phonons.

D. Linewidth Studies

Another example of where increased flux is important is in increased resolution. Even people like myself, who come from a background of optical spectroscopy originally, sometimes forget, after they have been doing neutron-scattering for a while, exactly how poor the energy resolution of neutron spectroscopy is. Typically, resolutions are something like a part in a hundred, whereas even a poor optical experiment typically has resolution of a part in 10^4. Increases in flux can be converted directly to increased resolution by tighter collimation. What could you do with this better resolution? You could study excitation linewidths, for example. To be specific consider the case of superconductivity and its effect on linewidths of phonons. In a superconductor, the effect of the conduction electrons on the phonon linewidth disappears below the

superconducting transition temperature so long as the phonon frequency is below that of the superconducting gap; that is, the phonon does not have enough energy to break a Cooper pair at that point, so the linewidth narrows. Fig. 10 shows an example of that effect in niobium, the narrowing of the phonon linewidth upon passing below the superconducting transition temperature.[11] These measurements provide very important information about the frequency-dependence of the electron-phonon interaction. However, because of the limited resolution of neutron spectroscopy at the present time, only very strongly coupled superconductors like niobium and Nb_3Sn can be studied by this method. Increased intensity would allow the same experiments to be done on a much wider class of more weakly coupled superconductors.

E. Spinwaves in Itinerant Ferromagnets

Now I would like to shift gears and discuss some applications of the epithermal neutrons that are so efficiently produced by the new spallation sources that are becoming operational around the world. In most magnetic materials the moments are associated with electrons that are closely localized around the atoms. But in some metals, Fe and Ni for example, the moment is better thought of as a modulation of the spin density of the conduction electrons. Correspondingly, the spin waves are a kind of special excitations of this electron gas. Since these excitations carry little or no charge density, they are not well studied by x-rays, but can be studied by neutrons. But the dispersion of these modes is very steep, as is appropriate for electronic excitations, and the kinematics of the situation require that very energetic neutrons be used in order to study them. This is where spallation sources come to the fore. In Fig. 11 the dotted line represents the measurements on spin waves in iron using thermal neutrons. The solid curve represents new data using higher energy neutrons from a spallation source.[12] I want to point out that some theories had predicted that at about 120 milli-electron volts or so these spin waves would disappear due to interaction with other conduction electrons, the so-called Stoner continuum. You can see from these data that this has not occurred.

F. Recoil Spectroscopy

Another area where spallation sources excel is in recoil spectroscopy; that is, where the neutron has such high energy that it interacts with a single particle rather than causing a collective excitation. In this so-called impulse-approximation region, the cross-sections are related exactly to the distribution of momenta of the particles in the unperturbed sample and thereby, if desired, through some further transformations, to the single particle potential. Recoil spectroscopy should be very interesting in determining very anharmonic potentials, for example, in hydrogen bonds. It has already proved useful in studying the momentum distribution of quantum fluids and solids, and very shortly there should be some new spallation source data available on what is the canonical problem in momentum-distribution spectroscopy; the Bose condensate in superfluid helium. I remind you that the prediction is that the momentum distribution in superfluid helium should contain a finite concentration of zero-momentum particles.

I want to show you just a single example of some raw recoil spectroscopy data that are taken from a spallation source on solid He.[13] (Fig. 12) The first peak that you see represents the recoil from aluminum in the sample container. The higher peak represents the recoil of the solid helium. The information about the momentum distribution of helium atoms is contained in the line shape of this recoil peak.

G. Nuclear Magnetism

Finally, I want to mention some experiments that are of special interest because they make use of the unique properties of the neutron in novel ways. The first has to do with nuclear magnetism. Systems which have electronic singlet ground states, and which consequently are incapable of conventional magnetism may, nevertheless, undergo spontaneous nuclear-spin alignment if the temperature is low enough. Usually it is an extremely low temperature indeed, ($\sim 10^{-6}$ K) but occasionally residual hyperfine interactions with the electrons can enhance this interaction and cause spontaneous nuclear alignment to occur at an attainable temperature. Because the neutron is sensitive to the spin state of the nuclei, neutrons are a uniquely designed probe for this effect. Fig. 13 shows the result of some recent measurements of the spontaneous nuclear alignment of $PrCu_2$ at low temperatures.[14] I must point out that this is a true milestone. In 30 years of neutron scattering research this is perhaps the first example of an experiment that suffers from a neutron flux that is too high. The limiting factor in determining the temperature is the heating of the sample due to neutron absorption.

H. Summary:

Table II is a list of some of the more important opportunity areas for neutrons in condensed matter physics as I see them. I've tried to indicate where new instruments and higher flux or both are most critical. In order to effectively address these opportunities three things are required:

a) We must upgrade instrumentation at our existing high performance reactors.

b) We have to continue to ensure that we remain competitive with Western Europe in terms of spallation sources, and I am thinking now of the SNS spallation source, which is due to come up later this year in Rutherford Laboratory in Great Britain. And finally,

c) We have to plan for the next generation high-flux source. By 1990, our high-flux reactors are going to be 25 years old.

I think we have to carefully weigh the advantages of reactors and spallation sources in making these plans. We must also consider the possibility of broader international involvement. Canada and Japan have active neutron research efforts and informal contacts suggest that they would be very interested in exploring how they might fully participate in the design, construction and use of a next generation source.

DR. BIRGENEAU: Are there any questions?

QUESTION: Do you want to say a bit more about what the spallation sources would do for us, again? Or do you want to answer why shouldn't we be happy to go over to Rutherford if they get it (SNS) to work?

DR. AXE: In fact, present plans include a spalation source (WNR/PSR) to come on in 1986, which will be equivalent to the Rutherford source. What is necessary there is an enlargement of the instrument hall. I suspect the source issue will come up in the subsequent talks as well and as there are a wide range of opinions that have to be represented, I believe this will be more satisfactorily done in the panel discussion later today.

QUESTION: You would not care to go through your list and assess relative merits?

DR. AXE: I have chosen to list new opportunities as for cold, thermal and epithermal neutrons, rather than for reactor and spallation sources. In the epithermal neutron region, I think that nearly everyone agrees that a well-designed spallation source is going to be superior to a reactor source. The real questions are these. How much should the epithermal experiments be emphasized with respect to the others on the list? And to what extent can spallation sources be adapted to the needs of the other experiments as well? The latter subject involves a whole series of rather complicated technical questions that require answers.

DR. MONCTON: I have five or six questions, but I will only ask one. You said that in the inelastic polarized business that you would benefit from the higher fluxes of new sources. What payoff might there be for a much smaller investment of money in monochromators?

DR. AXE: A lot of effort has gone into increasing the efficiency of polarizing monochromators. Dr. Fender can tell you that there has been a group at ILL that has been working continuously since the early seventies on just that. I do not know that there is a theoretical limit that we are reaching in terms of performance--

DR. MONCTON: What are the performances of current monochromators in terms of reflectivity?

DR. AXE: For polarized neutrons, I don't know exactly -- Dr. Shirane knows these numbers better than I do. I guess it is something like 40 percent reflectivity?

DR. SHIRANE: If you include a factor of two that you throw away up front, you are down by ~20 relative to a good unpolarized neutron instrument.

DR. BIRGENEAU: John, really a comment more than a question, but I would like to hear your response to it. This is, I think, a characteristically conservative list. I mean, it seems to me that one of the crucial issues in current condensed-matter physics, especially in the

context of new materials, is very often new materials which have just been synthesized in the last several years, where the fundamental limit turns out to be the size of single crystals you get -- that certainly is dominant in biology.

For example, if one wanted to know about the lattice dynamics of the intercalate species in a variety of intercalate materials, I think it is true that current sources simply do not provide enough neutrons to measure phonon dispersion relations. A factor of 10 would make possible such experiments.

It seems to me there are a very large number of experiments in novel materials where one order of magnitude increase, especially in the cold-neutron flux, would have a revolutionary impact. I think saying whether or not you need a new instrument or higher flux, you assume that you have got cubic centimeters of material. DR. AXE: I agree that many experiments are limited by sample size.

QUESTION: In the earlier talks (on x-rays) we continually heard the word "brilliance" as being important, not simply flux. I do not hear that word discussed by any of the neutron people. I am just curious to know is this because you cannot focus well? We do not hear the word "brilliance." You keep saying: I need more flux. What is the subtle difference now that makes you not refer to that measure?

DR. AXE: Yes, it is much more difficult to produce a narrowly defined beam of neutrons. Neutrons are emitted isotropically and in order to pick out a very narrowly divergent beam, you have got to throw away a lot of neutrons, whereas in the synchrotron case, the advantage is that these relativisitic effects automatically do that for you. Brilliance, of course, is important to us, too, for many experiments. But in other cases narrow angular resolution is of secondary importance.

QUESTION: You do not have the reflectors that concentrate the neutron well enough --

DR. AXE: Only very crude ones, a factor of three or something like that.

QUESTION: I just wanted to comment here on the remark about focusing neutrons. When you focus the neutrons, you are not increasing the brilliance, because you are focusing down to a point, but at the cost of an angular resolution. I think, in many cases, when neutron-scatterers ask for increased flux, they need increased brilliance, but the only way to increase the billiance is, in effect, to increase the flux.

QUESTION: Your example with the surface dynamics you mentioned that an increase in flux of a factor of five enabled you to get phonon-dispersion curves, whereas previously --

DR. AXE: I said I could imagine that that might be the case.

QUESTION: But that is only a square root factor applied in the signal-to-noise ratio, which you might be able to make up just by increasing the counting time.

DR. AXE: That is partially true. But you get into human problems. Many people are too impatient to devote months to collecting data -- or more to the point, to waiting in line for someone else to do so. And while it is possible to do a few tour-de-force experiments in some area in this way, the overall level of activity might not be sufficient to attract a "critical mass" of scientific interest to allow the subject to develop. It's impossible to quantify, but I have the strong impression that there are a number of fully developed areas that would never have taken hold if we had been stuck with last generation neutron sources.

TABLE I

SOME MAJOR TECHNICAL & SCIENTIFIC ACCOMPLISHMENTS OF THE LAST DECADE

*1974	Cold Sources, Neutron Guides (W. Europe, ILL)
1974	Low Dimensional Magnetism (U.S.)
1975	Powder Profile Analysis (Netherlands, ILL)
1975	Neutron Interferometry (U.S., Austria)
1975	Charge Density Waves (U.S., ILL)
1975	Vibration, Tunnelling & Diffusion of H in Metals (U.S., W. Europe)
1976	Structure of Physi- & Chemi-sorbed Monolayers (U.S.)
*1977	High Energy Resolution Spectrometers (W. Germany, ILL)
1978	Bose Condensate in ^{4}He; Liq^{3}He (U.S., Canada, ILL)
1979	Coexistence of Magnetism & Superconductivity (U.S.)
1981	Pulsed Spallation Sources (U.S., Japan, G.B.)

TABLE II

NEW OPPORTUNITIES

	New Instruments	Higher Flux
1. COLD NEUTRONS		
critical dynamics	●	○
phonon linewidths	●	●
proton tunnelling	○	○
diffusion (H, ionic conductors, etc.)	●	○
2. THERMAL NEUTRONS		
polarized neutrons		●
surface dynamics		●
interferometry		○
special environments (P,T)	○	*
time dep. effects (e.g. reaction kinetics, pulsed fields, ballistic phonons)		●
3. EPITHERMAL NEUTRONS		
nuclear recoil spectroscopy	○	●
magnetic X(Q,E); .1<E<1eV	○	○
nuclear resonance detectors		●
liq. & amorphous struct. & dynamics		○

● essential ○ helpful

References

1. H. Ikeda and K. Hirakawa, Solid State Comm. 7, 529 (1974 .

2. Y. Endoh, G. Shirane, R. J. Birgeneau, P. M. Richards and S. L. Holt, Phys. Rev. Lett. 32, 170 (1974).

3. J. des Cloizeau and J. J. Pearson, Phys. Rev. 128, 2131 (1962).

4. R. Comés, B. Renker, L. Pintschovius, R. Currat, W. Gläser and G. Schreiber, Phys. Stat. Solidi 671, 171 (1975).

5. J. J. Rush, J. M. Rowe, and D. Richter, Z. F. Physik, to be published.

6. W. Thomlinson, G. Shirane, D. E. Moncton, M. Ishikawa, and Ø. Fischer, Phys. Rev. 23, 4455 (1981).

7. See, for example, F. Mezei, "The Neutron and its Applications -- 1982", P. Schofield, ed., Inst. of Physics Conference Series #64, Inst. of Physics, London (1983); p. 181.

8. F. Mezei, Phys. Rev. Lett. 49, 1096 (1982).

9. J. P. Wicksted, G. Shirane and O. Steinsvoll, J. Appl. Phys. 55, 1697 (1984).

10. B. H. Grier, J. Eckert, H. Patterson, D. Richter, R. J. Rollefson, and L. Passell, submitted to Phys. Rev. Lett.

11. S. M. Shapiro, G. Shirane and J. D. Axe, Phys. Rev. B12. 4899 (1975).

12. K. C. Loong, J. M. Carpenter, J. W. Lynn, R. A. Robinson, H. A. Mook, J. Appl. Phys. 55, 1895 (1984).

13. R. O. Hilleke, P. Chaddah, R. O. Simmons, D. L. Price and S. K. Sinha, Physical Review Letters 52, 847 (1984).

14. S. Kawarazaki, N. Kumitomi, R. M. Moon, R. M. Nicklow and H. Suzuki, to be published.

FIGURE CAPTIONS

Fig. 1 Regions of energy-momentum space probed by cold, thermal and epithermal neutrons. Magnetic excitations are in green, nuclear excitations in purple.

Fig. 2 Comparison of magnetic superlattice intensities with Onsager's prediction for 2d Ising model.

Fig. 3 Quantum mechanical effects cause spin 1/2 1d antiferromagnet to have spin wave energies larger than the classical value by the factor $\pi/2$.

Fig. 4 The longitudinal (LA) acoustic phonons in the quasi 1-d metal potassium chloroplatinate (KCP), show a pronounced frequency anomaly associated with charge density wave formation.

Fig. 5 The splitting of higher order local H vibrational modes in metals can be used to determine the anharmonicity in the vibrational potential.

Fig. 6 Comparison of neutron powder diffraction pattern for $Tb_{1.2}Mo_6S_8$, showing new low temperature phase with coexisting magnetic and superconducting long range order.

Fig. 7 Schematic representation of the neutron spin echo principle.

Fig. 8 Neutron spin echo measurements of critical scattering energy widths show large deviations from behavior extrapolated from measurements using conventional techniques.

Fig. 9 Although magnetic and nonmagnetic excitations are often well separated at low temperatures (a), polarized neutrons are nearly indispensible for such studies in the paramagnetic regime (b).

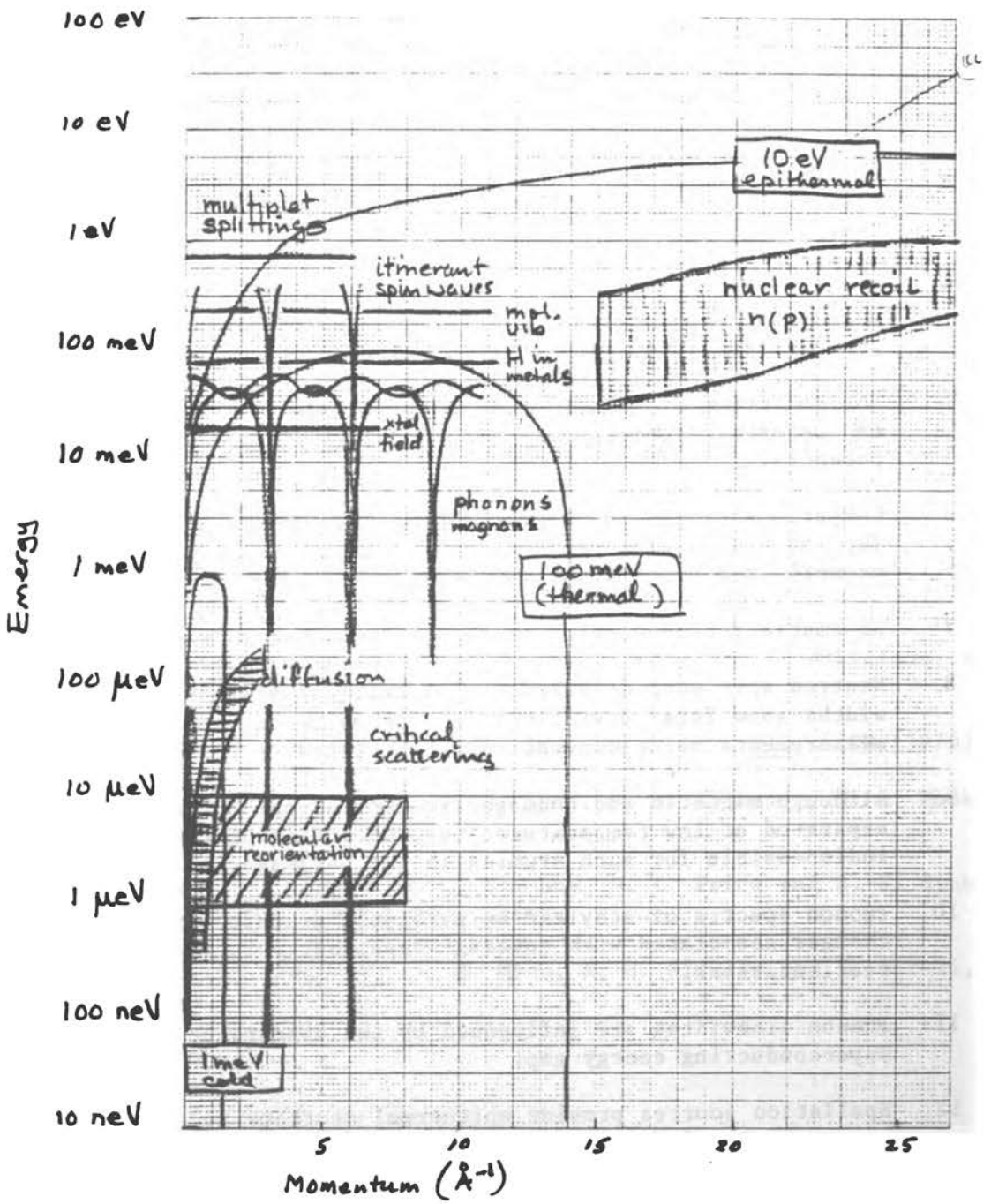
Fig. 10 Phonon spectra of ethylene on pyrolytic graphite show subtle changes associated with coverage dependent structural reorientations.

Fig. 11 Phonon linewidths are influenced by the appearance of the superconducting energy gap.

Fig. 12 Spallation sources provide epithermal neutrons to study high energy excitations, such as spin waves in Fe. Dotted line indicates previous measurements with reactor sources.

Fig. 13 A sample of neutron recoil spectroscopy data on solid He. The lower peak is Al recoil from the sample container.

Fig. 14 Superlattice reflections due to spontaneous nuclear magnetism in $PrCu_2$.


100 eV
10 eV
1 eV
100 meV
10 meV
1 meV
100 μeV
10 μeV
1 μeV
100 neV
10 neV
Energy
10 eV epithermal
multiplet splittings
itinerant spin waves
mpl. U6
H in metals
nuclear recoil
n(p)
xtal field
phonons magnons
100 meV (thermal)
diffusion
critical scattering
molecular reorientation
1 meV cold
5
10
15
20
25
Momentum (Å⁻¹)

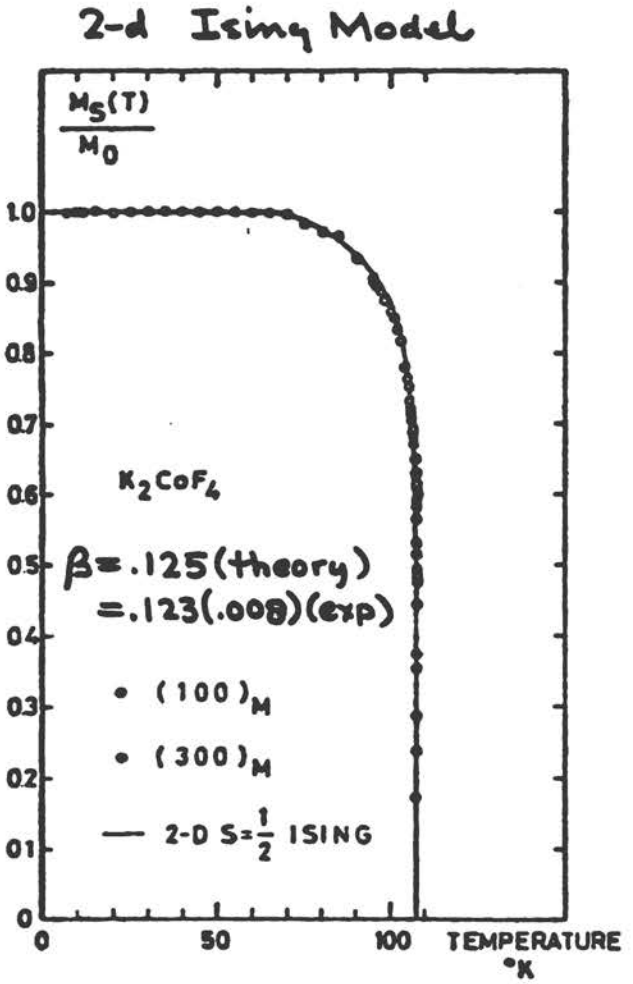
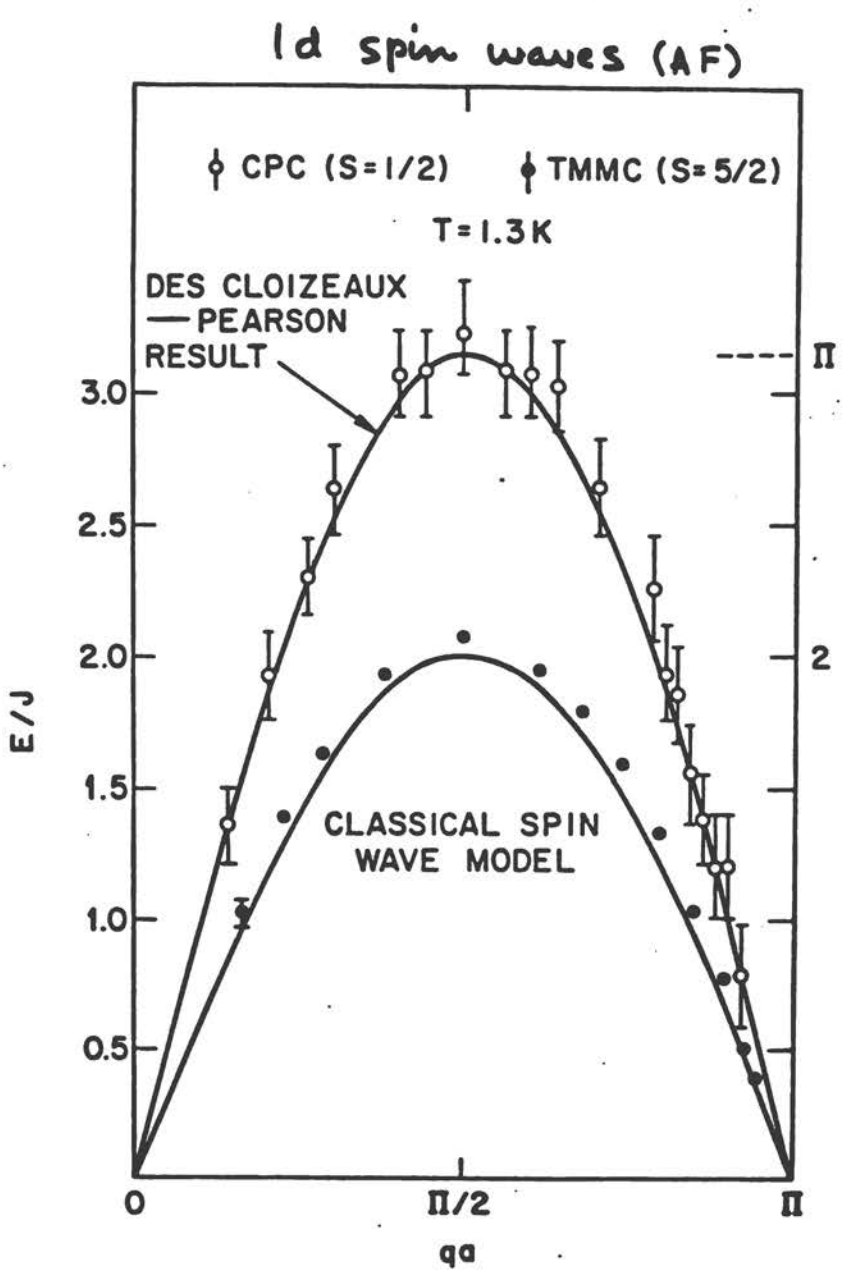
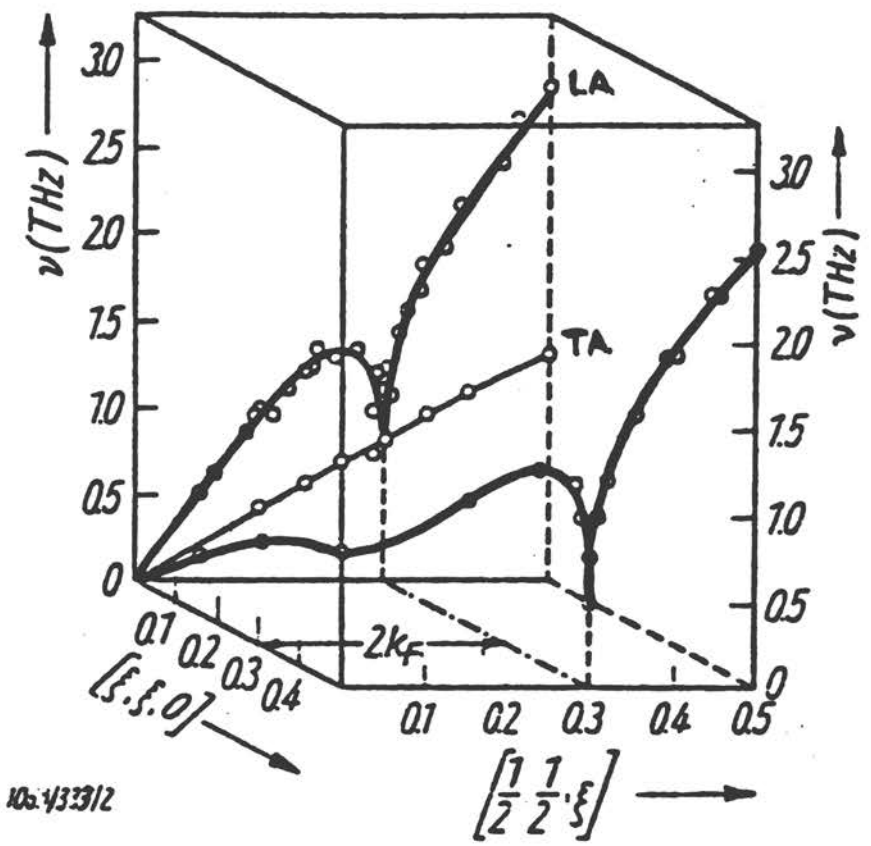


FIG. 1. Temperature variation of the normalized intensities of the $(100)_M$ and $(300)_M$ magnetic Bragg peaks for K_2CoF_4. The measured $(300)_M$ intensity had to be multiplied by 9.5 in order that it equaled the $(100)_M$ intensity at 4.2 K.


1d spin waves (AF)
CPC (S=1/2)
TMMC (S=5/2)
T=1.3K
DES CLOIZEAUX
— PEARSON
RESULT
CLASSICAL SPIN
WAVE MODEL
E/J
3.0
2.5
2.0
1.5
1.0
0.5
π
2
0
π/2
π
qa

KCP - a quasi 1d metal is unstable w.r.t a Peierls distortion

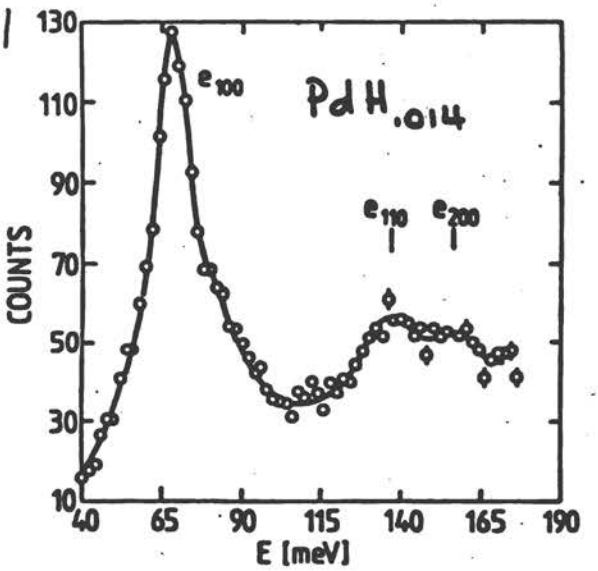


Superconductivity in PdH_x

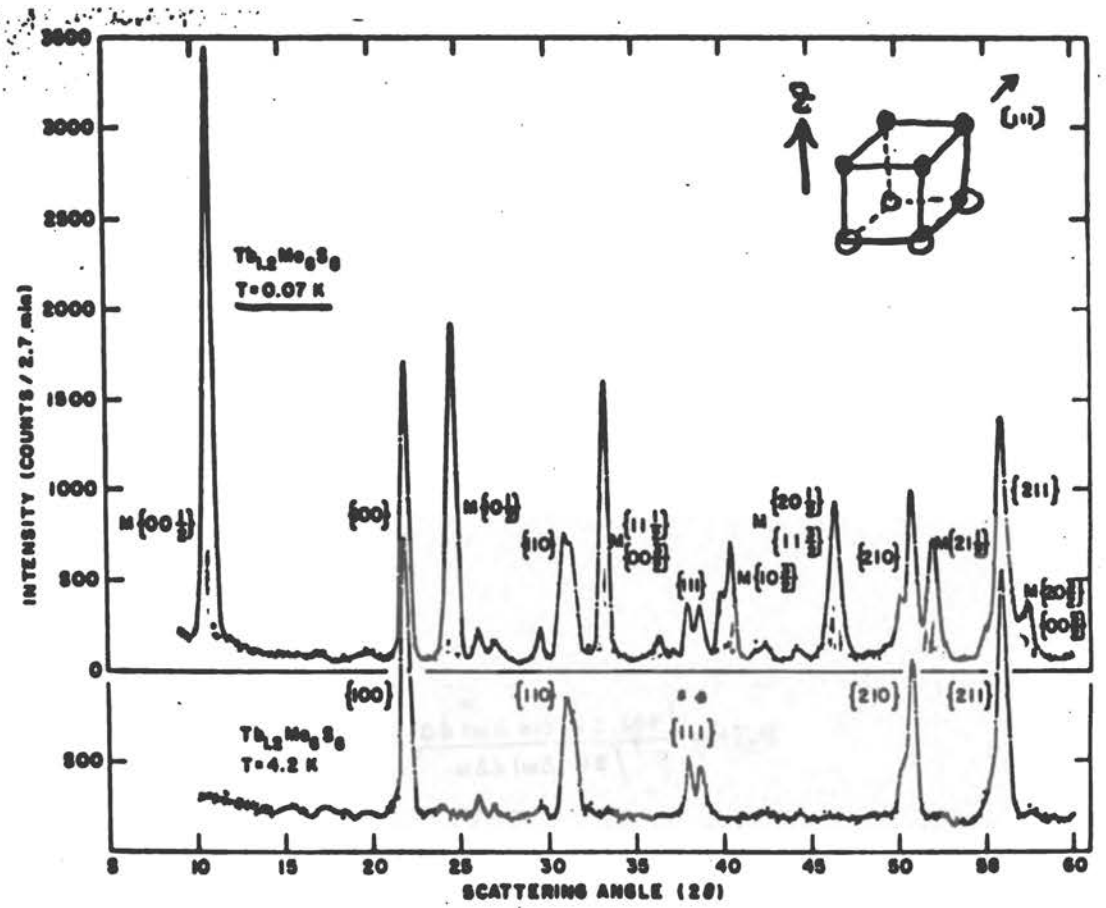
- Coupling to optic modes
- Inverse isotope effect $\left(T_c \sim \langle\omega\rangle \sim \frac{1}{\sqrt{M}}\right)$

$T_c(H) = 9\,K \quad T_c(D) = 11\,K$

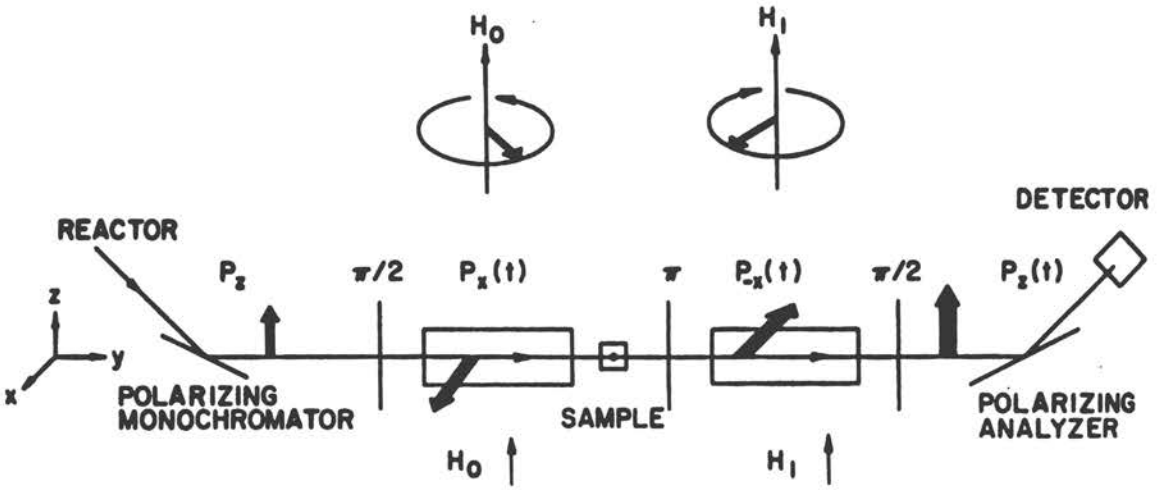
Q. Is potential isotope dependent?



A. No! Answer lies in strong anharmonicity


INTENSITY (COUNTS / 2.7 min)
SCATTERING ANGLE (2θ)
$Th_{1.2}Mo_6S_8$
T = 0.07 K
$Th_{1.2}Mo_6S_8$
T = 4.2 K
{100}
{110}
{111}
{210}
{211}
(111)

Neutron Spin Echo



$$P_z(t) = \frac{\int S(Q,\Delta\omega)\cos\Delta\omega t\, d\Delta\omega}{\int S(Q,\Delta\omega)\, d\Delta\omega} = \frac{S(Q,t)}{S(Q)}$$

$$\Delta\omega t = 2\pi(N_1 - N_f)$$

Conventional

$\Delta E_i \approx \Delta E_f \approx \Delta\omega$

NSE

$\Delta E_i \approx \Delta E_f \approx 10^5 \Delta\omega$

1 meV 10 neV

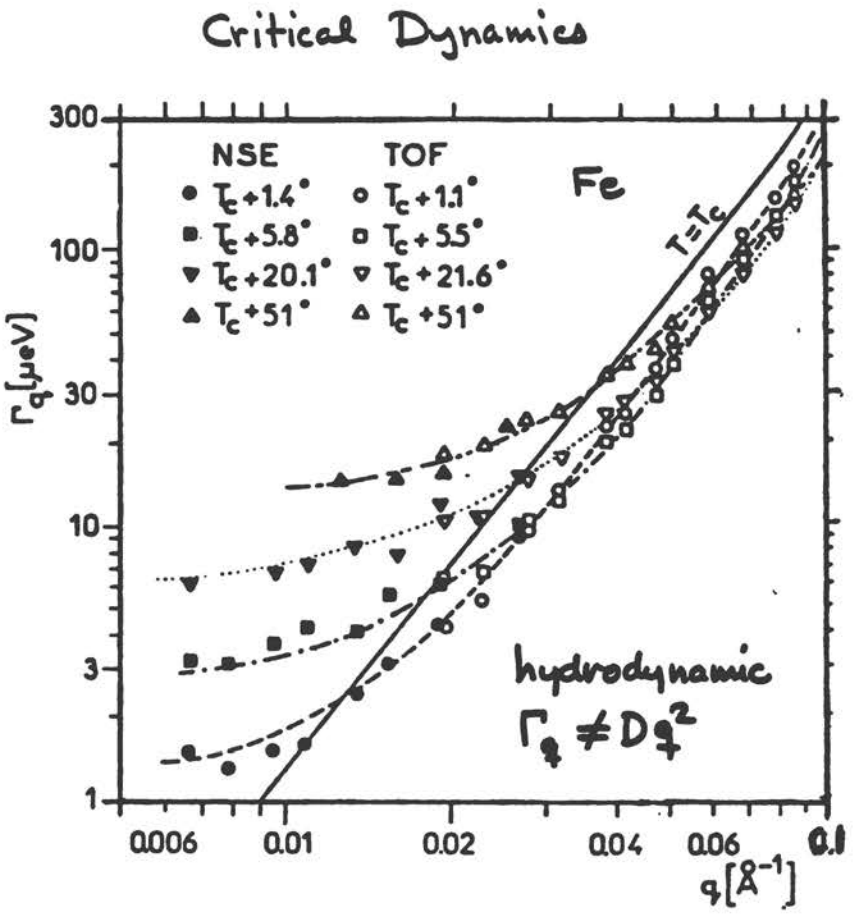
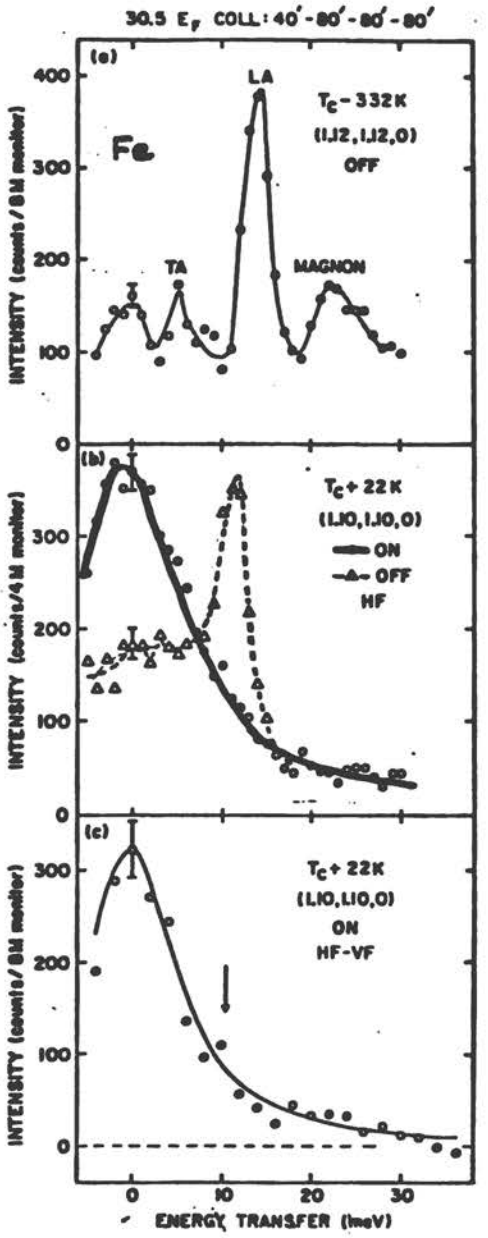
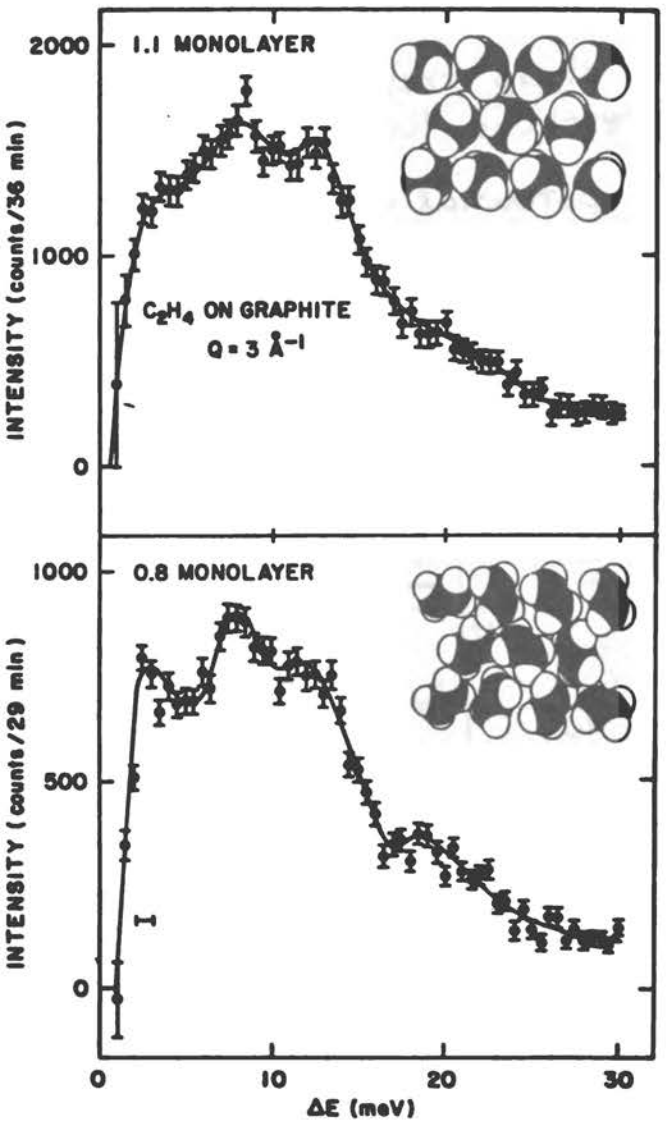


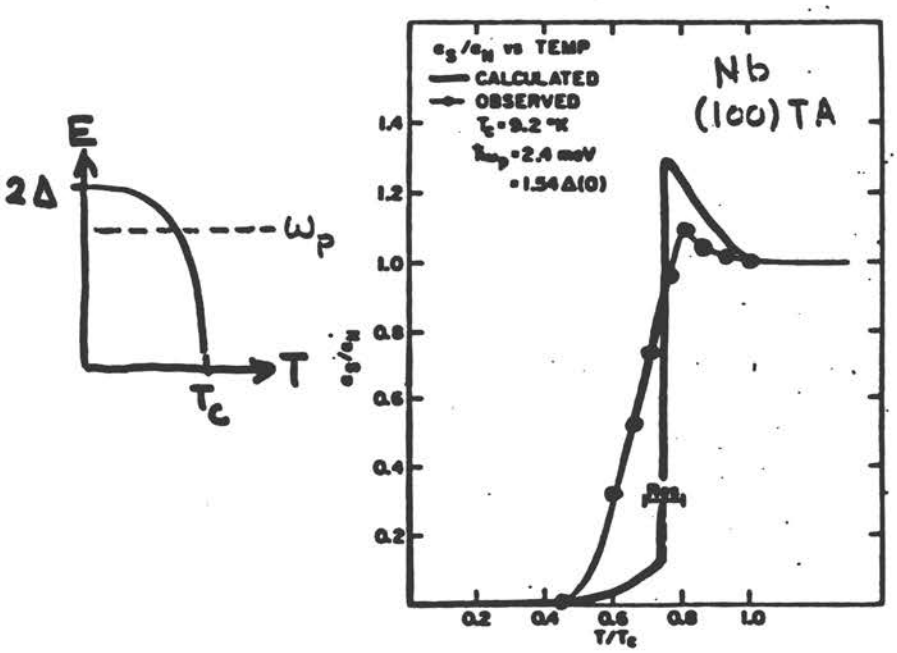
FIG. 2. Measured relaxation rates at various temperatures. For comparison the straight line is the same as in Fig. 1. The discontinuous lines were calculated from Eq. (6) for $T - T_C$ = 1.5, 5.6, 20, and 51 K, respectively.

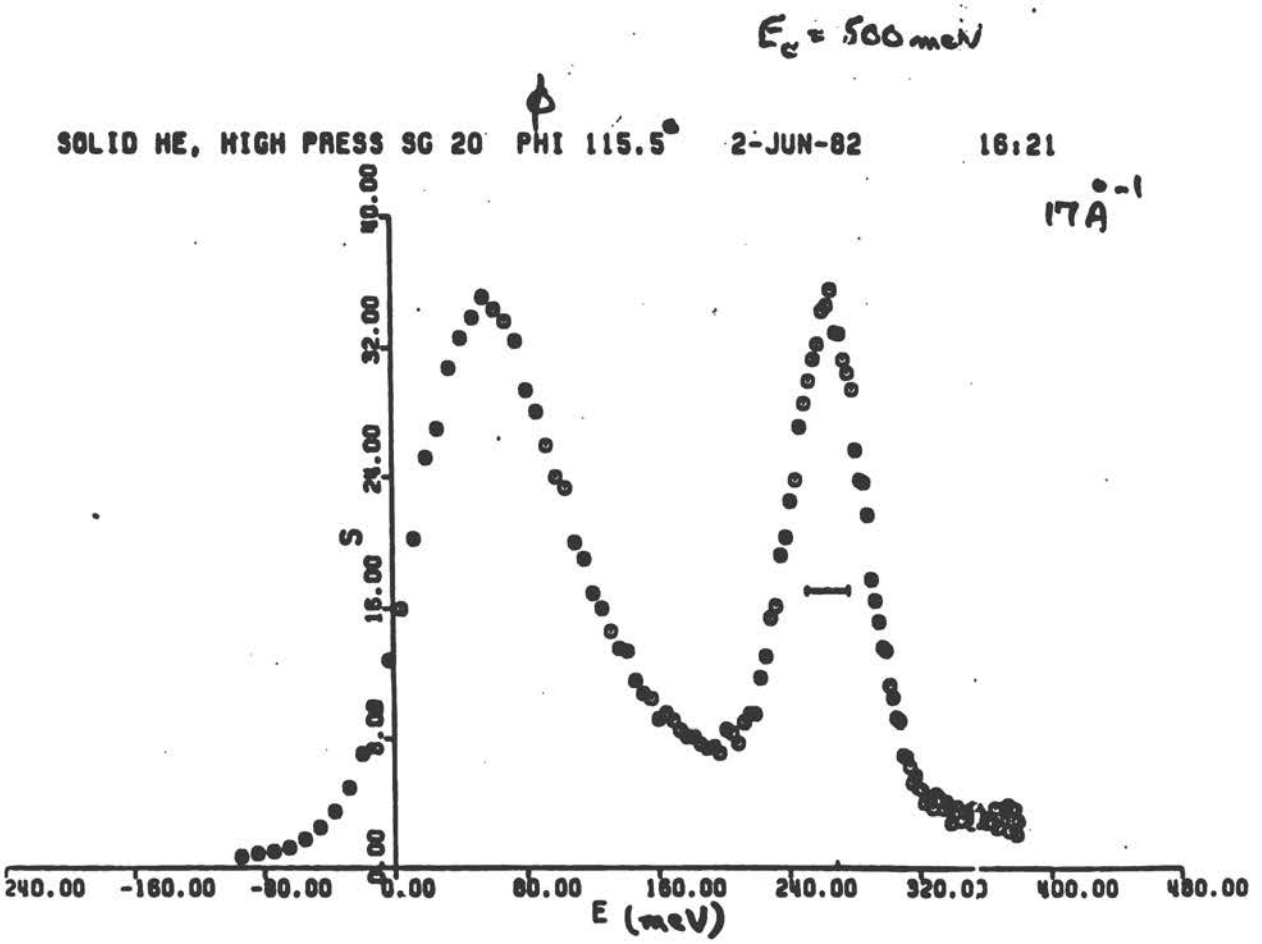

30.5 E_f COLL: 40'-80'-80'-80'
(a)
Fe
LA
TA
MAGNON
T_c - 332K
(1,1,2, 1,1,2, 0)
OFF
(b)
T_c + 22K
(1,1,0, 1,1,0, 0)
ON
OFF
HF
(c)
T_c + 22K
(1,1,0, 1,1,0, 0)
ON
HF-VF
INTENSITY (counts / 8M monitor)
INTENSITY (counts / 4M monitor)
0
100
200
300
400
10
20
30
ENERGY TRANSFER (meV)


1.1 MONOLAYER
2000
1000
0
INTENSITY (counts/36 min)
C_2H_4 ON GRAPHITE
Q = 3 Å^{-1}
0.8 MONOLAYER
1000
500
0
INTENSITY (counts/29 min)
0
10
20
30
ΔE (meV)

Linewidth Studies

- Most "sharp" excitation linewidths are resolution limited.
- Much potential information in linewidths & shapes (E.g. phonons, magnons, H-in metals, x-tal fields in metals)
- Example. Effect of superconductivity on phonon linewidths

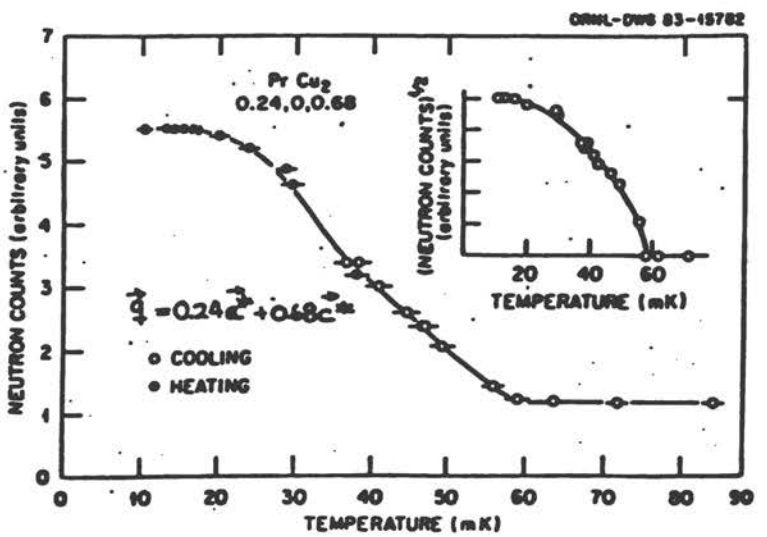



E_e = 500 meV
SOLID HE, HIGH PRESS SG 20 PHI 115.5° 2-JUN-82 16:21
17Å^{-1}
S
E (meV)
240.00
-160.00
-80.00
0.00
80.00
160.00
240.00
320.00
400.00
480.00

Spontaneous Nuclear Magnetism

- Nuclear ordering in electronic singlets can be drastically enhanced by hyperfine interaction.
- Neutron is sensitive to spin-state of nuclei.

$$b = \bar{b} + \Delta b \, \vec{I} \cdot \vec{\sigma}_n$$



SCIENTIFIC OPPORTUNITIES WITH NEUTRONS IN MATERIALS SCIENCE

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I am going to describe a number of applications of neutron scattering to problems in materials science, applications which either have proved to be very fruitful or promise to be very fruitful in answering materials-related questions.

Because this presentation has to be rather condensed and I am supposed to be discussing metals, ceramics and polymers, I have chosen to describe a few experiments which illustrate the various attributes of neutrons which make them especially well suited to the study of materials problems. First, however, it is useful to review some of the special properties of neutrons which make neutron scattering techniques so useful in materials science research. These properties are summarized in Table 1.

One very remarkable feature of neutrons is their great penetration depth. Specimens used in scattering experiments have a thickness of millimeters or even centimeters. Consequently it is possible with neutrons to look at properties as a function of position. This is a useful capability, especially when investigating stress states. The large penetration depth permits surveying over many grains in a sample. Obviously this is essential in a study of grain boundary cavitation or intergranular microcracking but there is another, more subtle benefit. Components seldom consist of a single crystal. The behavior of real materials is profoundly affected by their polycrystalline nature. For example, the constraint of neighboring grains alters deformation; environmental attack is strongest at the surface. Even if the distortions introduced by specimen thinning for x-ray or electron microscopic examination could be eliminated, the measurements would not be representative of bulk behavior. Certainly many important processes occur at the surface, but often it is essential to be able to examine what is going on inside of a specimen without the distortion introduced by the presence of a surface.

Large penetration depths make possible the examination by neutron scattering of large microstructural features, features say $\gtrsim$ 10 μm in size. Such features are frequently important in materials (e.g., pores in metals and ceramics).

Cold neutrons used in scattering have a low energy and therefore are nondestructive.

The nuclear scattering length of neutrons is not a monotonic function of atomic number, as is the case with x-rays. This random variation of scattering length makes possible the study of a number of alloys containing elements close together in the periodic table. (Note that many important alloys consist of transition elements, whose x-ray scattering lengths are similar.) Of far greater importance is the fact that a number of light elements are excellent neutron scatterers. Both hydrogen and deuterium are strong scatterers, and their scattering lengths differ significantly from one another. This fortunate circumstance makes neutron scattering a powerful, unique tool for studying polymeric materials. In the last few years a wealth of information on chain morphology and other details of polymer structure have been obtained which could only be speculated about before the advent of neutron scattering experiments.

Neutrons "see" materials through their magnetic moments and so can be used to deduce magnetic structures. Furthermore, if we are examining ferromagnetic material by small angle scattering, neutrons provide additional information as a result of the fact that we are dealing with magnetic as well as nuclear scattering contrasts. An example of the use of this extra information will be given later. There is another class of experiments in which it is advantageous to interact with a specimen through its nuclei rather than its electrons. In structural determinations neutron scattering gives information directly as to positions of the nuclei in the crystal whereas with x-rays this information is convoluted with the electron positions.

EXAMPLES OF NEUTRON SCATTERING IN MATERIALS RESEARCH

We now turn to the description of a number of experiments which illustrate the use of neutron scattering to investigate materials problems. (See Table II for a more extensive listing of such problems.)

Grain Boundary Cavitation.

It seems as if a high proportion of materials research concerns damage accumulation in various forms, e.g., microcracking, microstructural degradation, radiation damage, accumulation of stress or strain. An important damage mechanism at high temperatures is grain boundary cavitation. A large number of metals and alloys, when subjected to deformation at elevated temperatures, develop small voids on their grain boundaries. These voids grow under continued deformation and eventually may coalesce, thereby causing failure. Cavitation is an important engineering problem but it also is of considerable scientific interest. How do voids nucleate? Why do they grow under certain conditions? A great deal of effort has been expended on the theory of cavitation but almost no data exist of the type which would permit the testing of the theories. The sort of information needed includes the number of densities of

the voids and their size distributions as functions of time, temperature and deformation parameters. For reliable results a large number of voids should be included in the sample. In the small angle neutron scattering (SANS) experiments I'm going to describe 10^6 - 10^{12} voids were included in each measurement. The voids nucleate only at grain boundaries, so their total volume fraction is quite small. It is possible with SANS to measure void volume fractions which are less than 10^{-6}. We would like our observations of voids to begin as close as possible to the nucleation event, but since nucleation is continuous it also is necessary to be able to include large voids. Void sizes in the range of a few nanometers to somewhat less than a micrometer can be detected by SANS and analysed by diffraction theory. Of great importance, it is possible with SANS to separate void nucleation from void growth so that we can distinguish these two phenomena. (For a review of the theory and experimental techniques of SANS and methods of data analysis, see Kostorz, 1979; Glinka et al., 1980; Weertman, 1981.)

An extensive study of grain boundary cavitation in a model system, high purity copper, has been carried out with SANS (Page et al., 1980, 1982; Yang et al., 1984a,b, in press). Figure 1 shows the development of void volume fractions in copper subjected to a fully reversed cyclic (fatigue) stress of 34.0 MPa amplitude and frequency of 17 Hz. Temperatures of fatiguing ranged from 678 K (1/2 the melting temperature) to 840 K. Note that void volume fractions of less than 10^{-6} were measured and that cavitation was detected after only 15 s of fatiguing. If these data were plotted on linear rather than logarithmic coordinates it would be seen that there is no measurable incubation time required for fatigue-induced cavitation. It is possible to derive size distributions for the voids from the scattering results. In the case of cyclic stressing it was found that the distributions peak at a void size of 30 to 40 nm radius. The location of the peak does not change appreciably with continued fatigue. However the void number densities increase rapidly. The size distributions which result from time independent (creep) loading at 678 K under a stress of 27.6 MPa are shown in Fig. 2 (curves A). A number of significant differences from the fatigue distributions are evident, such as the absence of small voids, movement of the distributions to larger void sizes, much lower void densities. The detailed information provided by the SANS measurements (e.g., nucleation rates, average void spacings) permits the modeling of these distribution curves using various growth theories (curves B, C, D). Thus, for the first time, it is possible to make a quantitative evaluation of the merits of the various cavitation models. (Of course the SANS results also can be used as guides in the development of new cavitation mechanisms.) The information obtained from the SANS measurements is quite unique and should prove to be of great value in the investigation of cavitation processes.

Ceramics as well as metals cavitate and the methods described above have been used to study the phenomena in a number of ceramic materials (Page and Lankford, 1983; Page et al., in press a,b).

It should be emphasized that all the measurements described above of neutron scattering in copper were carried out at the Institut Laue Langevin. There is no facility in the United States which is capable of performing such experiments. Both the fluxes of long wave length neutrons and the range in measurable scattering vectors at the U. S. facilities are too low. (The scattering vector q is defined as $4\pi \sin \theta/\lambda$, where θ is 1/2 the scattering angle and λ is the neutron wave length.

With improved instrumentation and higher fluxes we could get closer and closer to actually watching nucleation events. In situ experiments would be possible. An obvious next step in the series of cavitation experiments is to study the effect of complex stress patterns on cavitation. We have an idea of the behavior of fatigue-induced cavitation and are beginning to acquire data on creep cavitation. Now we can combine these two modes of deformation, one leading to a high void nucleation rate, the other to a high growth rate, to see what happens under a complex loading cycle. This is not a trivial problem. A vast amount of effort has gone into trying to devise methods for predicting mechanical behavior at elevated temperatures under the complicated cycling patterns encountered in real life situations. Since grain boundary failure is an important failure process at high temperatures, an understanding of the influence of cycle pattern on the rate of cavitation would make a valuable contribution to life prediction modeling.

Microcracking.

The next experiment I would like to describe briefly concerns microcracking in a ceramic (Case and Glinka, 1984). This particular ceramic, $YCrO_3$, undergoes a phase transformation at 1100°C. Microcracking on the grain boundaries is produced as the material cools through the transformation temperature. Prolonged annealing below 1100°C heals the cracks whereas annealing above this temperature reintroduces the cracks in a reproducible manner. Material with this behavior is ideally suited for SANS measurements: subtracting the scattering of a specimen in its healed state from the scattering when it is cracked eliminates the contributions from all other sources, such as the surfaces. The resultant data can be fit to the curve of scattering expected from an ensemble of randomly oriented thin disks. From the SANS measurements combined with measurements of the elastic constants it was possible to determine the average radius and thickness of the disks and their number density n/v (Fig. 3). Note that the diameter of the cracks is about 6 μm, which is quite beyond the dimensions normally thought of as in the diffraction regime. (It was verified that the scattering was indeed governed by diffraction, not refraction.)

The results of the $YCrO_3$ experiment demonstrate that SANS can be used to detect the onset of microcracking in brittle materials as well as quantify the extent of damage. It is likely that grain boundary cracking in metals (including crack-like voids in the later stages of cavitation) also can be studied by SANS. As mentioned in the preceding section, higher fluxes would permit experiments to be carried out in situ, so that the kinetics of cracking could be studied directly.

Radiation Damage.

Radiation damage frequently appears in the form of voids. We already have seen how this type of damage can be studied by neutron scattering. I am going to describe another form of radiation damage which occurs in precipitation-hardening iron and steel containing a small percentage of copper. These materials become embrittled after exposure to neutron irradiation. It was suspected that the embrittling agents were either small voids or copper-rich clusters produced by the radiation but the features were too small (<2 nm) to be detected by transmission electron microscopy in a ferromagneitc material. This problem has been studied by SANS (Frisius et al., 1983) and further work is in progress (Odette et al.).

Since iron is ferromagnetic the neutrons in a SANS experiment are scattered not only by heterogeneities in the composition of the specimen but also by its magnetic domains. To eliminate the complication of superimposed domain scattering the specimen usually is magnetized in the plane perpendicular to the neutron beam (Fig. 4). In the expression for the differential scattering cross section $d\Sigma/d\Omega$ from such a magnetized ferromagnetic specimen the factor $(\Delta\rho_{nuc})^2$ is replaced by $[(\Delta\rho_{nuc})^2 + \sin^2\alpha\ (\Delta\rho_{mag})^2]$. Here $\Delta\rho_{nuc}$ and $\Delta\rho_{mag}$ are the differences in nuclear and magnetic scattering length density between matrix and scattering entity and α is the angle between the imposed magnetic field $\underline{H}$ and the scattering vector $\underline{g}$. The ratio of $d\varepsilon/d\Omega$ measured perpendicular to $\underline{H}$ to its value parallel to the field gives directly the quantity $[(\Delta\rho_{nuc})^2 + (\Delta\rho_{mag})^2]/(\Delta\rho_{nuc})^2 = A$. Measured values of A were compared with the calculations based on scattering arising from Cu precipitates (A = 11.1) and from voids (A = 1.3). For iron containing small amounts of copper, A was found to equal 11.1, indicating that the scattering is caused by copper precipitates. Size curves derived from the SANS data gave a value of 2.2 nm for the precipitates induced by fast neutron irradiation. This experiment is a good illustration of the additional information provided by the magnetic scattering length densities in neutron scattering from magnetic materials.

Residual Stress Measurements.

Another application of neutron scattering to materials research which has considerable scientific and technological potential is the measurement of residual stresses. Because of the large penetration depth of neutrons it is possible to use a slit system to measure stress as a function of position (Fig.

5). Thus stress states can be determined through the thickness of a component without destroying it. The validity of the method has been verified by experiments on test bars in which the stress state is known (Schmank and Krawitz, 1982; Prask and Choi, to be published).

I'll mention just one residual stress investigation, carried out at the Intense Pulsed Neutron Source at Argonne National Laboratory to measure stresses in cermets (Krawitz et al., 1983; Krawitz et al., in press). Cermets are very hard materials consisting of small pieces of a hard carbide in a soft binder, in this case tungsten carbide in a cobalt nickel alloy. Because of the large difference in the thermal coefficients of expansion between tungsten carbide and the binder, tremendous hydrostatic stresses are built up during fabrication of the material: tensile in the binder and compressive in the carbide. In this particular experiment the effect of various forms of applied stress on relaxing the large hydrostatic stresses was investigated. It was found that modest amounts of straining or cycling produce relaxations of the order of GPa's. Such a change in the internal stress state under loading certainly must affect the behavior of the cermets during service. A result which makes the data seem very convincing is the fact that the volume averages of the measured stress changes are zero (to within experimental error), as indeed they should be.

Residual stress measurements by neutrons should be useful in the examination of welds, to study load sharing, the effects of heat treatment, mechanical treatment. Improved instrumentation and increased neutron fluxes would improve the spatial resolution, currently about 1 mm^2. With these improvements it could become possible to examine the stress field around a crack. Note that this could be the stress field in the interior of the material, not the surface stress usually measured which is known to differ significantly from the interior value. It would be of great interest to observe, in real time, the build up of stresses under various forms of loading.

Porosity

I have mentioned the fact that the ability of neutrons to penetrate substantial thicknesses of material opens the door to the possibility of investigation by neutron scattering of "large" microstructural features. In general, the scattering of neutrons with the wave lengths ordinarily used in SANS experiments follows the theory of diffraction if the scattering entities are less than a few tenths of a micrometer. Refraction is dominant in the case of heterogeneities larger than about 10 μm. In the intermediate size range scattering occurs by a mixture of diffraction and refraction. The theory of scattering in this intermediate range is currently being developed (Berk and Hardman-Rhyne, 1984, to be published), so that the range of features which may be studied and analysed by neutron scattering is opening up to the point of overlap with other NDE techniques. This new development is proving to be especially valuable in the

study of porosity and sintering in ceramics. From the measurements of beam broadening as a function of neutron wave length in direct beam experiments it is possible to determine the average radius of the scatterers and their density. Figure 6 is a plot of the full width at half maximum of the scattering angle as a function of wave length λ obtained from a beam broadening experiment on a "green" compact of the ceramic $YCrO_3$ (Hardman-Rhyne et al., to be published). It can be seen that the agreement between the data and diffraction/refraction theory is excellent. An average pore radius of 0.17 Mm and a void density ratio of 0.42 was obtained from the fit of the broadening curve. This density ratio compared well with the overall density ratio of 0.43.

The extension of scattering theory to include refraction effects will permit the investigation by scattering of such features as large pores in metals and ceramics, and magnetic domains. Increased fluxes and improved instrumentation will permit the process of sintering to be followed in real time.

Polymers.

The large difference in the scattering lengths b of hydrogen and deuterium has already been mentioned ($b_H = -0.37 \times 10^{-12}$ cm vs $b_D = +0.66 \times 10^{-12}$ cm). Because of this difference, together with the fact that both hydrogen and deuterium are strong scatterers, it is possible to investigate a large number of problems in polymer configuration by means of neutron scattering. Indeed, neutron scattering has proved to be an excellent, unmatched technique for examining polymeric structures. Typically a fraction of the chains, or segments of chains in a specimen are made with deuterium in place of hydrogen. The deuterated material then is mixed with the ordinary protonated polymer. Measurements by SANS of the radius of gyration of the deuterated chains in such a mixture settled a long standing controversy regarding the molecular conformation in amorphous polymers. Are the chains arranged in random (Gaussian) coils as proposed by Flory and co-workers, or in quasi-parallel bundles? (See Allen and Petrie, 1976.) Such experiments have been extended to the intermediate q range in order to examine the local chain conformation over distances of the order of 1-10 nm.

Table III lists a number of areas of active research in polymeric structures which are being investigated by neutron scattering. Interactions in blends of polymers in which one species is deuterated are examined by SANS to determine the compatability of the constituents. Information on the morphology of two phase blends can be used to optimize processing variables. Diffusion in polymers is being measured by noting changes in scattering as a function of time and temperature from samples prepared by alternating layers of deuterated and protonated polymers (Bartels et al., 1983, to be published).

As larger neutron fluxes become available it will be of great interest to follow the dynamics of changes in chain configuration during deformation.

CONCLUSION

Because of their unique properties, cold neutrons are remarkably well suited to the investigation of a large number of problems in materials science. In many cases, neutron scattering is the only technique available which can yield the desired information. The elucidation of polymeric structures is an example par excellence of this point. Even with the current below the state-of-the-art facilities in the United States a number of experiments of the highest quality are being carried out. (Other, more demanding experiments have required the use of European laboratories.) With increased fluxes and improved instrumentation the range of problems that can be studied by neutron scattering will open up. Of especial interest will be real time studies of the dynamics of processes: precipitation, phase decomposition, polymer chain deformation, microcracking, cavity nucleation, etc., etc.

REFERENCES

Allen, G., and S. E. B. Petrie 1976. The Physical Structure of the Amorphous State. G. Allen and S. E. B. Petrie, eds. Marcel Dekker.

Bartels, C. R., W. W. Graessley, and B. Crist 1983. Measurement of self-diffusion coefficient in polymer melts by a small-angle neutron scattering method. J. Polymer Sci.: Polymer Letters Edn. 21: 495-499.

Bartels, C. R., B. Crist, and W. W. Graessley to be published. Self-diffusion coefficient in melts of linear polymers: chain length and temperature dependence for hydrogenated polybutadiene.

Berk, N. F., and K. Hardman-Rhyne 1984. Theory of multiple small angle neutron scattering from a monodisperse medium of large particles. Bull. Amer. Phys. Soc. 29: 549. Also, to be published.

Case, E. D., and C. J. Clinka 1984. Characterization of microcracks in $YCrO_3$ using small-angle neutron scattering and elasticity measurements. J. Mats. Sci. 19: in press.

Frisius, F., R. Kampmann, P. A. Beaven, and R. Wagner 1983. Influence of copper on the defect microstructure and radiation strengthening of iron. pp. 171-174 in Dimensional Stability and Mechanical Behavior of Irradiated Metals and Alloys, British Nuclear Energy Society, London.

Glinka, C. J., H. J. Prask, and C. S. Choi 1980. Neutron diffraction and small angle scattering as nondestructive probes of the microstructure of materials. Pp 143-164 in Mechanics of Nondestructive Testing, W. W. Stinchcomb, ed. New York: Plenum Press.

Hardman-Rhyne, L., N. F. Berk, and E. D. Case, to be published. Porosity of sintered and green compact $YCrO_3$ using small angle neutron scattering. Proceedings of the Symposium on NDE, Philadelphia, PA 1983. O. Buck and S. M. Wolf, eds. Metals Park, OH: American Society for Metals.

Krawitz, A. D., E. F. Drake, R. L. DeGroot, C. H. Vasel, and W. B. Yelon 1983. Neutron diffraction studies of cemented carbide composites. Pp. 973-990 in Science of Hard Materials. New York: Plenum Press.

Krawitz, A. D., R. Roberts, and J. Faber, in press. Residual stress relaxation in cemented carbide composites studied using the Argonne Intense Pulsed Neutron Source. Adv. in X-ray Analysis 27.

Odette, G. R., G. Lucas, and C. J. Glinka, work in progress. Radiation enhanced precipitation hardening in steel.

Page, R., J. R. Weertman, and M. Roth 1980. Investigation of fatigue-induced grain boundary cavitation by small angle neutron scattering. Scripta metall. 14: 773-777.

Page, R., J. R. Weertman, and M. Roth 1982. Small angle neutron scattering study of fatigue induced grain boundary cavities. Acta metall. 30: 1357-1366.

Page, R. A., and J. Lankford 1983. Charactrization of creep cavitation in lucalox alumina by small angle neutron scattering. J. Am. Cer. Soc. 66: C-146-148.

Page, R. A., J. Lankford, and S. Spooner in press a. Nucleation and early-stage growth of creep cavities in hot-pressed silicon carbide. Acta metall.

Page, R. A., J. Lankford, and S. Spooner in press b. Small-angle neutron scattering study of creep cavity nucleation and growth in sintered alumina. J. Mats. Sci.

Prask, H. J., and C. S. Choi to be published. NDE of residual stress in uranium bymeans of neutron diffraction.

Schmank, M. J., and A. D. Krawitz 1982. Measurement of a stress gradient through the bulk of an aluminum alloy using neutrons. Metall. Trans. A 13A: 1069-1076.

Weertman, J. R. 1981. Identification by small angle neutron scattering of microstructural changes in metals and alloys. Pp. 147-168 in Nondestructive Evaluation: Microstructural Characterization and Reliability Strategies, O. Buck and S. M. Wolf, eds. Warrendale, PA: The Metallurgical Society of AIME.

Yang, M., J. R. Weertman, and M. Roth 1984a. Use of small angle neutron scattering to study grain boundary cavitation. Pp.149-156 in Proceedings of the Second International Conference on Creep and Fracture of Engineering Materials and Structures, B. Wilshire and D. R. J. Owen, eds. Swansea, UK: Pineridge Press.

Yang, M. S., J. R. Weertman, and M. Roth 1984b. A test of grain boundary void growth theories by small angle neutron scattering. Scripta metall. 18: 543-548.

Yang, M. S., J. R. Weertman, and M. Roth in press. Small angle neutron scattering studies of microstructural changes in copper deformed at elevated temperatures. Fifth Risø International Symposium on Metallurgy and Materials Science, 3-7 September 1984, Roskilde, Denmark.

TABLE I.

UNIQUE FEATURES OF NEUTRONS IN MATERIALS SCIENCE RESEARCH

- Penetration depth in mm's
  - properties measured as function of (x,y,z)
  - survey over many grains
  - distortion caused by surface minimized
  - large features can be measured (refraction)
  - NDE capabilities
- Scattering length
  - not monotonic function of atomic number
  - many light elements are good scatterers (H vs D)
- Magnetic information
  - magnetic structure
  - additional information: perpendicular, parallel to H
  - direct determination of position of nucleus

TABLE II

TOPICS IN MATERIALS SCIENCE AND ENGINEERING WHICH HAVE BEEN STUDIED BY NEUTRON SCATTERING

- Damage accumulation
  - cavitation
  - microcracking
  - microstructural degradation
  - radiation damage
  - stress/strain changes
- Residual stress, texture
- Phase transformations
- Porosity (sintering)
- Polymers, colloids, micelles
- Amorphous metals, short range order
- Materials processing

TABLE III

ACTIVE AREAS OF RESEARCH IN POLYMER STRUCTURES

- Polymer-polymer interactions in blends
  - compatibility
  - morphology of second phase
  - optimize processing
- Diffusion of polymers
- Colloidal systems
- Micelles
- Response to deformation
  - individual chains
  - crystalline polymers

FIGURE CAPTIONS

Figure 1. Development of void volume fraction with increasing fatigue time in copper subjected to fully reversed fatigue (from Page et al., 1982)

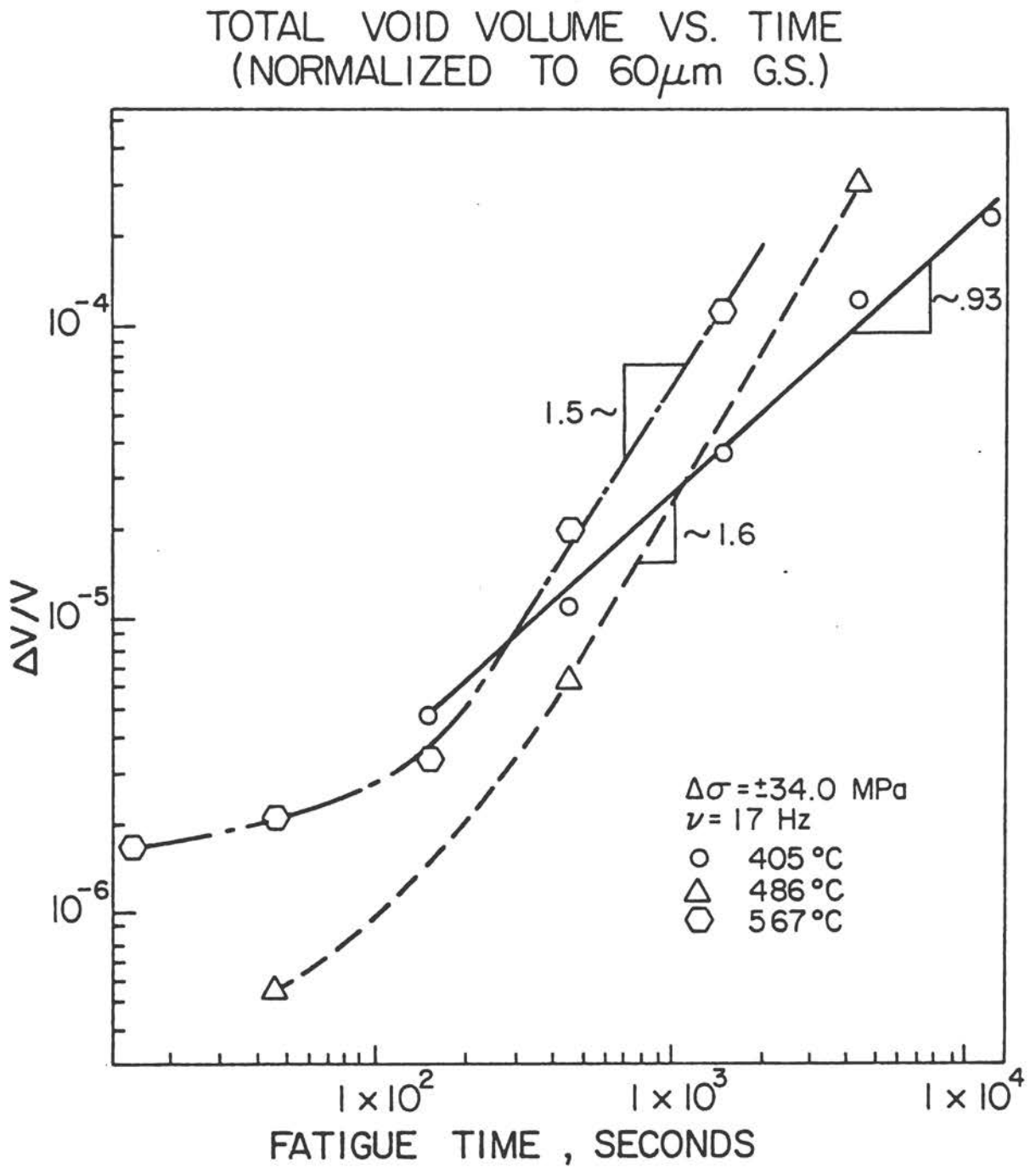
Figure 2. Size distribution curves of creep cavities measured directly by SANS (curves A), or modeled using data obtained from the SANS measurements together with various theories of void growth (curves B, C, D). (Taken from Yang et al., 1984b.)

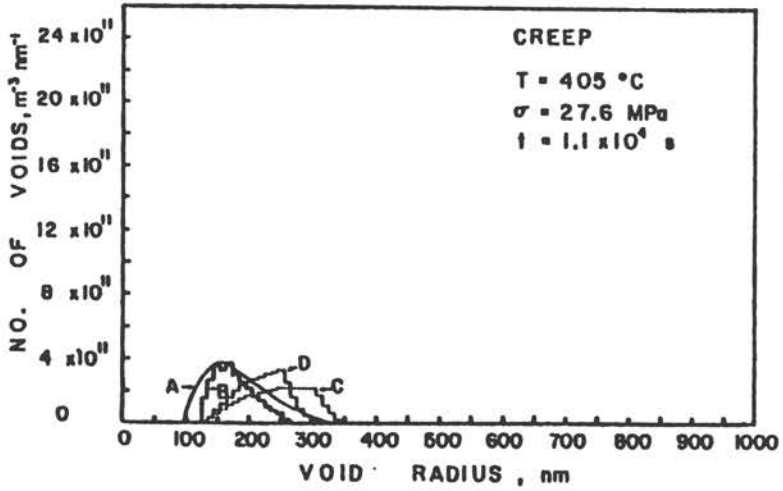
Figure 3. Curve of scattering intensity vs scattering vector for $YCrO_3$ containing microcracks. Data points are from SANS measurements. The curve is a least-square fit to the data of the scattering function for randomly oriented thin disks of thickness 2H (Case and Glinka, 1984).

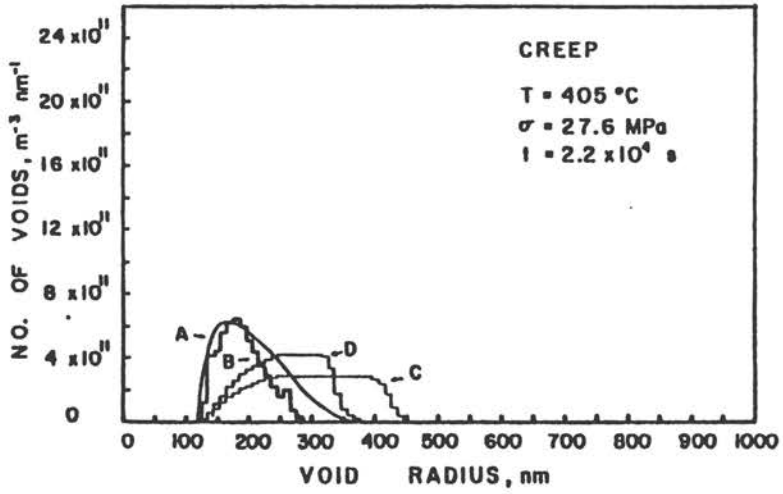
Figure 4. Experimental arrangement for SANS measurement of a ferromagnetic material.

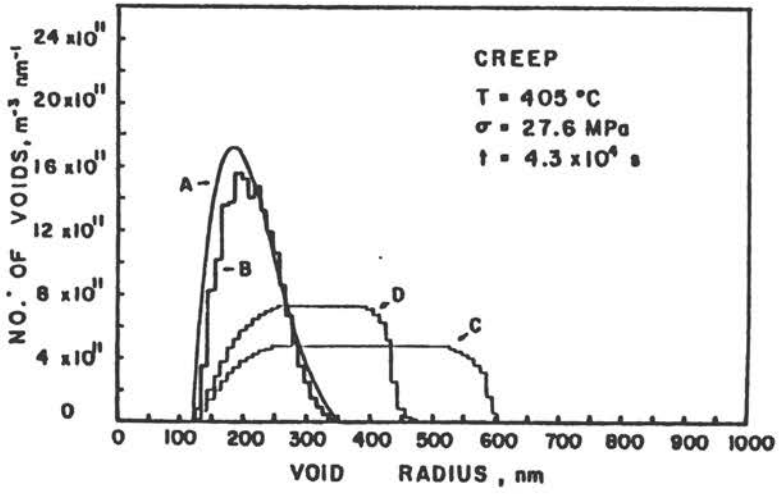
Figure 5. Slit arrangement to allow SANS measurements to be made over a small defined region of a specimen (from Prask and Choi, to be published).

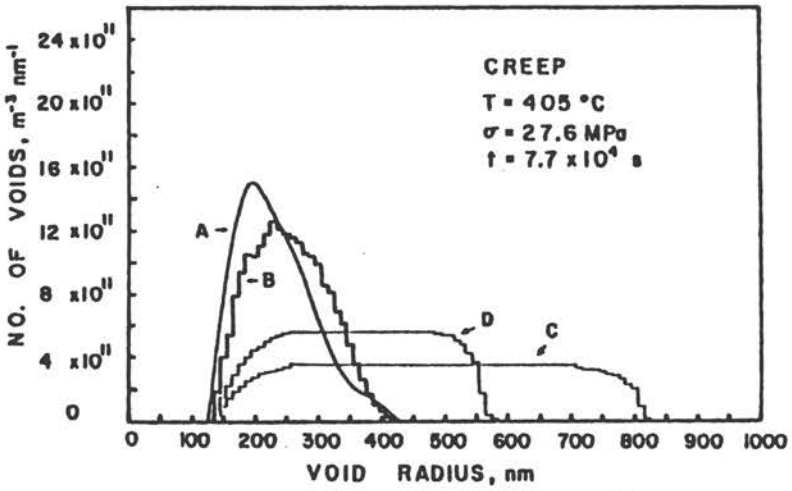
Figure 6. Curve of the full width at half maximum (in radians) as a function of neutron wave length for voids in a "green" compact of $YCrO_3$. Squares are data points and circles are values calculated from theory (from Hardman-Rhyne et al, to be published).

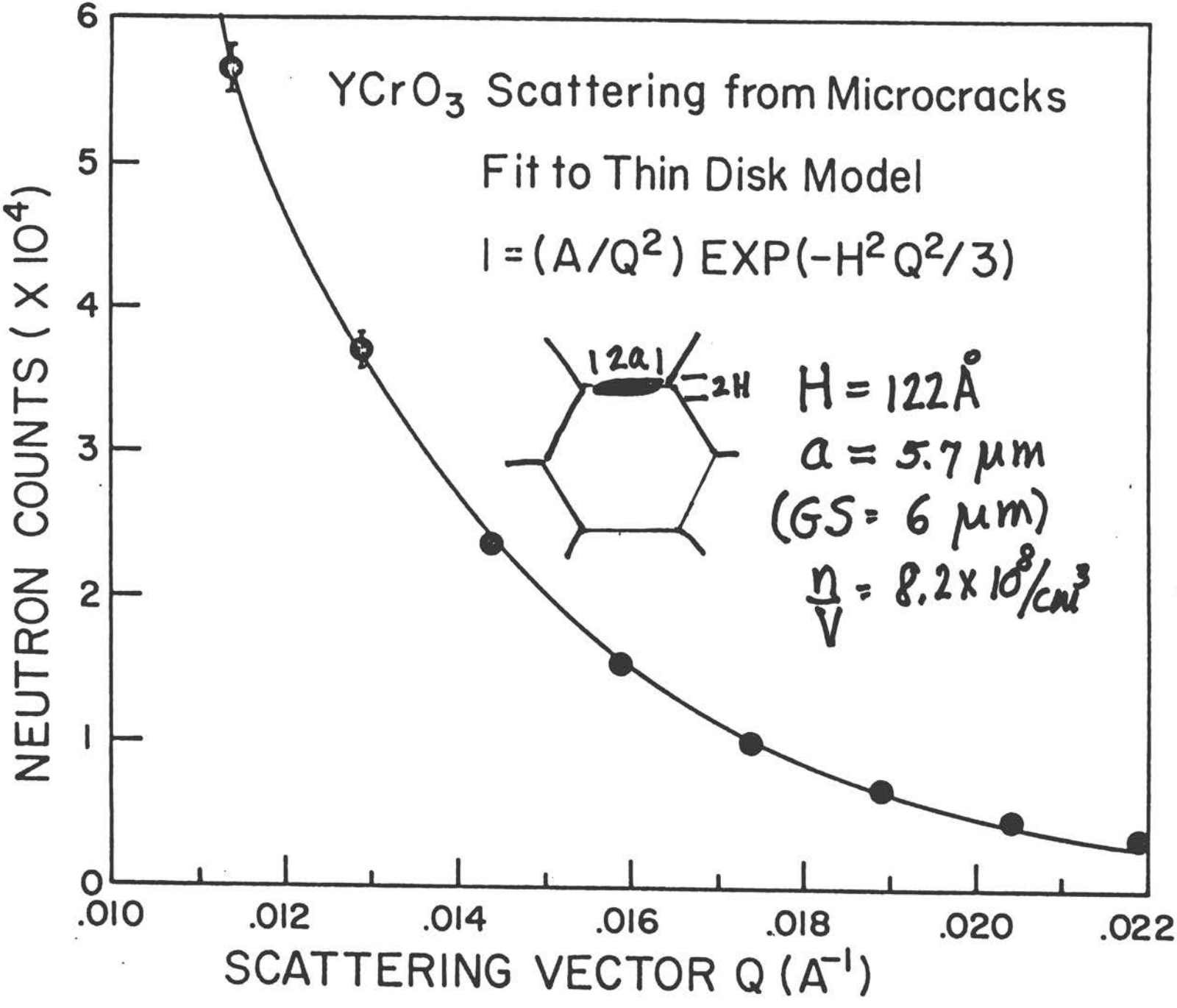

TOTAL VOID VOLUME VS. TIME
(NORMALIZED TO 60μm G.S.)
ΔV/V
10^-4
10^-5
10^-6
1.5~
~1.6
~.93
Δσ=±34.0 MPa
ν=17 Hz
405°C
486°C
567°C
1×10^2
1×10^3
1×10^4
FATIGUE TIME, SECONDS

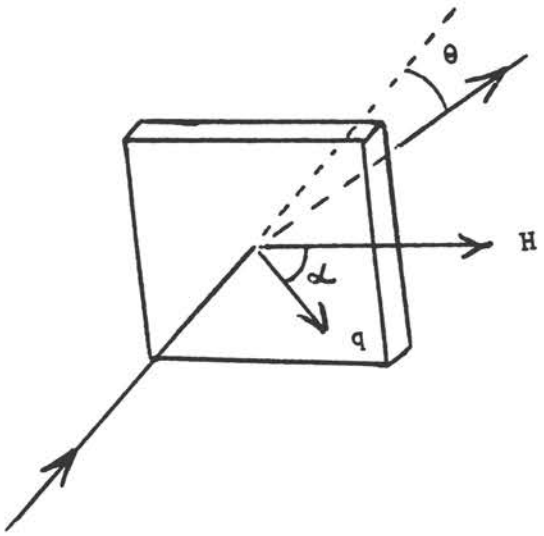

CREEP
T = 405 °C
σ = 27.6 MPa
t = 1.1 x10⁴ s
NO. OF VOIDS, m⁻³ nm⁻¹
VOID RADIUS , nm
A
B
C
D

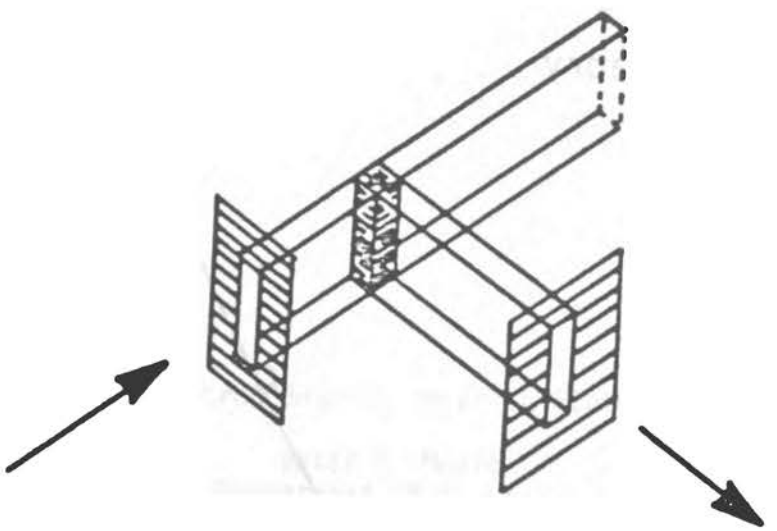

CREEP
T = 405 °C
σ = 27.6 MPa
t = 2.2 x10⁴ s
NO. OF VOIDS, m⁻³ nm⁻¹
VOID RADIUS, nm
A
B
C
D

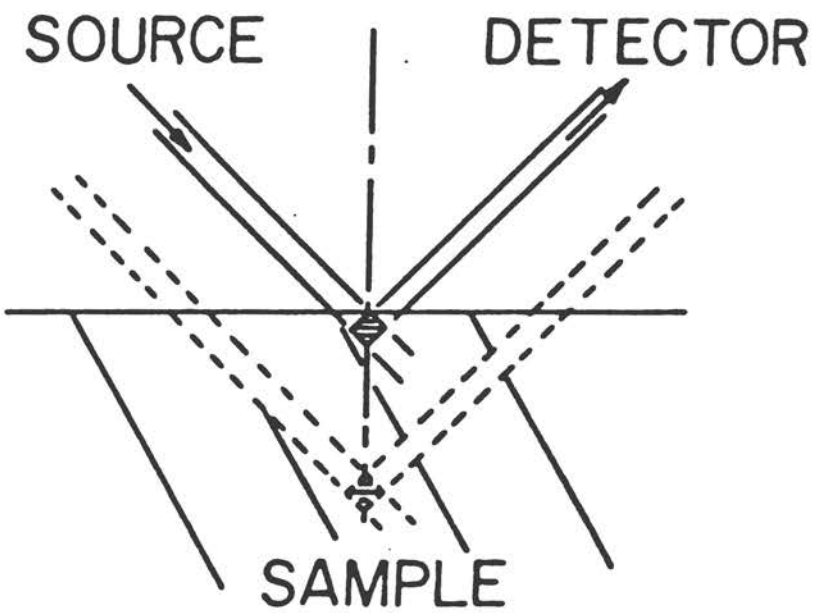

CREEP
T = 405 °C
σ = 27.6 MPa
t = 4.3 x10⁴ s
NO. OF VOIDS, m⁻³ nm⁻¹
VOID RADIUS , nm
A
B
C
D

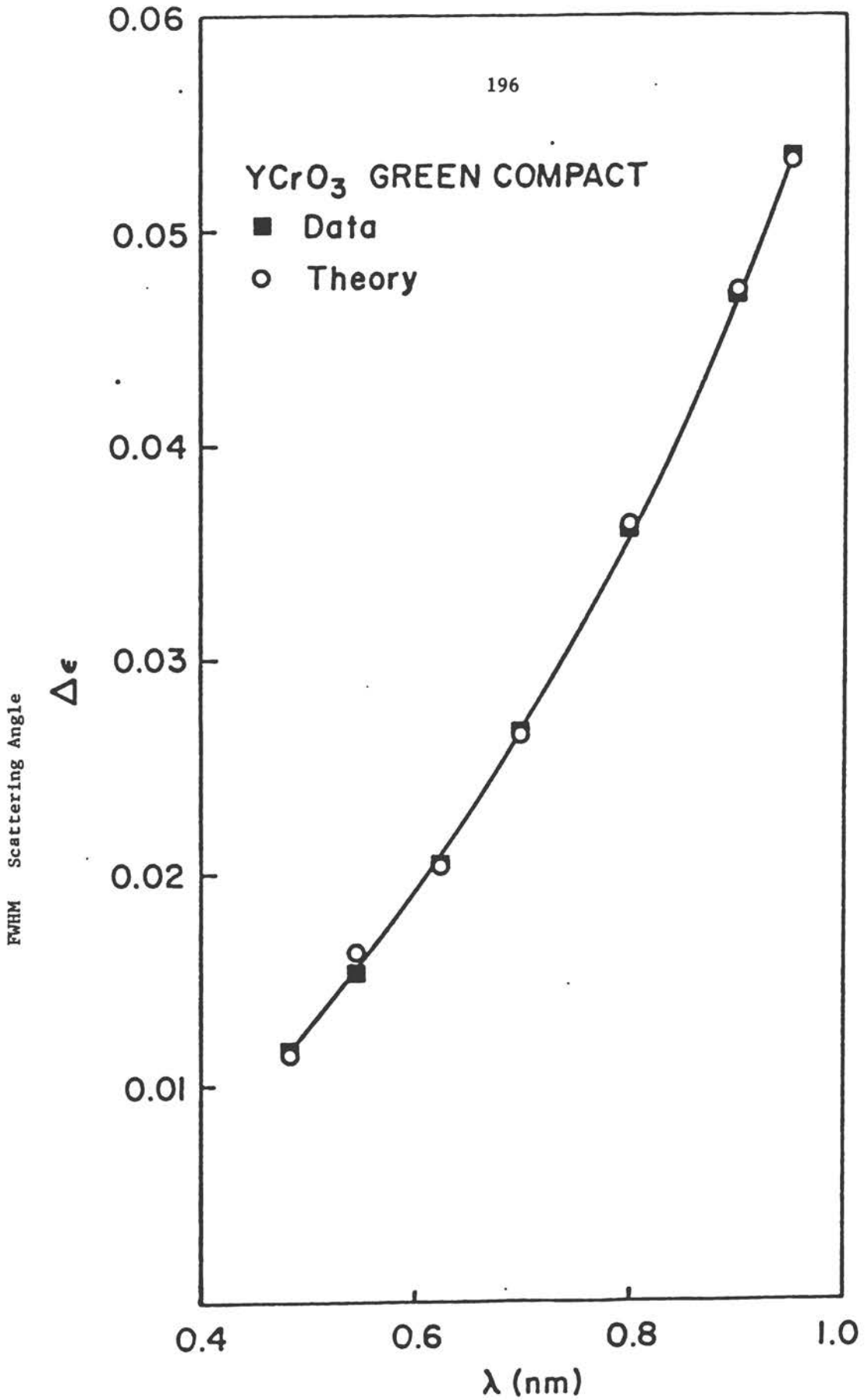

CREEP
T = 405 °C
σ = 27.6 MPa
t = 7.7 x10⁴ s
NO. OF VOIDS, m⁻³ nm⁻¹
VOID RADIUS, nm
A
B
C
D


YCrO3 Scattering from Microcracks
Fit to Thin Disk Model
I = (A/Q²) EXP(-H²Q²/3)
12a1
2H
H = 122Å
a = 5.7 μm
(GS = 6 μm)
n/V = 8.2 x 10⁸/cm³
NEUTRON COUNTS (X 10⁴)
SCATTERING VECTOR Q (A⁻¹)
0
1
2
3
4
5
6
.010
.012
.014
.016
.018
.020
.022


θ
H
α
q




SOURCE
DETECTOR
SAMPLE


YCrO3 GREEN COMPACT
Data
Theory
0.06
0.05
0.04
0.03
0.02
0.01
Δε
FWHM Scattering Angle
0.4
0.6
0.8
1.0
λ (nm)

Application of Neutron Beam Research in Biology and Medicine

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Introduction

The report which follows is an edited version of remarks made to the Committee on Major Materials Facilities in Washington, D.C., April 17, 1984. The purpose of the presentation was to give the Committee a brief summary of the contributions neutron science has made to biology and medicine, and a prediction of the directions this work is likely to take in the future. Brief summaries are difficult to make; the emphases given different areas, not to speak of the omissions made for brevity's sake, are matters of personal evaluation and liable to criticism. Furthermore, history shows that the future deals harshly with scientists foolish enough to try to predict it. Indeed, any field of science whose future is predictable is a disappointing one.

Those wishing to read further, and form independent judgements will find two published symposium proceedings of great value, one which appeared in 1976 (Schoenborn, 1976), and the second in 1984 (Schoenborn, 1984). No attempt will be made below to provide exhaustive references for all the points made; only a few key references will be provided in each case. The symposia give all the depth of coverage one might require.

Medical Applications. It is perhaps easiest to begin this discussion by a consideration of medical applications of neutrons, a field very much in its infancy. Clinical investigators have made little use of neutron beam facilities so far. Some thought has been given to the design of drugs which will concentrate in specific organs of a live animal, carrying with them elements with high neutron absorption cross sections. Bombardment of these organs with a neutron beam following uptake of the drug could produce a localized dose of ionizing radiation which would be of value in cancer therapy. Much remains to be done before the utility of such enterprises can be evaluated.

(In the discussions which followed the verbal presentation of this report, the author was reminded that high flux reactors, which have been the main sources of neutron beams for the research community, are also used to generate radioisotopes. While these substances may appear to one who works with beams to be incidental byproducts of ongoing activities, their importance to biology and medicine cannot be overstated. The introduction of radioisotopes into biochemistry in the 1940's accelerated its progress by revolutionizing one's ability to detect processes occuring at low levels; biochemistry without them is virtually inconceivable today. A wide variety of therapeutic and diagnostic techniques based on radioisotopes are in routine use in hospitals around the world, and there is a substantial commerce in the manufacture and sale of radioisotopically labelled compounds for biomedical purposes. If any biomedical application of neutron generating facilities can alone justify their construction and operation, this is it.)

Structure in Biology. The primary use of neutron beams in biology to date has been as an experimental tool for determination of structure.

Three dimensional structure has always been a central concern of biologists. They pursue it at many levels, ranging from the gross morphology of extinct reptiles to the determination of the placement of methyl groups in proteins. On occassion the results of structural investigations have had momentous impact on the development of biology. A case in point would be the discovery of the structure of DNA, an event which launched the science of molecular biology into an orbit from which it has yet to descend.

Because structure is so important to biology, it will always be true that any time the physical and chemical communities develop a new way of studing it there will be a few biologically inclined scientists interested in finding out what the new method can do for them. So it was that in the mid-1960's, when the current generation of high flux beam reactors were being commissioned or built, that a few biophysical chemists asked for, and were given access to beam time and instrumentation. The literature produced by these pioneers and their followers over the past 15 years, is our best guide to what neutrons can do for biology.

The Relationship of Neutron Beams and Biological Structure. Typical thermal neutron sources generate neutron beams of useful flux between about 1A and 10A in wavelength. Using radiation in this wavelength range, one can study the structures of objects having maximum linear dimensions as large as 500A, the size of some viruses and macromolecular aggregates. Provided the material of interest crystallizes appropriately, a neutron study can lead to a description of its structure at atomic resolution.

Both in terms of the resolution achievable and the size range of objects accessible, there is a strong overlap between the capability of x-rays and of neutrons. Moreover, biologists have a second technique available for studying the structure of objects on the large size of this range, electron microscopy. Both conventional x-ray generators and electron microscopes are trivially cheap compared to the instrumentation needed to produce and utilize neutron beams. Why should biologists study structures with neutrons when cheaper more convenient alternatives exist?

Why Neutrons? The justification for what might seem at first glance an outrageous extravagence, the study of biological structure using neutrons, is contained in a single word, "hydrogen." Biological neutron experiments are done for two purposes only. They are done at high resolution to determine the placement of hydrogen atoms in biological molecules and, at lower resolution, they are done to exploit in one way or another the sensitivity of neutron radiation to the difference between hydrogen and deuterium to discover the location of components in large structures.

Hydrogen. The end product of an x-ray crystallographer's work is a description of a molecule in terms of an electron density map. Hydrogen, having only a single electron, is never conspicuous in such maps. Even in a well-determined, small molecule structure the placement of hydrogens is subject to substantial error. Unfortunately the electron density maps obtained in x-ray crystallographic studies of biological macromolecules seldom have the resolution or the favorable ratio of data measured to parameters determined characteristic of small molecule electron density maps. In such low quality electron density maps, hydrogen simply disappears.

Table I compares the scattering lengths of atoms of biological significance for both x-rays and neutrons. While scattering lengths for x-rays are proportional to atomic number making C, N and O far more conspicuous than H, in the neutron case, the magnitude of ^{1}H's scattering length is within a factor of 2 of other atoms. The negative sign of its scattering length implies that the neutron wave produced by scattering from ^{1}H is 180° out of phase with respect to the wave produced when a C, for example, scatters a neutron from the same location in space. Thus in a neutron scattering length density map

of a molecule, ^1H will appear as a negative hole while other atoms are represented as positive peaks. Negative or not, however, ^1H will be detected more easily in a neutron experiment than in an x-ray one and ^1H is visible in the (relatively) low quality maps produced when macromolecular crystals are solved by neutron techniques.

A second point which emerges from Table I is the striking difference in scattering length between ^1H and ^2H. The former is negative while the latter is positive. If ^1H is substituted by ^2H, at high resolution, all the ^1H scattering length density holes will be replaced by positive peaks. In the context of low resolution experiments it should be born in mind that most biological materials contain more hydrogen atoms than all other atomic species put together. Thus very strong perturbations in the total scattering length of a biomolecule can be achieved by ^2H labelling. Only modest alterations in the chemical properties of the substances accompany ^2H labelling. Indeed, there is no other combination of labelling method and radiation choice which achieves so much at so little cost to the integrity of the material under study. We shall see what use can be made of this fact below.

The Motivations for High Resolution Studies. Perhaps the major objective of those who started biological work with neutrons in the late 1960's was the determination of the crystal structures of proteins at as high resolution as possible. A number of issues stimulated this interest. The first had to do with hydrogen bonds. The three dimensional structure of proteins is stabilized in part by hydrogen bonding. (For overviews of protein structure see; Cold Spring Harbor Symposia on Quantitative Biology, V 36, 1972; Schulz and Schirmer, 1979.) It is, in fact, an embarrassment for the x-ray derived protein structures that hydrogen bonds are not observed directly because of the invisibility of the shared hydrogen atoms. The existence of these bonds is inferred from the proximity of appropriate donor and acceptor groups. In a neutron study, these interactions are directly observable. Ability to visualize hydrogen bonds directly was also attractive for those interested in enzyme mechanism, as opposed to structure as such, because the catalytic configurations of these molecules commonly involve complex hydrogen-bonded networks, and alterations in proton chemistry often accompany enzyme action.

A second issue, closely related to the first, had to do with solvent structure. It has been known for a long time that the water which immediately surrounds a macromolecule in solution has properties which distinguish it from bulk solvent. Since solvation is believed to be an important influence in the folding of macromolecules, one wanted to see how water is structured around the surfaces of biological macromolecules in detail. In an x-ray structure, such water is observable because O is visible. The problem is that these solvent structures are seldom perfectly ordered, and many H_2O sites commonly have occupancies less than one, as one might anticipate. At some point in the analysis there comes a stage where it is difficult to distinguish a partially occupied, single atom water position from noise in the map. In a neutron map, all three atoms in H_2O can be seen and the shape of the molecule helps distinguish it from noise.

A third reason for solving protein structures at high resolution was discovered by accident, I suspect. Biological molecules contain a lot of H and most prefer to exist in aqueous media which are also hydrogen rich. The

presence of so much hydrogen brings with it a burden. In addition to having a reasonably large coherent scattering length, hydrogen also has an exceptionally large incoherent cross-section (Bacon, 1975). Hydrogen incoherent scatter contributes a large background to any scattering or diffraction measurement which might be done on samples containing it. In addition, its presence effectively limits the permissible thickness of biological specimens to a few mm. A simple expedient which alleviates both problems is to replace ^1H_2O in the solvent with ^2H_2O.

An interesting process begins as soon as the solvent is changed to ^2H_2O. Many of the protons in biological molecules are chemically labile, and these begin exchanging with ^2H. What is observed is that not all groups chemically capable of exchange succeed in doing so; some are protected from exchange by their position in the molecule.

The pattern of protection is far more interesting than that expected from simple steric hindrance considerations based on the molecular structure (e.g. Wlodawer and Sjolin, 1982). Some groups apparently well protected from solvent exchange; others do not. Thus what is discovered from the exchange pattern is evidence about the dynamic properties of the molecule since flexibility is clearly required to permit exchange of interior groups. Neutron data collected in ^2H_2O readily distinguishes exchanged from unexchanged sites and thus gives valuable data on the long time limit of the exchange process.

There are a number of other techniques which are used to get information on these processes. Tritium exchange experiments have been done for years (Woodward and Hilton, 1979). While tritium exchange can give good kinetic data, it is hard to discover which groups are exchanging by this method (e.g. Rosa and Richards, 1981). NMR can also be used for studies of this kind. For smallish macromolecules (MW 10,000) where assignments can be made, NMR can identify the slowly exchanging groups and measure their exchange rates (e.g. Wagner & Wuthrich, 1979). The neutron method is not size limited like the NMR technique, but presently gives no kinetic data.

The fourth and final motivation came from the recognition that one might be able to distinguish O and N in a neutron map (see Table I). These are a number of residues in protein, like asparagine, which terminate in amides. In an x-ray map it is hard to distinguish the carbonyl side of an amide group from its amine side. The difference between N and O is larger in a neutron experiment than in its x-ray counterpart and so the distinction can be made, and the groups correctly placed in space.

Protein Crystallography. In the early days it was hard to collect neutron data from protein crystals. Neutron sources produce beams of low flux, and so, in order to get appreciable data collection rates, one selected proteins for study which would form very large crystals. Myoglobin was studied in the early days using a crystal of 24 mm^3 in volume, which is exceptional for a protein crystal (Norvell and Schoenborn, 1976). One was trying to compensate for the low flux by placing large crystals in the beam. Substantial progress has been made in the techniques used for protein data collection, which has reduced the need for exceptionally large crystals, and hence broadened the range of problems which can be approached. A crystal 1 mm^3 in volume will yield useful data in an acceptable length of time today.

(An interesting feature of neutron crystallography is that neutrons, unlike x-rays, don't damage crystals because their energies are only kT, much too little to rupture chemical bonds. Crystals last "forever" in a neutron beam.)

About six proteins have been studied by neutron crystallography at Brookhaven, the National Bureau of Standards and the Institute Lae u-Langevin (see Schoenborn, 1984). What is clear from the data published so far is that all the promises and hopes which led to the development of this field are going to be fulfilled. But what is also evident is that the exchange properties and solvent structures evident in the protein examined so far are so diverse that it is hard to deduce any general principles. We are going to have to see more examples. It is also clear that it would be interesting to attempt to measure exchange kinetics. Perhaps using cryogenic methods and higher flux sources it would be possible to get some data of this kind.

It should be noted that no one has developed methods for solving macromolecular structures using neutron data alone. Only those protein crystals are studied by neutrons which have already been solved using x-rays. The neutron structure is derived by a refinement. Neutron analysis is, in fact, a method for extending the scientific impact of having solved a protein crystal structure by x-ray methods. It is an "end game" technique, and the justification for it is that the x-ray problem still takes man-years to solve. A few months of data collection on a neutron spectrometer, followed by some computation, is cheap compared to the investment necessary to get the x-ray structure in the first place, and the extra information gained is substantial.

There will undoubtedly be a steady flow of biochemists bringing protein crystals to reactors in the future motivated by issues such as the one described above. One hope is that a nucleic acid crystal will be attempted soon. Nucleic acids are densely charged polyelectrolytes and the surrounding solvent region may be quite interesting.

Low Resolution Studies. In my mind there is little doubt that the results which are obtained using neutrons crystallographically will in the long run be the most significant contribution of neutron research to biology. Nevertheless, as you examine the literature of the past 15 years, for every crystallographic paper there have been 10 or more describing the use of neutrons to study structures at much lower resolution. All of these experiments exploit the ^{1}H - ^{2}H difference in one way or another.

In a low resolution experiment, by definition, individual atoms are not visualized. What is of interest are not the scattering lengths of individual atoms but bulk, average scattering properties, which can be conveniently characterized in terms of scattering length densities. A few scattering length densities for substances of biological interest are given in Table II. H_2O has a scattering length density close to zero; its two hydrogens ($b = -0.374 \times 10^{-12}$ cm) just about cancel out the positive contribution ($b = +.667 \times 10^{-12}$ cm) due to its oxygen. The scattering length density of $^{2}H_2O$, on the other hand, is strongly positive because the negative contributions of the hydrogens have been replaced with positive scattering lengths due to deuterium You will notice that the different biological materials differ in scattering length density. These differences reflect the relative abundances of hydrogen in these substances. In every case perdeuteration produces striking increases in scattering length density.

Many biological objects are composites consisting of two different chemical species and hence varying significantly in scattering length density within their volumes. One can obtain low resolution information on the disposition of the two materials in such a structure by the now classical solution scattering method called "contrast variation" (Stuhrmann, 1982). In effect, by adding D_2O to the H_2O solvent in which the structure is dissolved one can arrange it so that the difference in scattering length density (the contrast) between one of the components and the solvent is zero. In this solvent, the unmatched component will dominate the scatter, and information can be gained about its size and shape, etc. Reversal of the contrast to match the second component will yield comparable information about the first.

Contrast variation experiments are easy to implement biochemically and data collection is straight forward. Large numbers of such experiments have been reported. Among the successes achieved by this method one would have to count the studies done on nucleosomes (Pardon et al., 1977; Suau et al., 1976). Nucleosomes, which consist of DNA and protein, are the unit of structure in chromosomes. The neutron contrast variation work done on this material led to a low resolution model for its structure which has now been confirmed crystallographically (Klug, 1983).

Contrast variation has also been done on viruses. Viruses cyrstallize and the structures of some are now known at high resolution (see Rossmann et al., 1983). The problem with these structures is that what is crystallizing is their outter protein coats. The nucleic acid they contain is not ordered with respect to the coat, and so while the crystal structures in hand are very informative about the protein coat, they tell us next to nothing about the placement of the nucleic acid. The technique of contrast variation has been used to get (low resolution) information on this point (see Cusak, 1984). Contrast variation has also been helpful in the analysis of the structures of lipid bilayers containing protein.

An application of contrast variation which is particularly intriguing has been explored by Zaccai and Jacrot at I.L.L. They have been doing contrast variation studies on tRNA and have strong evidence for the existence of an electrostricted layer of water around these molecules (Li et al., 1983).

Experiments Based on Specific Deuteration. At the risk of being accused of personal bias, let me say that the most elegant low resolution neutron experiments are those involving direct deuteration of the object under investigation. Localized deuteration experiments are low resolution analogues of the isomorphous replacement experiments which are used to phase macromolecular crystal data. The result of the analysis of isomorphous replacement data in an x-ray experiment is determination of the placement of a heavy atom in a crystal. In the low resolution neutron case the atoms whose positions are determined are the deuteriums used as label.

A number of incisive experiments have been done in this way. Among them one would certainly include the series of experiments done to position lipid molecules in membrane bilayers (see Buldt, 1984). In this case bilayers were formed from lipids chemically labelled with ^2H at specific positions. The perturbation in bilayer diffraction caused by the ^2H incorporated into them revealed the locations of the deuterated position of the lipid molecules in the structure.

Several macromolecular aggregates have been, or are being now investigated by specific deuteration methods to determine the position of macromolecular subunits within these structures. A full study has been completed on RNA polymerase, a five subunit structure from E. coli (Stoechel et al., 1979). The 30S ribosomal subunit from E. coli, containing 22 macromolecular components, is being studied by similar methods; 15 of its components have been located (Ramakrishnan et al., 1984). The 50S subunit of the ribosome is being examined as well in a set of experiments just getting underway at I.L.L. Nierhaus et al., 1983).

The production of appropriately labelled samples for experiments of this kind places heavy demands on biochemical technology. A specific deuteration experiment is typically 95% sample preparation, and 5% data collection and analysis. The number of structures known well enough biochemically to permit the production of suitable amounts of appropriately labelled material is small at the present time. There s a "learning curve" connected with the preparation and manipulation of any biochemical system, however. So it is reasonable to anticipate that as time goes on, more and more structurally interesting systems will get to the stage where the kind of information specific deuteration experiments can give is interesting, and the technical means of doing the work are in hand.

While counterparts to many of these experiments can be thought of in the context of electron microscopy or x-ray scattering, and some have been attempted, none work as well as their neutron cousins. These are experiments where the peculiar properties of neutron radiation happen to fit the biological problem particularly well.

Inelastic Scattering. In the past few years some work has begun on inelastic scattering from biological polymers (see Engelman et al., Middendorf et al., 1984). Very little experience has been gained so far; the data acquisition rates possible with biological materials are slow, and the competing demands for time on the few existing instruments suited for such work have limited what the biologists could do.

What is clear from the data is that proteins have inelastic modes that correspond to whole molecule vibrations and that these low frequency modes respond in interesting ways to biologically significant alterations in molecular state, such as substrate binding. It is unclear how this field will develop; the spectra are seriously overlapped and assignment is going to be very difficult. There is, however, a connection between these kind of measurements and the theoretical area of molecular dynamics. A lot of effort has been made in the past decade to simulate the dynamic properties of proteins and nucleic acids computationally. These calculations in effect predict the inelastic spectra biological macromolecules should have. A comparison of theory with data in this area would be extremely helpful.

Summary and Conclusions. There is no doubt that neutron beams have proven useful tools for biophysical chemists in the last decade and a half. In evaluating the progress to date it should be born in mind that the total number of beam lines used for biological work in the whole world over this period has never been greater than about 6, and that many of these have been shared with scientists working in other disciplines. The effort has been limited in its size, as perhaps it should have been in view of its

status as a field attempting to prove its scientific right to resources. In view of these limited resources, the level of acheivement has been gratifying.

It is fair to conclude that there is a future for neutron beam studies of biological materials. At the very least, there should be a continuing market for data of the kinds obtainable from the experimental approaches already in use. One can hope, and, indeed, anticipate the development of new ways for exploiting neutrons to characterize biological materials. It is reasonable, therefore, to plan future neutron beam facilities with biological users in mind. They will form part of the constituency which justifies such facilities.

In thinking about neutron facilities one should not lose sight of the fact that most biological experiments are limited by data acquisition rate. Data rate is dependent not only on the characteristics of the source, but on how well the neutrons it generates are utilized. The dominance of I.L.L. in small angle neutron work does not arise from exceptionally high flux in its reactor, although its flux is excellent, to be sure, but from the efficiency with which neutrons are delivered to the counter at the D-11 small angle station. Instrument design should be given the same level of thought and support as the design of the source itself.

References

1. Bacon, G.E. 1975. Neutron diffraction. 3rd Edition, London: Oxford University Press.

2. Büldt, G. 1984. Specific deuteration and membrane structure. op cit 16 pp. 189-199.

3. Cusack, S. 1984. Neutron scattering studies of virus structure. op cit 16 pp 173-187.

4. Engelman, D.M. and P.B. Moore. 1975. Determination of quaternary structure by small angle neutron scattering. Ann. Rev. Biophys. Bioengin. 4: 219-241.

5. Engelman, D.M., A.J. Dianoux, S. Cusack and B. Jacrot. 1984. Inelastic neutron scattering studies of hexokinase. op cit 16 pp. 365-380.

6. Klug, A. 1983. Nucleosome structure & chromatin superstructure. pp. 91-112 in Nucleic Acid Research, K. Mizobucki, I. Watanabe and J.D. Watson, eds., Tokyo: Academic Press.

7. Li, Z.Q., R. Giege, B. Jacrot, R. Oberthür, J.-C. Thierry and G. Zaccai. 1983. Structure of phenylalanine-accepting transfer ribonucleic acid and of its environment in aqueous solvents with different salts. Biochemistry 22:4380-4388.

8. Middendorf, H.D., J.T. Randall and H.L. Crespi. 1984. Neutron spectroscopy of hydrogenous and biosynthetically deuterated proteins. op cit 16 pp. 281-400.

9. Nierhaus, K.H., R. Lietzke, R.P. May, V. Nowotny, H. Schulze, K. Simpson, P. Wurrnbach and H.B. Stuhrmann. 1983. Shape determination of ribosomal proteins *in situ*. Proc. Natl. Acad. Sci. USA 80:2889-2893.

10. Norvell, J.C. and B.P. Schoenborn. 1976. The structure of carbon monoxide myoglobin: real space refinement. Op cit 15, pp II-12-II-21.

11. Pardon, J.F., D.L. Worcester,J.C. Wooley, P.I. Cotter, D.M.J. Lilley, and D.M. Richards. The structure of the chromatin core particle in solution. Nucleic Acids Res. 4:3199.

12. Ramakrishnan, V.R., M. Capel, M. Kjeldgaard, D.M. Engelman and P.B. Moore. 1984. Positions of proteins S14, S18 and S20 in the 30S ribosomalsubunit of *E. coli*. J. Mol. Biol. 174:000-000

13. Rosa, J. and R.M. Richards. 1981. Hydrogen exchange from identified regions of the S-protein component of ribonuclease as a function of temperature, pH and the binding of S-peptide. J. Mol. Biol. 145:835-851.

14. Rossman, M.G., C. Abad-Zapatero, M.A. Hermodson, and J.W. Erickson. 1983. Subunit interactions in southern beam mosaic virus. J. Mol. Biol. 166:37-83.

15. Schoenborn, B.P. 1976. Neutron scattering for the analysis of biological structures. Brookhaven Symposia in Biology 27, Brookhaven National Laboratory, Upton L.I., NY (BNL 50453).

16. Schoenborn, B.P. 1984. Neutrons in biology. Proceedings of the 32nd Brookhaven Symposia in Biology. Basic Life Sciences V 27, Hollander, A., genrl. ed. New York:Plenum Press.

17. Schulz, G.E. and R.H.Schirmer. 1979. Principles of protein structure. New York: Springer Verlag.

18. Stoeckel, P., R. May, I. Strell, Z. Geha, W. Hoppe, H. Henmann, W. Zillig and H.L. Crespi. 1979. Determination of intersubunit distances and subunit shape parameters in DNA-dependent RNA polymerase by neutron small-angle scattering. J. Appl. Crystallogr. 12:176-185.

19. Stuhrmann, H.B. 1982. Contrast Variation. pp. 197-214 in Small Angle X-ray Scattering, O. Glatter and O. Kratky, eds., London: Academic Press.

20. Suau, P., G.G. Kneale, G.W. Braddock, J.P. Baldwin and E.M. Bradbury. 1977. A low resolution model for the chromatin cor particle by neutron scattering. Nucleic Acids Res. 4:3769-3786.

21. Wagner, G. and K. Wüthrich. 1979. Correlation between the proton exchange rates and the denaturation temperatures in globular proteins related to the basic pancreatic trypsin inhibitor. J. Mol. Biol. 130:31-37.

22. Wlodawer, A. and L. Sjolin. 1982. Hydrogen exchange in RNase A: neutron diffraction study. Proc. Nat. Acad. Sci. USA 79:1418-1422.

23. Woodward, C.K. and B.D. Hilton. 1979. Hydrogen exchange kinetics and internal ot in proteins and nucleic acids. Ann. Rev. Biophys. Bioengin. 8: 99-127.

Table I. Scattering Lengths of Biologically Important Elements and Isotopes for Neutrons and X-rays.

	Neutrons ($b \times 10^{12}$ cm)	X-rays ($b \times 10^{12}$ cm)*
^{1}H	-0.374	0.28
^{2}H	+0.667	0.28
C	+0.665	1.69
N	+0.94	1.97
O	+0.58	2.25
P	+0.51	4.23
S	+0.28	4.50

*X-ray scattering lengths are given for a scattering angle of zero.
[Data taken from Bacon (1975).]

Table II. Average Scattering Length Densities for Selected Biological Materials.

Substance	^{1}H substituted	^{2}H substituted
H_2O	-0.55	+6.36
Protein	+3.11	+8.54
Nucleic Acid	+4.44	+7.44
Carbohydrate	+4.27	+8.07
Fatty Acid	-0.01	+6.89

Scattering length densities are given in units of 10^{-14} cm/Å^3 or 10^{10} cm^2. These average values are obtained by summing the scattering lengths of all atoms in a molecule and dividing the result by the molecular volume. For ^{2}H substituted materials it is assumed that all exchangeable hydrogen sites are occupied by ^{2}H. (Data from Engelman and Moore, 1975.)

SUMMARY OF THE RUSH REPORT ON NEUTRONS

PRESENTATION BY DR. WERNER

Last spring, the Solid-State Sciences Committee of the National Research Council commissioned a study of the current status of neutron scattering research facilities in the United States. This turned out to be very important and timely. Jack Rush of the National Bureau of Standards was the chairman of the committee, and by all rights, he should be up here telling you about his report. I will refer to the report as the Rush Report, and I assume, from now on -- until we build a new reactor or a new pulse source -- it will be referred to as the Rush Report.

Vu-graph 1

This is the title page of the report. It turns out that the recommendations in the report have not yet been okayed by the National Academy. But, as far as I can tell, I can tell you about them, which I will go on to do today.

The committee consisted of an appropriate mix, I think of people who I would say are cognoscentès -- some people are more cognoscentè than others -- people representing special interest groups, and there were a few skunks. I will show you the list. Vu-graph 2. You can read the names. It was a very good committee. It worked very well. Jack Rush did a very large fraction of the work. He really deserves a lot of credit for a very good report, I believe.

We were not asked to assess particular proposals, those of the type that you heard about today, nor did we attempt to rate or prioritize the various ideas that exist in this field, for upgraded sources, new instruments, and that sort of thing. However, we were very much aware of these proposals, after all. Of course, they influenced our thinking with regard to future possibilities and opportunities of neutron scattering in America.

Neutron sources in the United States serve a wide variety of scientific and technological purposes and needs which are unrelated to neutron scattering. Ralph Moon mentioned a few of those in his talk. I would like to just give you a list and make a comment on that.

Vu-graph 3.

In fact, the one that he talked about, I noticed when I was looking through these vu-graphs, I missed, - the generation of transuranic elements. You can say it is in here in some way, but it is not explicitly in here.

Other applications of sources used for neutron scattering -- that is, those sources on which we do neutron scattering; there are other reactors and sources which produce radioisotopes and so on -- radiopharmaceuticals, radioisotopes, transmutation doping of silicon. Now, something like 100 tons of silicon goes through our reactors (worldwide) per year, something like a third of it in this country -- neutron activation analysis and chemistry, radiation dosimetry and standards, radiation damage, and so on; many other things, nuclear physics and fundamental neutron physics.

If you add all these up -- it is hard to do it exactly -- it turns out that these programs; these additional programs, support roughly one-half of the cost of running these sources. So they are very important to us as neutron scatterers. Although it was not in our study, and it was not our commission to assess these other applications of neutron sources, I think we must be very much aware of them when we are planning new sources to be built in the 1990s. These applications are not only scientifically interesting, they are technologically important, and they make money for our sources.

I will assume the members of the Committee have a copy of the report. I will not assume that you have read it. Over the past six years, it turns out that there have been two or three other neutron scattering studies in the United States. It depends upon how you count. Brinkman-1, Brinkman-2, I count that as one. There was one in 1977, a National Academy study. Then there was the study in 1980 sponsored by the DOE, centered on the facilities funded directly by the Department of Energy.

Both of these reports emphasized the much greater investment and facility advances that were being made in Europe. They recommended that steps be taken to assure an internationally competitive position for the United States in this field.

While some of these recommendations have been addressed - and I will come back to that and show you that some have -- at least in part, most have not. Total funding in real dollars has shown no real increase over the last six years. It should therefore be no surprise that there are currently critical gaps in U.S. neutron research capabilities with respect to modern facilities. We have been hearing about that these two days. It is obvious. The long-range scientific and technological ramifications of not maintaining state-of-the-art research facilities in fields as important as neutron and x-ray scattering can be severe.

The report is a 90-page document. It consists of six major sections. I have a vu-graph of the table of contents. Vu-graph 4. There are six major sections: conclusions and recommendations -- and I will come back to that at the end -- you have already heard the introduction; current status of neutron scattering facilities in the United States; facilities description; the user community; comparison with the European community; overseas neutron scattering sources -- and I will show you a listing of the reactors and pulsed neutron sources there -- recent neutron scattering research in the United States, comparisons with Europe. This is the scientific part of the report, which is the big part, and I assume that most of you will enjoy reading that the most.

Yesterday you had four talks on the main sections of the scientific reports: condensed matter physics, chemistry, biology, polymer and colloid science, materials science, and engineering.

There is one additional section, too; neutron optics, which was not covered. I was the main author of that section, so there is some temptation for me to say something about it. But I will refrain. However, if anyone would like to ask me a question on gravitationally-induced interference - those sorts of experiments, I would be delighted.

Then there is a section on future opportunities, facilities and research at the end.

Since the scientific part is the justification for why we do neutron work, and it has already been given yesterday, I will not say much about that. What I will do now is give you some summary data; where we stand, where the reactors are, so we have an overall view toward the field.

Just to make sure, again, that you are all tuned in on the same wavelength and the same frequency, I want to remind you again of the fundamentals. Vu-graph 5. Neutron people love to come back to these fundamentals. Very quickly, neutrons are marvelous. The wavelength of thermal neutrons is about equal to the interatomic d-spacing of atoms in solids and liquids. The energy is about the same as thermal excitation energy. Neutron "see" hydrogen -- and you have been told about the hydrogen-deuterium contrast, selective labeling, and magnetism. Neutrons are the "cat's meow" in magnetism. Anybody who does not believe it, look at the literature. Contrast of elements adjacent in the periodic table -- that

is because of the variability of the scattering lengths of the elements, and their various isotopes. The interactions and cross-sections are generally known, and they are simple. The neutron probe is weakly interacting. Special environments are routine. Experiments down to millikelvin in temperature, up to 30 kilobars pressure, fields as high as 100 kilogauss, are routinely done. The neutron is a general probe of condensed matter.

The reason of Q and ω space accessible to neutrons -- it is seven orders of magnitude in energy. John Axe is usually conservative, and he gave it eight yesterday. He gave the pulsed-neutron people another decade. In the wavevector Q it is about five orders, five decades.

The lower three decades here, about a tenth of a microvolt to a tenth of a millivolt, we cannot access in the United States right now. That is what all this cold neutron business is all about.

Where are we with regard to facilities right now, as of 1984, in the United States? Vu-graph 6. You all know this already, but I will try to bring it back into focus, where things are. The high-flux isotope reactor at Oak Ridge is a 100-megawatt reactor. The high-flux beam reactor at Brookhaven is a 60-megawatt reactor. The National Bureau of Standards reactor is currently 10 megawatts and will be increased to 20 megawatts this summer. The University of Missouri reactor is now 10 megawatts, and there is consideration for increasing its power level to 20 megawatts. Then there is the 30-megawatt Oak Ridge research reactor and the 5-megawatt MIT reactor. Those basically are the six reactors that we have where serious neutron scattering work is carried out at some level.

Then we have these two-pulsed neutron sources, the IPNS at Argonne, which you have already heard about, and the facility WNR at Los Alamos. You heard nice programs for upgrading both of these sources today. It is clear that if either or both were increased, productivity in the pulsed-neutron business in the United States would be enhanced by a lot.

You should really look again at this second column here: the commissioning years. You will note that all of the reactors were built in the 1960s. In the decade of the 1960s, we had basically six nice reactors built in the United States, none since then. That is a serious problem. These reactors are getting older. We do not know when the maintenance costs will cross the line when we decide it is just too expensive to continue to maintain them; we will either shut them down or build something new. No one really knows those things for sure. But we do know that the maintenance costs will continue to go upward, and by the mid 1990s things will really be critical.

I would also like to call your attention, just to remind you, to the flux levels. The flux levels in American reactors are comparable to reactors in Europe. They range from an order of one to ten, in units of 10^{14} neutrons/cm^2/sec. So, in innate flux, our reactors are just as good as the reactors in Western Europe.

Then, to summarize, we have six reactors, two pulsed-neutron sources, and on all of these sources, we currently have a total of 53 instruments. Some are better than others. There is a wide diversity of instrumentation on these reactors and pulsed sources.

Over the last decade, neutron scattering research worldwide has shown a rapid expansion in both the number of users and the diversity of disciplines and sciences to which neutron methods are being applied. You have been hearing about that these past two days. In the United States that is also true. Vu-graph 7. I show here -- I think you have already seen this vu-graph; I think Jack Rush has shown it to you in an earlier meeting -- the change in the number of neutron users in the United States. These users are

hands-on people. That is, it does not include crystal growers back home, or theorists that are involved in the project. It is hands-on users only. During the past six years, the number of users has roughly doubled. I think the number is 510 as of last year.

The publications have also gone up during this period of time. There are good reasons for why this has gone on, not only that there has been a rapid expansion in Europe, but there has been improvement in instrumentation here in the United States; even with level budgets. For example, there have been four modern SANS facilities built at four of our reactors. Of course, during this time, the IPNS at Argonne came on line. I will come back to those improvements that have occurred in neutron instrumentation at our reactors and at our pulse sources.

I point out that there is a sort of canonical number; namely there should be roughly two users per publication, something like that. At least that is my canonical number.

Let me show you also the distribution of users amongst the various fields in the United States. Vu-graph 8. The traditional area where neutron scattering began and still remains strong is in condensed matter physics. It is now 35 percent; chemistry, 24 percent; materials science, 15 percent; polymer science and biology each 13 percent. The trend is that these sorts of nontraditional areas are growing more rapidly than condensed matter physics.

Total users is 510. Of those, 30 percent come from federal laboratories and agencies, 60 percent from universities, and 10 percent from industry.

I would like to give you a feeling for the neutron facilities in other Western countries, mainly in Western Europe, but on this list there is also the NRU reactor in Canada and the JAERI reactor in Japan.

Vu-graph 9.

It turns out, if I count right, that there are 12 reactors that do serious neutron scattering research in Europe. Some of them are listed here, and some of them are listed below. Fluxes are about the same as reactors in the United States. Where we are really behind is in this last column, "Special Characteristics". That has been pointed out over and over again during the past two days.

Cold sources: The Institute Laue-Langevin has a cold source, another one under construction, a guide hall, a hot source, 26 instruments, and 8 more under development. This is the sort of thing that is going on, not only there, but other places also. That is the thing that must be of considerable concern to all of us.

Vu-graph 10.

Here is a comparison table of the United States and Western Europe alone. I have already said in the United States we have 53 neutron instruments. In Western Europe there are 114. Under development in the U.S. are 16, and 10 at the pulse sources, 50 under development in Western Europe, 10 at the pulse source, the SNS. Cold source instruments: two in the United States, 30 in Western Europe, and 20 under construction. This is where we really see the big gap. Hot sources, and so on.

Neutron research budgets: These numbers are difficult to come by. I understand that you are going to have some more discussions and explanations of how these numbers are derived, not only for neutron facilities, but also for synchrotrons, which I do not know much about. But for neutrons, I have gone over these things with Jack Rush, and I believe that they are essentially correct. If you add the numbers up in different ways, you come out roughly with the same message.

During the period '75 to '83 in the United States, the expenditure for permanent facilities was $32 million. In Western Europe, it was of the order of $250 million, which is probably on the low side. $50 million more has now been approved. For science and operations last year, 1983, in the United States it was $27 million, in France, Germany, and the U.K. only, $80 million.

You see that there is an investment gap. Roughly speaking, the publication rate points that up also. In other words, in this field, like in many other fields of scientific research, you get basically what you pay for. People here are no smarter or no more stupid than they are in Europe.

Vu-graph 11.

So we have some gaps in our capabilities. The clearest one is cold neutrons. I am not going to try to explain to you why we have that enormous gap in cold neutrons. there are all kinds of reasons for it. We need this whole new generation of instruments that goes along with cold neutron sources -- guide tubes, large-scale and continuously adjustable focusing monochromators, supermirrors, all this sort of ancillary equipment that goes along with doing high-quality neutron work. We need much more of it. You just heard this afternoon that we need more work on advanced neutron source design efforts, both on the pulsed neutron side and on the reactor side. I was really pleased to see that that is now going on at an embryonic stage.

The panel believed that the United States is still internationally competitive in chemical and biological crystallography, thermal neutron triple-axis spectroscopy, and pulse source research, at least for the present.

Vu-graph 12.

I said I would come back to what the new instruments are that we built here in the United States over the last seven years or so. There are four SANS instruments, at the National SANS Center at Oak Ridge, funded by the NSF, at the Bureau of Standards, at Brookhaven, at the University of Missouri. There are new high-resolution powder diffraction and biological crystallography spectrometers at ANL, BNL, MURR, and NBS, improved three-axis spectrometers at Brookhaven, the National Bureau of Standards, and Oak Ridge, neutron inter- ferometers at the University of Missouri, at MIT, and pulsed source develop- ment has been going on very actively at Argonne and Los Alamos.

With regard to this gap that we talk about in neutrons and that I pointed out -- it looks like it might be getting worse. I do not see anything that we can do right now that is going to change the flow of things. The gap is going to get larger for awhile. Vu-graph 13. Not to scare you, but this is a sort of summary of what is going on in Western Europe: the SNS source at Rutherford Laboratory, the 10^{16} source, with 15 new instruments, to come on line with operating instruments by 1987; new cold source/guide hall at the Institute Laue-Langevin -- I have already mentioned that -- a $40 million upgrade of the Berlin reactor, to 20 megawatts, a cold source, a hot source, and a guide hall; an upgrade of the KFA reactor in Julich, cold neutron facilities and guide hall; upgrade of the Studsvik reactor in Sweden and the Petten reactor in the Netherlands; and there is a $7 million per year design effort at KFA on a new neutron source for Germany.

In Japan, there is a $150 million replacement of the JAERI reactor, which will be a 20-megawatt reactor with cold source and guide hall. This goes back to the importance of reactors of the intermediate power level; if you properly instrument them with cold sources and state-of-the-art

instrumentation, they are very valuable. There is also a design study for a pulse source at Tsukuba.

I would like to tell you what the conclusions of the panel were, and then I would like to tell you what the recommendations are. I again say that the recommendations, as currently stated, have not yet been approved by the National Academy. I do not see any reason why they will not be approved. They are not that bizarre.

Vu-graph 14.

Conclusions: I will read these to you. One: During the last decade, neutron scattering research worldwide has shown a rapid expansion in the number of users and the diversity of disciplines and sciences to which the neutron methods are applied. The number of users in Europe during the decade of the seventies increased by a factor of 3. It is 1250 now. The number of users in the United States during the last six years has gone up by a factor of 2 to the present number of 510.

Number two: The U.S. has fallen far behind Western Europe in the development of advanced facilities at research reactors, especially cold sources, guide tube technology, focusing monochromators, spin echo, and back-reflection spectrometers. We all know about these things now. The U.S. remains competitive in thermal neutron three-axis spectroscopy, chemical and biological crystallography, and, for the present, pulsed-neutron source research.

The last conclusion: Current U.S. reactors remain world-class in terms of available neutron beam intensities. Immediate opportunities exist, as you heard about today, at these sources for achieving an internationally competitive status in instrumentation for both cold and thermal neutron scattering research. Finally, I point out again, these sources will be 20 to 25 years old by 1990.

Those are the facts. Vu-graph 15.

The recommendations of the panel are these -- I will read these to you. One: That an immediate commitment be made to develop and install new state-of-the-art instrumentation at our high-performance research reactors to take advantage of the opportunities in high-resolution and high-sensitivity neutron spectroscopy, small-angle scattering and diffraction, medium-resolution macromolecular diffraction, and diffuse scattering. These things will require an extensive development and application of modern cold source and guide tube technology, focusing and polarizing monochromators, and area detectors.

Two: Adequate support be provided to allow full investigation and development of new pulse source instrumentation required to exploit the opportunities provided by the pulse structure, high fluxes of epithermal neutrons, and expanded wavevector range.

Three: Funding be provided for serious, competitive design efforts to be started immediately for the next generation of sources, so that full proposals are available by fiscal year '88. These designs should then be reviewed by a broadly based user group appointed by the National Academy, to recommend a coherent plan for new source construction.

The last recommendation you might have some question about. The panel talked about that in some detail. I cannot give you all the reasons for appointing this group to oversee a coherent plan. But basically, the general philosophy is that the current broadly-based user community should be involved at an early stage in the decision-making process of instrument selection, design, type of source, and siting.

DR. STEVENS: Did you consider putting any suggestion of budgets behind those recommendations, how much per year for how many years?

DR. WERNER: Yes, we discussed where to put that in the report. If you read to the end of the report, there is a number. It says an additional $75 million expended over five years. Whether that fits in with what is being proposed here I don't know -- that was a rough number.

DR. STEVENS: Your recommendations had to do with instrumentation and design studies. Is that $75 million for the composite whole?

DR. WERNER: That is right, $75 million expended over five years for instrumentation and source improvement. Is that right, Jack?

DR. RUSH: Yes, but it did not include design studies for new sources. one of the panel members, who was one of the skunks, who should remain nameless, suggested very strongly that something like that be included, because he said Don Stevens is going to ask that question. The $75 million figure referred, Don, to the upgraded instrumentation and experimental halls and so forth. It would be required to achieve some kind of parity while we got on with the new source.

DR. WERNER: We can give you an estimate for new source design costs. We have our personal views about how much these design studies should cost. But you can get those from people on your panel, as well as from me. Those will only be estimates.

DR. RUSH: There is something very good about that, and that is that all those recommendations were worked out by people, a number of whom are in this room, before the Seitz Panel actually became known. So it is not in any way directly related to these issues. I suppose one could go over what that means later.

DR. FISHER: I was struck by the fact that getting to the state-of-the-art seems to mean reproducing in the United States now what was innovative in Europe 15 years ago, in some cases.

DR. WERNER: Sort of, yes. It is basically catch-up.

DR. EISENBERGER: Sometimes when one falls behind, one can take an advantage. One can skip a stage of evolution. Is there something that goes beyond where they have already invested their instrumentation money?

DR. WERNER: Yes, I think both of the proposals this afternoon (reactors and pulsed sources), in fact, go beyond that. We cannot get to those sorts of things quickly. After all, to design and construct a reactor is like a 12-year process.

DR. EASTMAN: Peter is talking about instrumentation, for example, the spin echo experiment and the other experiment.

QUESTION: Are there next-generation instrumentations that would offer advantages over current ones that Europe has, that if we invested our money now, would give us the hope of not just catching up, but give us the hope of having some advantages?

DR. RUSH: All of the proposals that generally related to upgrades included instruments that have no analog or exceed current capabilities in Europe.

QUESTION: Is that in your report, what advantages those might give in terms of capabilities?

DR. RUSH: Those instruments are not in our report. They were in the Brookhaven and Los Alamos and NBS proposals, which did not see the light of day until the powers that be saw fit to create this body.

DR. SHIRANE: Whenever we design a new instrument, we always look at everything available. In that sense, we are building upon the improvements.

DR. EASTMAN: Let me repeat Peter's perception. It is my perception to some degree as well. We did not get clear indications in a number of cases of trying to quantify or qualify how a new spin echo spectrometer would be

better than the one which is at ILL, that kind of thing. That tone did not come through in a number of cases.

DR. WERNER: I think that the spin echo machine that Mike Rowe is designing at NBS is of that quality. We know what they do in Europe. Obviously we will not just do it exactly that way. We will make it at least a bit better. If you want really novel instrumentation, like neutron interferometers -- that was novel, but you are not going to get those every day.

DR. FISHER: Isn't there a point that responds to that? My understanding of the evidence that has been presented is that in Europe they have had developmental funds, which is why you can hope for some of these distinct breakthroughs every now and then. Your question really has to be translated the other way. Shouldn't we be investing so many million a year so that the next breakthrough will be here? You cannot program a breakthrough, but you can at least say we will put some of our resources into doing that. That is what has not been done.

DR. EASTMAN: I would hope that, if this kind of a recommendation for building more instrumentation were to occur, budget-wise, you would then go back, once there are real dollars committed, and find the best people, and something new would happen in a period of years, presumably.

QUESTION: I do not think things happen unless you put money into them and say you have a program.

DR. STEVENS: In order to do all this, there is the matter of manpower. If there is a manpower pool available to then start up an instrumentation R&D program and so on, that is great. If there is not, that means that some of the researchers at the present time will be diluting their efforts in order to fill this gap. Did you look into these things?

DR. WERNER: We did not look into that in detail. What you say is certainly true, that people who are currently doing their own physics experiments or chemistry experiments must devote some time to instrumentation development. Do you have any feeling about that, Jack, whether there are enough people around?

DR. RUSH: I think the answer is that people can be found. In particular, if you do not move in this direction, there will not be any people around in the next decade or at the end of the century at all to keep hacking away at the triple-axis spectrometers and the powder diffractometers. There is a chicken and egg here.

DR. WERNER: For example, we turn out roughly two students a year at the University of Missouri in neutron scattering. Of those, one goes into the field, and the other one goes somewhere else, basically because there have not been places to go to get new jobs in instrument development and that sort of thing. They go and find other things that are more financially rewarding.

DR. MOON: I think it is generally true -- certainly it is at Oak Ridge -- that we are shorthanded as far as scientists per instrument. But in one aspect, namely detector development, there is manpower available today. At Oak Ridge, for example, our Instrumentation and Controls Division is not really directly funded. They exist as a service organization. In that case, it takes just some money to actively engage some people there.

DR. SILVER: We now have 12 scientists associated with our program, most of whom came on board in the last three years. So we are finding new people.

DR. EASTMAN: Okay, thank you very much.

CURRENT STATUS OF NEUTRON SCATTERING RESEARCH AND FACILITIES IN THE UNITED STATES

"RUSH REPORT"

REPORT OF THE SUBCOMMITTEE ON NEUTRON SCATTERING

SOLID STATE SCIENCES COMMITTEE

NRC - NAS

JAN. 1984

Subcommittee on Neutron Scattering

JOHN D. AXE
BROOKHAVEN NATIONAL LABORATORY

ROBERT J. BIRGENEAU
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

WALTER L. BROWN
BELL LABORATORIES

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LOS ALAMOS NATIONAL LABORATORY

DONALD M. ENGELMAN
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GERARD H. LANDER
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RALPH M. MOON, JR.
OAK RIDGE NATIONAL LABORATORY

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ROBERT ULLMAN
FORD MOTOR CO.

JULIA R. WEERTMAN
NORTHWESTERN UNIVERSITY

SAMUEL A. WERNER
UNIVERSITY OF MISSOURI

OTHER APPLICATIONS OF SOURCES USED FOR NEUTRON SCATTERING

- RADIO-PHARMACEUTICALS, RADIOISOTOPES
- TRANSMUTATION DOPING OF Si
- NEUTRON ACTIVATION ANALYSIS
- RADIATION DOSIMETRY/STANDARDS
- RADIATION DAMAGE
- NEUTRON RADIOGRAPHY/TOMOGRAPHY
- PRODUCTION OF MICRON-PORE FILTERS
- PRODUCTION OF PORTABLE NEUTRON SOURCES - ^{252}Cf
- NEUTRON DEPTH PROFILING
- PRODUCTION OF γ-SOURCES FOR SCATTERING EXPERIMENTS, MEDICINE, ETC.

- NUCLEAR PHYSICS
- FUNDAMENTAL NEUTRON PHYSICS

THESE PROGRAMS SUPPORT ROUGHLY 1/2 OF COST OF RUNNING THE SOURCES.

CONTENTS

1. CONCLUSIONS AND RECOMMENDATIONS

2. INTRODUCTION

3. CURRENT STATUS OF NEUTRON SCATTERING FACILITIES IN THE UNITED STATES
   - FACILITY DESCRIPTIONS
   - THE USER COMMUNITY
   - COMPARISON WITH THE EUROPEAN COMMUNITY

4. OVERSEAS NEUTRON SCATTERING FACILITIES
   - RESEARCH REACTORS
   - PULSED NEUTRON SOURCES

5. RECENT NEUTRON SCATTERING RESEARCH IN THE UNITED STATES COMPARISONS WITH EUROPE
   - CONDENSED MATTER PHYSICS
   - NEUTRON OPTICS
   - CHEMISTRY
   - BIOLOGY
   - POLYMER AND COLLOID SCIENCE
   - MATERIALS SCIENCE AND ENGINEERING

6. FUTURE OPPORTUNITIES: FACILITIES AND RESEARCH

APPENDIX: INSTITUTIONAL SPONSORS OF USERS OF MAJOR NEUTRON SCATTERING FACILITIES IN THE UNITED STATES (JULY 1982 - JUNE 1983)

FUNDAMENTALS

NEUTRONS ARE MARVELLOUS!

- WAVELENGTH $\lambda \sim$ INTERATOMIC SPACING, d, OF ATOMS IN SOLIDS AND LIQUIDS AND ENERGY $E \sim$ THERMAL EXCITATION ENERGIES, $\hbar\omega$
- SEES H, H/D CONTRAST SELECTIVE LABELLING.
- MAGNETISM
- CONTRAST OF ELEMENTS ADJACENT IN PERIODIC TABLE.
- INTERACTIONS/CROSS-SECTIONS KNOWN. WEAKLY INTERACTING.
- EXTREME ENVIRONMENTS ROUTINE, T, P, H.
- GENTLE PROBE.

REGION OF Q, ω SPACE ACCESSIBLE TO NEUTRONS:

ENERGY: 10^{-7} - - - ->- - 1 EV.

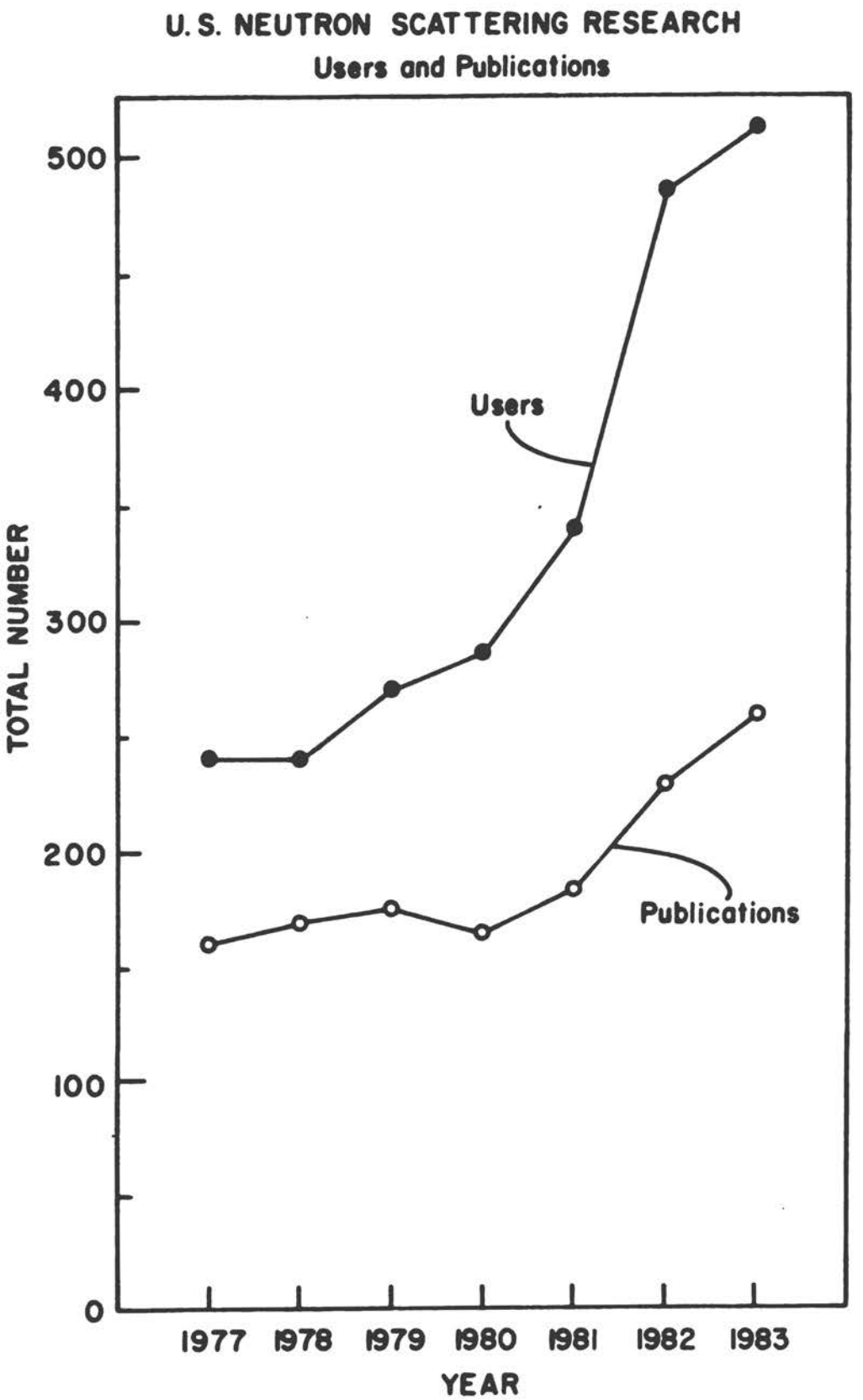
WAVEVECTOR: 10^{-4} - - - ->- - 50 A^{-1}.

MAJOR NEUTRON SCATTERING FACILITIES IN WESTERN COUNTRIES

RESEARCH REACTORS	POWER	COMMISSIONING YEAR	AVERAGE THERMAL FLUX (10^{14} N/CM^{2}SEC)	SPECIAL CHARACTERISTICS
INSTITUT LAUE-LANGEVIN (GRENOBLE, FRANCE)	57 MW	1972	10	COLD SOURCES (1 UNDER DEVELOPMENT), GUIDE HALL, HOT SOURCE, 26 INSTRUMENTS (8 UNDER DEVELOPMENT)
ORPHEE REACTOR (SACLAY, FRANCE)	14 MW	1981	2.5	2 COLD SOURCES, LARGE GUIDE HALL, HOT SOURCE, 25 INSTRUMENTS (SOME UNDER DEVELOPMENT)
KFA REACTOR FRJ-2 (JULICH, GERMANY)	20 MW	1962	~1	COLD SOURCE, GUIDE HALL EXPANSION UNDERWAY
NRU REACTOR (CHALK RIVER, CANADA)	35 MW	1959	~3	
RISO DR-3 REACTOR (ROSKILDE, DENMARK)	10 MW	(60'S)	1	COLD SOURCE
HARWELL RESEARCH REACTOR (GREAT BRITAIN)	20 MW	1957	1	COLD SOURCE
JAERI RESEARCH REACTOR (JAPAN)	10 MW	(60'S)	.8	

MANY OTHER REACTOR FACILITIES: E.G., STUDSVIK (SWEDEN), PETTEN (NETHERLANDS), KJELLER (NORWAY), BERLIN REACTOR (GERMANY), SAPHIR REACTOR (SWITZERLAND)

PULSED SOURCES		PEAK THERMAL FLUX
NS (RUTHERFORD LABS, U.K.)	1984-6	1×10^{16} (50 HZ) 15 INSTRUMENTS PLANNED
KENS (TSUKUBA, JAPAN)	1977	$.6 \times 10^{14}$ (20 HZ)


U. S. NEUTRON SCATTERING RESEARCH
Users and Publications
TOTAL NUMBER
500
400
300
200
100
0
Users
Publications
1977
1978
1979
1980
1981
1982
1983
YEAR

U.S. NEUTRON SCATTERING USER COMMUNITY (1983)

		Trend ('77-'83)
Condensed Matter Physics	35%	+33%
Chemistry	24%	+100%
Materials Science	15%	+150%
Polymer Science	13%	
Biology	13%	

Total Users 510

Federal laboratories and agencies	30%
Universities	60%
Industry	10%

MAJOR NEUTRON SCATTERING FACILITIES IN WESTERN COUNTRIES

SEARCH REACTORS	POWER	COMMISSIONING YEAR	AVERAGE THERMAL FLUX (10^{14} N/CM^{2}SEC)	SPECIAL CHARACTERISTICS
ISTITUT LAUE-LANGEVIN GRENOBLE, FRANCE)	57 MW	1972	10	COLD SOURCES (1 UNDER DEVELOPMENT), GUIDE HALL, HOT SOURCE, 26 INSTRUMENTS (8 UNDER DEVELOPMENT)
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MANY OTHER REACTOR FACILITIES: E.G., STUDSVIK (SWEDEN), PETTEN (NETHERLANDS), KJELLER (NORWAY) BERLIN REACTOR (GERMANY), SAPHIR REACTOR (SWITZERLAND)

PULSED SOURCES		PEAK THERMAL FLUX
IS (RUTHERFORD LABS, U.K.)	1984-6	1×10^{16} (50 HZ) 15 INSTRUMENTS PLANNED
KENS (TSUKUBA, JAPAN)	1977	$.6 \times 10^{14}$ (20 HZ)

SUMMARY COMPARISON OF MAJOR U.S. AND EUROPEAN FACILITIES

NEUTRON SCATTERING FACILITIES

	U.S.	WESTERN EUROPE
TOTAL INSTRUMENTS	53	114
UNDER DEVELOPMENT	16 (10 PULSED SOURCE)	~50 (10 PULSED SOURCE)
COLD NEUTRON INSTRUMENTS	2	30 (+20 UNDER CONSTRUCTION)
COLD SOURCES	1(+1 UNDER CONSTRUCTION)	8
HOT SOURCES	0	2
GUIDE HALLS	0	5

NEUTRON RESEARCH BUDGETS

	U.S.	WESTERN EUROPE
EQUIPMENT & FACILITIES (1975-83)	≃32$M	~250$M (+50$M APPROVED)
SCIENCE & OPERATION (1983)	≃27$M	≃80$M (FRANCE, GERMANY, U.K.)

GAPS IN U.S. CAPABILITIES

- COLD NEUTRONS - NEW GENERATION OF INSTRUMENTS
- GUIDE TUBES, LARGE SCALE, CONTINUOUSLY ADJUSTABLE FOCUSSING MONOCHROMATORS, SUPERMIRRORS, ETC.
- ADVANCED NEUTRON SOURCE DESIGN EFFORTS

U.S. CURRENTLY INTERNATIONALLY COMPETITIVE

- CHEMICAL AND BIOLOGICAL CRYSTALLOGRAPHY
- THERMAL NEUTRON TRIPLE-AXIS SPECTROSCOPY
- PULSED SOURCE RESEARCH

NEW U.S. NEUTRON FACILITIES

(1976-83)

- SANS - ORNL (NSF), NBS, BNL, MURR
- High Resolution Powder Diffraction, Biological Crystallography - ANL, BNL, NBS
- Improved 3-Axis Spectrometers - BNL, NBS, ORNL
- Neutron Interferometers - MURR, MIT
- Pulsed Source Development (ANL, LANL)

CURRENTLY FUNDED DEVELOPMENT PROJECTS: EUROPE AND JAPAN

WESTERN EUROPE

- SNS PULSED SPALLATION SOURCE (RUTHERFORD LAB., U.K.)
  10^{16} N/CM^{2}SEC PEAK FLUX, 15 INSTRUMENTS BY 1987
- NEW COLD SOURCE, GUIDE HALL, INSTITUTE LAUE-LANGEVIN
- 40$M UPGRADE OF BERLIN REACTOR: 20 MW POWER, COLD SOURCE, HOT SOURCE, GUIDE HALL
- UPGRADE OF KFA, JULICH COLD NEUTRON FACILITIES AND GUIDE HALL
- UPGRADE OF STUDSVIK (SWEDEN) AND PETTEN (NETHERLANDS) REACTORS
- 7$M/YEAR DESIGN STUDY AT KFA FOR ADVANCED WEST GERMAN SPALLATION SOURCE (10^{17}N/CM^{2}SEC PEAK FLUX)

JAPAN

- 150$M REPLACEMENT OF JAERI REACTOR
  20 MW POWER, COLD SOURCE, GUIDE HALL
- DESIGN STUDY FOR >100$M 10^{16}N/CM^{2}SEC PULSED SOURCE AT TSUKUBA

CONCLUSIONS

(1) DURING THE LAST DECADE NEUTRON SCATTERING RESEARCH WORLDWIDE HAS SHOWN A RAPID EXPANSION IN THE NUMBER OF USERS AND THE DIVERSITY OF DISCIPLINES AND SCIENCES TO WHICH NEUTRON METHODS ARE APPLIED.

	EUROPE (1970-1980):	X3	≈1250 (1983)
USERS			
	U.S. (1977-1983):	X2	≈510 (1983)

(2) U.S. HAS FALLEN FAR BEHIND WESTERN EUROPE IN THE DEVELOPMENT OF ADVANCED FACILITIES AT RESEARCH REACTORS. ESPECIALLY:

- COLD SOURCES, GUIDE TUBE TECHNOLOGY
- FOCUSSING MONOCHROMATORS, SPIN ECHO AND BACK-REFLECTION SPECTROMETERS

U.S. REMAINS COMPETITIVE IN THERMAL NEUTRON 3-AXIS SPECTROSCOPY, CHEMICAL AND BIOLOGICAL CRYSTALLOGRAPHY, AND (FOR THE PRESENT) PULSED SOURCE RESEARCH.

(3) CURRENT U.S. REACTORS REMAIN WORLD-CLASS IN TERMS OF AVAILABLE NEUTRON BEAM INTENSITIES. IMMEDIATE OPPORTUNITIES EXIST AT THESE SOURCES FOR ACHIEVING AN INTERNATIONALLY COMPETITIVE STATUS IN INSTRUMENTATION FOR BOTH COLD AND THERMAL NEUTRON SCATTERING.

- THESE SOURCES WILL BE 20-25 YEARS OLD BY 1990.

RECOMMENDATIONS

(1) IMMEDIATE COMMITMENT BE MADE TO DEVELOP AND INSTALL NEW STATE-OF-THE-ART INSTRUMENTATION AT OUR HIGH PERFORMANCE RESEARCH REACTORS TO TAKE ADVANTAGE OF THE OPPORTUNITIES IN:

- HIGH RESOLUTION AND HIGH SENSITIVITY NEUTRON SPECTROSCOPY
- SMALL ANGLE SCATTERING AND DIFFRACTION
- MEDIUM RESOLUTION MACROMOLECULAR DIFFRACTION AND DIFFUSE SCATTERING

- WILL REQUIRE EXTENSIVE DEVELOPMENT AND APPLICATION OF:
  - MODERN COLD SOURCE AND GUIDE TUBE TECHNOLOGY
  - FOCUSSING AND POLARIZING MONOCHROMATORS
  - AREA DETECTORS

(2) ADEQUATE SUPPORT BE PROVIDED TO ALLOW FULL INVESTIGATION AND DEVELOPMENT OF NEW PULSED SOURCE INSTRUMENTATION REQUIRED TO EXPLOIT THE OPPORTUNITIES PROVIDED BY:

- PULSE STRUCTURE
- HIGHER FLUXES OF EPITHERMAL NEUTRONS
- EXPANDED WAVE VECTOR RANGE

(3) FUNDING BE PROVIDED FOR SERIOUS, COMPETITIVE DESIGN EFFORTS, TO BE STARTED IMMEDIATELY, FOR THE NEXT GENERATION SOURCES, SO THAT DEFINITE PROPOSALS ARE AVAILABLE BY FY 88. THESE DESIGNS SHOULD THEN BE REVIEWED BY A BROADLY-BASED USER GROUP, APPOINTED BY THE N.A.S., TO RECOMMEND A COHERENT PLAN FOR NEW SOURCE CONSTRUCTION.

Report on The Planning Study for Advanced National Synchrotron Radiation Facilities

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In August 1983 we were asked by the Department of Energy, Office of Energy Sciences to make a critical review of the status and future prospects for synchrotron radiation science and to establish a ten-year road map for the development of synchrotron radiation facilities. As part of that charter, we were also asked to examine the Advanced Light Source proposed by Lawrence Berkeley National Laboratory.

The committee we chose to do the study has a very broad range of disciplines represented, and a uniform representation of universities, industry, and government labs. Roughly one-third of the committee are outside of the synchrotron radiation field.

To make the study an open and comprehensive process virtually everyone in the synchrotron community was invited to give us their opinions. We began with a 2-day general meeting in Albuquerque, in which roughly 80 people participated, where applications, facilities, and users were thoroughly discussed.

We then solicited additional technical information, opinions and ideas, from which we received hundreds of letters and other communications comprising well over 1000 pages of information. We then held three executive sessions to discuss our general strategy, to evaluate the material we had gathered, to arrive at our decisions and to prepare the report. The final report contains contributions by over 100 people. These people worked very hard and were most cooperative with us. We are most grateful for their assistance.

Our report discusses the physics of synchrotron radiation, and its applications to science and technology, which is really the bedrock of the report, and which we feel is very, very exciting. We present a rather complete survey of our existing facilities and the facilities in the rest of the world. We estimate costs for new facilities and how we would like these facilities organized to better handle the needs of their users.

Finally, we discuss some of the alternative sources, such as laser plasmas, x-ray lasers, and free-electron lasers.

Scope of the Study

Our judgements regarding facilities development were based on the new science and technology that will be available with a new generation of high brilliance sources. As discussed in the synchrotron science presentations there is a wide range of exciting new science possible with these machines, divided roughly into three classes. The first class would be analytical continuations of techniques we use now; that is, the information we now derive for bulk materials and surfaces we can think of deriving with greater resolution and for smaller particles and grain boundaries, for weaker phenomena, in and more dilute systems. The second class involves things not possible before. Things like inelastic and magnetic scattering, the various types of microscopies and microprobes, and areas such as plasma physics, new gas phase spectroscopies and actinide chemistry. It will open up new areas of experimentation and draw new groups to the field. Finally, there are the unanticipated breakthroughs that will occur because of the availability of these high brilliance sources. The excitement and challenge the imaginative use of these sources will present to the bright young scientists we want to draw to the materials sciences is impossible to quantify, but has to be a major factor in our ultimate decision to build them. Crucial to the question of new science is whether gains in brilliance translate into something useful at the sample. The answer is yes, in many ways as described in the synchrotron science discussions.

We also examined the technical limits to the use of higher brilliance. You can say you want to put more and more photons on a smaller and smaller spot, but there are limits to what you can do, based on the ability to handle power and the fundamental limits of available optics.

Finally, we examined the issues that affect development and use of these machines, e.g. how does this community organize itself to focus towards something like a 6-GeV machine and once it is built how do we make it readily usable to both the specialist and the broader community.

Status of Facilities and the User Community

Table I presents a list of the present and planned facilities in the United States. There are six dedicated or partially dedicated storage rings. From the .28 GeV SURF-NBS ring to the two new rings at NSLS. There are two proposed facilities. Over 100 beam lines will be available when all the existing facilities are operational. The Tantalus ring will go out of operation when the Aladdin ring comes up.

An important factor for the future is the rather limited inventory of available straight sections for insertion devices utilization; four at Aladdin, four operational at SPEAR, with an eventual inventory of twelve, CHESS has one, and at Brookhaven, the XUV ring

Table 1

STATUS OF FACILITIES IN USA

	Energy	Beamlines	Operation
SURF-NBS	.28	11-UV, XUV(B.M.)	Ded.
Tantalus - U. Wisc.	.25	11-UV, XUV(B.M.)	Ded.
Aladdin - U. Wisc.	1.0	35-UV, XUV(B.M.) 4-(I.D.)	C/Ded.
SSRL(SPEAR)-Stanford	1.8-3.5	19-UV, XUV, XR 4(12)(I.D.)	P-Ded.
SSRL(PEP)-Stanford	15	1-(I.D.)	C
CHESS - Cornell	5.5	6-XR 1(3)-(I.D.)	Par.
NSLS-I - Brookhaven	.75	23-UV, XUV(B.M.) 2-(I.D.)	Ded.
NSLS-II - Brookhaven	2.5	32-(B.M.) 4(5)(I.D.)	C/Ded.
ALS	1.3	12-(I.D.)	Prop.
6 GeV	5-6	30-(I.D.)	Prop.

Ded. = Dedicated, Prop. = Proposal, C = Under Construction or Commissioning, B.M. = Bend Magnet, I.D. = Insertion Device, present (potential).

Table 2

SYNCHROTRONS AROUND THE WORLD

Country	Number	Status
Brazil	1	F.S.
China	2	C
England	1	Op
Europe	1 (ESRF)	P
France	3	2-Op, 1-C
Germany	3	2-Op, 1-C
Italy	1	Op
Japan	7	4-Op, 2-C, 1-P
Sweden	1	C
Taiwan	1	P
USA	11	7-Op, 2-C, 2-P
USSR	6	4-Op, 1-C, 1-P
	38	20-Op, 9-C, 6-P 1-F.S.

Op = Operational
C = Construction
F.S. = Feasibility Study
P = Proposal

has two, while the x-ray ring has five. The new rings will have a larger complement of straight sections, and that is one of the prime reasons for wanting to build them.

One question on everyone's mind regards the commissioning of the new machines at Brookhaven and Stoughton. Just exactly what is the problem that is causing the delay. We feel most people do not appreciate that, although these machines are smaller than high-energy machines, they are still state of the art; they are technically very, very challenging.

A further problem is that there were several critical omissions in the name of economy. For instance, NSLS and the Stoughton rings were built without adequate diagnostics in addition to other shortcomings. Most difficulties are in execution, not design. One lesson that has been learned is that for high brightness rings, at-energy injection is virtually a necessity.

Finally, our community was inexperienced at building and commissioning such faciities and as we now know, it is not a trivial exercise.

Most importantly, we do not want to repeat this process; any future project must be adequately funded and managed to reach commissioning within a reasonable timeframe.

Table II lists the synchrotron inventory around the world. The number of facilities is increasing dramatically; at present, there are 38 facilities in various stages of development. Twenty are operational, nine are under construction, six are proposed, and one is in the feasibility study stage. Europe has one in the proposal stage, the ESRF, which is the equilvalent of our 6-GeV ring. The French have an important ring under construction, Super-ACO, which is a scaled down equivalent of our ALS.

It is evident that excitement over synchrotron radiation is worldwide in scope and capabilities are growing rapidly.

Table III presents the count of users and publications for the last three years, for SSRL, Stoughton, Brookhaven, NBS, and Cornell. There is a very rapid growth in the number of users over the last three years, which we expect to continue as the new facilities come to full operation.

The publication rate is high and the impact is very broad. Also shown in Table III is the breakdown in terms of discipline for the users at SSRL for 1983. The range of users, now weighted toward the fundamental interests, is expected to move toward more applied areas as beamtime availability increases.

While facilities in the next generation are going to be more expensive and complex, the money will be well spent. The science that has come out of the relatively modest investment we have had in this area has been very dramatic, and it justifies going ahead.

Table 3

Summary of Users and Their Publications (1981-1983)

	Users			Publications		
	1981	1982	1983	1981	1982	1983
SSRL	167	249	275	136	168	162
SRC	135	130	96	78	84	78
NSLS	-	-	398[a]	-	-	40
SURF	57	39	39	30	42	20
CHESS	15[b]	186	249	4	30	36[c]
TOTALS	374	604	1057	248	324	336

[a]Includes x-ray PRT members who would have been using the facility if it had been operating; 124 users actually took data on the VUV ring.
[b]Operation started in December 1981.
[c]70 more publications are presently in print.

A general idea of the SR-demand distribution across disciplinary boundaries can be obtained from the current breakdown of SSRL proposals, which is as follows:

Physical sciences	35%
Materials sciences	28%
Biology and medicine	21%
Chemical sciences	16%

Synchrotron Radiation

The frontiers in science are defined by our capabilities. Electromagnetic radiation is the most effective and versatile of exploratory probes for looking at structural properties and physical phenomena. Synchrotron radiation is easily the most versatile of electromagnetic radiation sources, covering eight decades of the spectrum, with high intensity, small source size, coherence, collimation, polarization, and time structure.

We now have an opportunity for a revolutionary jump in our capabilities.

The use of synchrotron radiation (SR) began in the late 1960s and early 1970s, using bending magnet radiation from storage rings that were designed for high-energy physics. They gave us orders-of-magnitude gain in brightness over existing standard x-ray sources, and many scientific frontiers were crossed by that capability.

The second generation of storage ring, designed specifically for SR, have higher beam currents and lower emittance, i.e., smaller electron beam crosssection and divergences. The second generation of machine was designed before the importance of insertion devices was realized, so they are still primarily bending-magnet machines. However, they still provide a quantitative gain of one or two orders of magnitude in brightness over the first generation of rings.

The third generation will demand still lower emittance, and numerous straight sections to accommodate insertion devices. It will give us one to four orders of magnitude gain in brilliance over present day machines and will make a qualitative difference in our capability.

Technical Features of Synchrotron Radiation

A simple pedagogical exercise will explain the features of these devices that led us to our conclusions.

If the path of a "bunch" of ultra relativistic electrons of energy $E = \gamma mc^2$ circulating in a storage ring is bent with a magnetic field into a radius R it will emit radiation into a cone of width $1/\gamma$. The radiation will have a critical wavelength, which is given by

$$\lambda_c \doteq R/\gamma^3.$$

For a 3-GeV ring, with $\gamma = 6 \times 10^3$ and a typical radius of 20 meters, the critical wavelength is ~ 1 Å or an energy of about 12 keV. The opening angle is $\sim 2 \times 10^{-4}$ radius or roughly 40 seconds of arc. In a bending magnet a fan of radiation is formed as this beam sweeps through the magnet.

The spectral dependence for bending magnet radiation from a 1.3 GeV machine is shown in Fig. 1. The spectrum is continuous and extends from very low energies, the infrared and below, to a few times the critical energy where it drops sharply in intensity. The source brightness far exceeds that of any traditional photon source through virtually all of that range.

The time structure of such a device is defined by the bunch length and the orbital period. In SSRL, for example, the bunch of electrons is roughly 10 centimeters long. It takes 300 picoseconds to pass the aperture of a beamline, yielding a 300-picosecond pulse of photons. The orbital period is 780 nanoseconds.

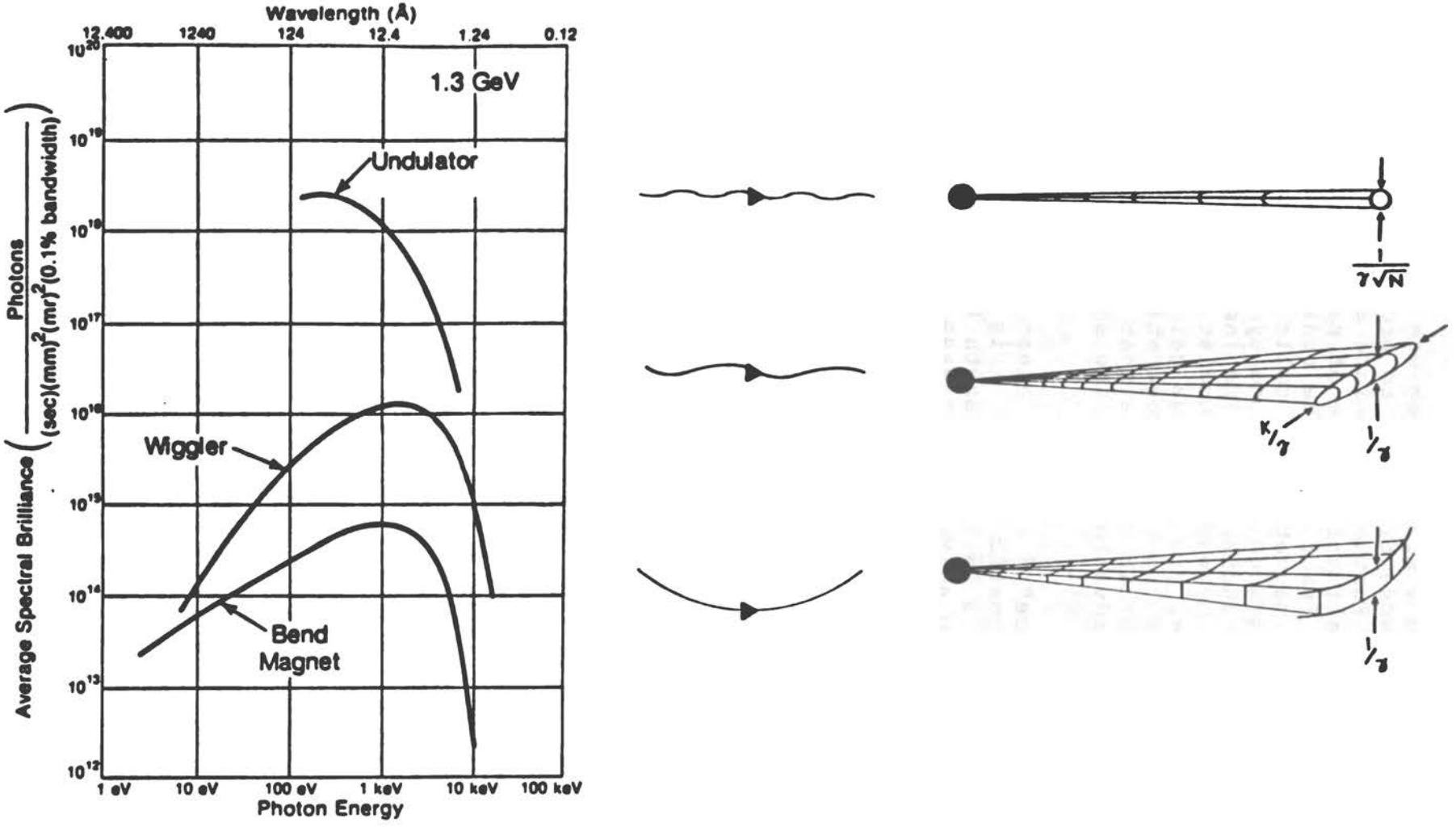


Figure 1. A Bending Magnet/Wiggler/Undulator Comparison. Left: The spectral brilliance as a function of photon energy for a bending magnet, wiggler, and undulator on a 1.3-GeV ring (the ALS design). The undulator curve is actually an envelope; the detailed spectral dependence is shown in Figure 2. Right: The approximate relationship between the electron-beam oscillations for the bending magnet (bottom), wiggler (middle), and undulator (top), and the respective angular distributions of their radiation. Undulator radiation is emitted in an intense laser-like beam.

The bending magnets in a storage ring are designed to control the electron orbit and crosssection, not to produce synchrotron radiation to the optimum. Furthermore, since experimental beamlines can accept only a small solid angle of radiation, a few milliradians, only a small fraction of the radiation emitted while the electron traverses the magnet arc is collected. Magnetic structures specifically designed to produce synchrotron radiation, so-called wiggler and undulators, which are inserted into long straight sections of the ring where the undisturbed path of the electron is a straight line, provide large gains in photon beam quality and intensity. The functional separation of the magnets that control the electron orbit and those that produce the radiation is an important strategic advantage allowing source design innovations to be implemental at will.

In an "insertion device" a straight electron trajectory is wiggled in a transverse magnetic field that is alternating, say N times, along the path in a device of length L. These insertion devices immediately provide an N-fold increase in intensity because the radiation from each of the N magnetic sources is superimposed in the forward direction. If the electrons path deviates by an angle which is less than the natural opening angle of the SR, $1/\gamma$, the device is called an undulator. Devices having larger deviations are called wigglers. In addition to enhanced brilliance, other characteristics of the photon beam can be controlled by varying the magnetic periods, $\lambda_u = L/N$, and the magnetic field B. A key parameter determining performance is $K = 0.93\ B(T)\lambda_u(cm)$. K is approximately the ratio of the angular excursion of the electron to the synchrotron opening angle $1/\gamma$. If $K<1$, the device is an undulator; for $K>1$ it is a wiggler. The behavior of both these devices can be described by the same theory, but their properties can be significantly different.

The total radiation produced by wigglers is similar to bending-magnet radiation in its vertical opening angle, $1/\gamma$, and its smooth spectral function. However, its horizontal opening angle is reduced to K/γ, and its intensity is multiplied by N. To understand the properties of undulators, one must take account of the interference of the radiation emitted by each of the 2N magnetic poles. This detailed interference theory is necessary as K decreases toward unity, but it is equally valid for high-K wigglers. The mathematical relationships that explain the precise properties of wigglers and undulators are contained in the footnotes below Figure 2. For the purposes of the following discussion, note that (1) undulator radiation has a structured spectrum consisting of peaks at the fundamental wavelength λ^1 and harmonics λ^m (Footnote 1), and (2) the fundamental radiation is emitted into a solid angle Ω (Footnote 2). With these definitions one can describe generally the performance of insertion devices. Figure 1 shows the spectral brilliance and the qualitative differences in the spatial character of the radiation from different sources. Spectra for two different undulators are depicted in Figure 2. Finally, Table 4 gives specific performance data for a number of different devices.

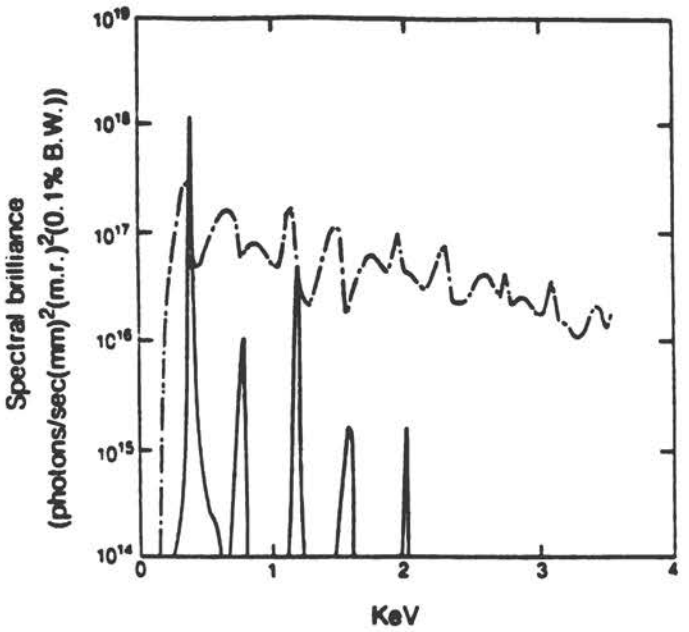


Figure 2. Spectral Brilliance as a Function of Photon Energy. Spectral brilliance through a pinhole aperture as a function of photon energy is shown for the 400-eV-fundamental-energy undulators of Table 1, for both the 1.3-GeV ring (solid line) and the 6-GeV ring (dashed line). The spectral brilliance and purity of the 1.3-GeV machine is diminished at 6 GeV, while the power to the optical element is increased.

Footnotes: Insertion-Device Properties

The fundamental wavelength λ_p of an undulator of period λ_u at an opening angle σ is:

$$\lambda_p^m = \frac{\lambda_u}{2\gamma^2 m}\left(1 + K^2/2 + \gamma^2\sigma^2\right) \qquad \text{(FN1)}$$

The radiation is emitted into an opening angle

$$\Omega = \left(1 + \frac{K^2}{2}\right)\frac{1}{N\gamma^2} = \frac{2\lambda_p}{L} \qquad \text{(FN2)}$$

The power in the fundamental is:

$$P\left(\lambda_p\right) \propto \frac{K^2 N}{1+K^2/2} \qquad \text{(FN3)}$$

The ratio of the total power to the power in the fundamental is:

$$\sum_m \frac{P_m}{P_1} = 1 + K^2/2 \qquad \text{(FN4)}$$

The total power from the device is:

$$P_T = 0.127\ (E(\text{GeV}))^2\ \langle B(\text{kG})\rangle^2\ L(\text{cm})\ I(\text{A}) \qquad \text{(FN5)}$$

Table 4

Undulator Performance on 1.3- and 6-GeV Machines

Conditions: The total power is constant in the comparison between the 1.3- and the 6-GeV rings at any energy, assuming that E^2B^2L is constant. That is, the beam current is fixed (at 400 mA) in the comparison.

Machine Energy (GeV)	E_1 (eV)	λ_u (cm)	B_o (T)	K	N	Total Power (W)	Power Density at 10 m (W/mm^2)	Power in the Central Spot (W)	Brilliance (photons/s·mm^2·$mrad^2$·0.1%BW)
1.3	100	10	0.12	1.1	50	30	0.7	1.6	3.2×10^{17}
6	100	95.5	0.0255	2.27	5	30	7	16	4.9×10^{16}
1.3	200	5	0.236	1.1	100	120	3.0	4.5	1.3×10^{18}
6	200	47.7	0.051	2.27	10	120	29	43.5	1.9×10^{17}
1.3	400	3.5	0.165	0.54	142	58	3.00	3	1.2×10^{18}
6	400	42.5	0.035	1.42	12	60	24	24	3.1×10^{17}
6	15,000	2.15	0.176	0.355	230	1400	1700	850	4×10^{18}

Generally, lower-K and higher-N devices (undulators) produce radiation with greater directionality. For a low-K undulator, the solid angle $\Omega = 1/\gamma^2 N$, and it contains a quasi-monochromatic beam with a fractional bandwidth $\Delta\lambda/\lambda$ equal to $1/N$. The total number of photons in this beam is increased by a factor of N and the brightness by a factor of N^2, compared with a beam from a bending magnet. Typically, $N = 100$, so the gains are substantial. As shown by Footnote 4, the power in the fundamental P_1 is a substantial fraction (two thirds) of the total device power P_{TOT} when $K = 1$, and $P_1/P_{TOT} \to 1$ as $K \to 0$. Therefore, the most efficient production of radiation in a narrow bandwidth around λ_p occurs for devices with $K \lesssim 1$. As K increases with fixed λ_p and L (by varying either λ_u or γ), the solid angle Ω remains constant. Thus, a high-K device is still capable of producing highly directional radiation of wavelength λ_p with N-fold intensity enhancement. However, this solid angle now includes substantial higher-harmonic power given by $P_1(K^2/2)$ and the bandwidth is increased to $(1 + K^2/2)/N$. This decrease in coherence is a direct result of the large angular excursions of the electron in a high-K device, which diminish the relative range of angles over which constructive interference occurs.

Before discussing the specific consequences of the behavior described above for the next generation of machines, one more point should be made. The brilliance of $K = 1$ undulator beams is potentially so high that their ultimate quality is strongly dependent on the emittance of the storage ring. First, the spatial size of the electron beam in a storage ring must be small enough so that at a reasonable distance d one can select out an area $d^2\Omega$ through which the first harmonic will pass. Second, the angular divergence of the electron beam should be on the order of $\Omega^{1/2}$ or smaller. For this reason, the next generation of storage ring will be designed with very low emittance.

Undulator Performance and Storage-Ring Design: The Need for Two Machines

Footnote 1 provides the basis for choosing the energy E of the machine necessary to produce a $K = 1$ device operating in the range $0.5\ \text{A} < \lambda_p < 1.0\ \text{A}$. For a fixed-length straight section, it is best to make the period λ_u as small as possible for $K = 1$. The limit on λ_u is determined by magnet technology and results in a machine-energy requirement of 6 GeV. There is a similar optimum energy of about 1.5 GeV for producing fundamental undulator radiation with $\lambda_p > 10$ A. Nevertheless, there is a basic asymmetry between the two machines: A high-energy machine can produce lower-energy undulator radiation by making λ_u or K larger, but a low-energy machine cannot produce first-harmonic radiation in the x-ray region because of the lower limit on λ_u. To use higher harmonics for this purpose requires large K and greatly diminished brilliance. Let us consider in more detail two important technical issues relevant to our recommendations: (1) the problems of producing

soft x-ray ultraviolet (XUV) (λ_p < 10 A) undulator radiation on a 6-GeV machine and (2) the thermal loads generated by hard-x-ray undulators on a 6-GeV machine.

(1) To produce λp = 10 A with E = 6 GeV requires a reduction in N (an increase in λ_u, for fixed L) and changes in either K or B or both. Table 4 compares XUV devices on the ALS machine with devices to produce the same λ_p on a 6-GeV machine. In this comparison K and B are changed in the device in such a way as to keep constant the total power produced. The result for the 400-eV device, for example, is a reduction in brilliance on the 6-GeV machine by a factor of four and a concomitant increase in the power in the central spot by a factor of eight. Clearly, the beam quality has diminished. Also, the power densities may exceed those tolerable on delicate XUV monochromators. In addition, the spectral purity is decreased, as shown in Figure 2.

(2) The power densities produced by hard x-ray undulators are clearly high, as demonstrated by the last entry in Table 4. This issue will be the subject of substantial research and development during the preparation of proposals for 6-GeV facilities. It is, however, already clear that the total power and power density can be withstood by properly engineered nonoptical components. This conclusion follows from considering the powers and power densities created in fixed-target x-ray tubes (~ 1/2 kW/mm^2). Starting from the power density of 2300 W/mm^2 at 10 meters that is listed in Table 1, adjustments should be made for the placement of components at larger distances from the source and and for the implementation of oblique-incidence geometries. Furthermore, for purposes of the comparison in Table 1, the same currents were used for both machines. It is unlikely that a 6-GeV machine would have such a high current. The combination of all these factors diminishes the expected power densities to a few tens of W/mm^2, well below known thermal limits for nonoptical components. Further research and development will be necessary to develop thermally robust optical components, but the situation is clearly less critical than for XUV optics.

To use a 6-GeV ring for soft-x-ray science, the higher-order power from the beam must be removed before the beam strikes the first focusing optical element. There exists in principle a solution to the higher-order-power problem, using total-external-reflection optics. The basic concept is that by properly chosing the mirror material and the angle of reflection, the unwanted high-energy photons can be absorbed on the first metal mirror. This is common practice in the hard x-ray region. For the XUV region, an aluminum mirror at 30-mrad incident angle would absorb the higher harmonics well at energies between 800 and 1000 eV. A fundamental difference between work in the XUV and the x-ray regions is that experiments in the XUV commonly span up to two decades in energy (e.g., 20 eV to 2000 eV), while in the x-ray they rarely span a factor of two. Utilizing the total-external-reflection phenomenon in the XUV region is thus much more complicated because for every factor-of-two energy range, a separate mirror is needed. Use of the total-external-reflection phenomenon in the XUV will be further complicated by

carbon contamination of the mirror, which is more of a problem in the XUV and which will occur at a higher rate on a 6-GeV ring. Research and development will be needed to determine the extent to which utilizing the total-external-reflection phenomenon can make a highenergy ring useful in the XUV region. While the above problems can be extreme on a new 6-GeV ring, they are much reduced on a 2.5-GeV machine like the NSLS.

In addition to the power-handling problem, the time structure of a 6-GeV machine will be worse than that of an ideally designed small ring by a factor of two to five. In principle, short pulses could be attained with a 6-GeV ring; this is accomplished with lattice changes and optics and rf-driver modifications that are more complex and expensive on a 6-GeV ring than on a 1.3-GeV ring. The cost of UV beamlines will also be higher on a 6-GeV ring, due to the scaling in size and the more complex optics.

Given these considerations, the need for for a 6 GeV ring as well as separate machines optimized in the hard and soft x-ray regions, respectively, becomes apparent. In determining the relative priority of the two machines, there are two factors to be considered.

1. There are no dedicated facilities where hard x-ray undulators can be developed, whereas some limited opportunities for developing XUV undulators do exist.

Of the two high-energy (E > 4 GeV) storage rings operating in the USA (PEP and CESR), neither has any prospect of dedicated operation. Nevertheless, important experience could be gained by developing undulators for research-and-development purposes on these rings. Such a device is now part of the SSRL (Stanford Synchrotron Radiation Laboratory) Enhanced Photon Flux Facility (SEPFF) construction project.

On existing dedicated lower-energy rings (the SPEAR, Aladdin, and NSLS rings), undulators to serve the XUV regime are now under design or construction. Because other undeveloped straight sections exist at these facilities, new construction could be undertaken to further increase the XUV capacity.

2. Although the low-energy ring cannot provide undulator capability in the x-ray region, the high-energy machine can access some of the XUV region, albeit with reduced performance.

The production of x-rays on a low-energy ring is limited to the use of high-field wigglers. Although these sources do not represent an improvement in flux over beams produced by bending magnets on SPEAR and at NSLS, they would represent an increase in capacity.

Soft x-ray undulator radiation produced on a high-energy machine would have a brilliance that is lower than that produced

on an optimal lower-energy machine but higher than that produced by existing devices. Therefore, in principle, the high-energy machine could provide new XUV capability. However, two substantial difficulties arise. First, the spectral purity is compromised, and second, the power in the central spot may exceed the power-handling limits of current optical technology.

Recommendations and Conclusions:

To meet the challenges and opportunities in both scientific-research and technological applications of SR, facilities will be needed that are dedicated to the utilization of insertion devices and that are readily accessible to the whole spectrum of university, industry, and defense interests. New machines dedicated to the utilization of insertion devices, even if they are developed on the most expeditious schedule, will not have significant impact until the late 1980s or early 1990s. Therefore, our recommendations include the full development of existing insertion-device capability, in parallel with the construction of new facilities specifically designed for the use of these devices.

I. Existing Facilities and Projects

The committee recommends that steps be taken to ensure the timely completion of the commissioning of the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory and the Synchrotron Radiation Center (SRC) at Stoughton, Wisconsin. We are encouraged by the actions at NSLS and SRC since our initial letter to the Department of Energy (DOE). To optimize utilization of existing facilities, we recommend providing operations funding, so that such facilities can provide a maximum of beam time in a "user friendly" mode, and continued research funding, so that it will be possible to take full advantage of the facilities.

To realize the full potential of existing facilities, the committee recommends expeditious completion of currently approved projects to construct insertion-device beamlines: the NSLS Phase II project at Brookhaven Laboratory and the SSRL Enhanced Photon Flux Facility (SEPFF) project at the Stanford Synchrotron Radiation Laboratory (SSRL). The future construction of additional insertion-device-based beamlines at existing facilities is strongly recommended.

II. Major New Facilities

The committee believes that major new programs based on the utilization of insertion devices are of central importance for effective progress in materials-science, physics, biology, and chemistry research over the next decade. The committee is therefore unanimous in its recommendations, which follow in order of priority.

1. The design and construction of a high-energy storage ring capable of providing fundamental undulator radiation in

the x-ray region of the spectrum up to 20 keV, with an early 1990s target date for full operation of the facility. To achieve this objective, appropriate research and development funding should be allocated now.

2. The construction of a second, lower-energy ring capable of providing fundamental undulator radiation in the soft x-ray region of the spectrum up to 2.0 keV. This machine should also provide picosecond (ps) timing capabilities. The Advanced Light Source (ALS) is such a machine.

The committee strongly recommends that no action based on the second-priority recommendation interfere with the timely pursuit of the first-priority recommendation.

III. Alternative-Source Facilities

Free-electron-laser (FEL), ultraviolet (UV)-laser, and laser-heated-plasma sources promise to make important complementary contributions at the low-energy end of the spectrum. To provide a complete full-spectrum capability, these sources should be developed in as timely a fashion as possible by their respective technical communities and funding agencies. However, the committee concluded that in the foreseeable future SR will continue to be the premier source of radiation in the soft x-ray and x-ray regions.

IV. Other Comments and Conclusions

The Need for Two Machines and their Relative Priority -- The physics governing the performance of undulators dictates that a machine designed to produce x-ray radiation at energies above 10 keV operate at a different energy level than a machine designed for the optimal production of soft x-ray ultraviolet (XUV) radiation at energies less than 2 keV. Using existing or anticipated technology, fundamental undulator radiation at 10 to 20 keV will require a 5 to 6-GeV machine, while optimized undulator radiation at less than 2 keV will require a machine operating at approximately 1.5 GeV. Factors governing the relative priority of these two machines include:

A. There are no dedicated facilities where x-ray undulators can be developed, whereas some limited opportunities for developing XUV undulators do exist.

B. Although the low-energy ring cannot provide undulator capability in the x-ray region, the high-energy machine can access some of the XUV region, albeit with reduced performance.

Commissioning of New Machines -- The difficulties being experienced in the commissioning of the newly constructed machines arise from overzealous attempts at economy, from some deficiencies in the project-management systems, and from a general lack of big-project experience in the materials-science community. These are

not fundamental technical problems and should be rectified in future projects.

Improving Access to Facilities -- The access to SR facilities is currently being restricted by two major factors. The first factor is the difficulty experienced by university-based groups in obtaining the funding necessary for participation. We recommend that beamline funding at future and existing facilities be provided in such a way that university-based groups can participate more readily. This cooperation would significantly broaden both the technical base that could contribute to innovations in instrumentation and the scientific base that could contribute to effective use of the facility. A proposal-based, peer-reviewed approach for the selection of outside participants is strongly recommended.

The second factor is the limitation on the participation of industry, university, and government laboratories that are performing applied research. In deciding which groups can participate in beamline usage, there is currently a bias towards fundamental research. The broadening of program-review committees to include applied interests, together with procedures to ensure more "user friendly" instrumentation and the protection of proprietary and classified interests, would increase the participation of applied-research groups.

Continuing Review -- The rapid developments in SR make it appropriate that a committee similar to ours convene periodically to review current developments in the entire field and to make recommendations for future actions.

Bibliography

Bienenstock, A. and Winick, H. "Synchrotron Radiation Research--An Overview." Physics Today. 36(6):48-56, 1983.

Brown, G. et al. "Wiggler and Undulator Magnets--A Review." Nuclear Instruments and Methods. 208:65-77, 1983.

Current Status of Facilities Dedicated to the Production of Synchrotron Radiation. Washington: National Academy Press, 1983.

Doniach, S. "Synchrotron Radiation: A Tool for Chemistry and Biology." Physica Scripta. T1:11-15, 1982.

Koch, E. E., ed. Handbook on Synchrotron Radiation. vol 1. Amsterdam: North Holland Publishing Co., 1983.

"Proceedings of the National Synchrotron Radiation Conference." Nuclear Instruments and Methods. 195, 1982.

Siegbahn, K., ed. "Proceedings of the International Conference on X-ray and VUV Synchrotron Radiation Instrumentation," Hamburg, 9-13 August 1982. Nuclear Instruments and Methods. 208, 1982.

Williams, G.P. "A Review of Synchrotron Radiation, its Uses and Special Technologies." Vacuum. 32(6):333-45, 1982.

Winnick, H. and Doniach, S., ed. Synchrotron Radiation Research. New York: Plenum Press, 1980.

ARGONNE PERSPECTIVE ON A 6-GeV SYNCHROTRON SOURCE

(Presented by K. L. Kliewer)

First of all, I wish to say that Argonne would like to build a 6-GeV source.

Let me then emphasize a point that, in my opinion, did not receive adequate emphasis yesterday, when the remarkable intensity from the 6-GeV source was almost invariably associated with undulators operating in the region around 10 kev. What I have shown in Figure 1 are spectra from three wigglers; one, the ALS spectrum, with a more or less typical wiggler -- we have taken the parameters out of published, or almost published, information; a similar spectrum for NSLS; and finally that for a 6-GeV ring with a 200-milliamp current.

What the cross-hatched region in Figure 1 emphasizes is that the 6-GeV source is going to provide, in addition to, of course, the range of high-enthusiasm undulator energy, also a regime of high energy/intensity that is essentially unavailable from other sources (CHESS being an energy exception). I think the high-energy radiation that is available with this particular system is something that should be kept in mind as we are thinking about sources for the future.

I would like to talk just briefly about a couple of the reasons that we feel this high-energy region is of particular importance, emphasizing the technological perspective as compared with the fundamental physics perspective. There is an elaboration on some of these results in the document that we provided to the Committee.

One of the vital questions in nuclear waste management is how to immobilize the appropriate atoms in glasses. There has been a recent study at Argonne in which uranium in various charge states in silicate glasses was investigated. The results obtained are really quite striking. If the uranium ions are in the +6 charge state, they order in sheets having roughly a uranyl character, as determined from EXAFS using the L_3 edge of uranium. Thus, the random distribution of uranium ions usually assumed is not valid; the uraniums cluster.

With the source that has been used to this point, namely a laboratory source, the clustering has been characterized, but not very well. What is needed to properly establish the size and character of these clusters is anomalous scattering, and such investigations require the level of intensity provided by the 6-GeV source.

If the charge state of the uranium ions changes to 5 or 4, which you can manage by controlling the chemistry in the preparation of the glass, then the world changes completely. No longer do the uraniums cluster. In addition, in the case of neptunium, you get a very lim-

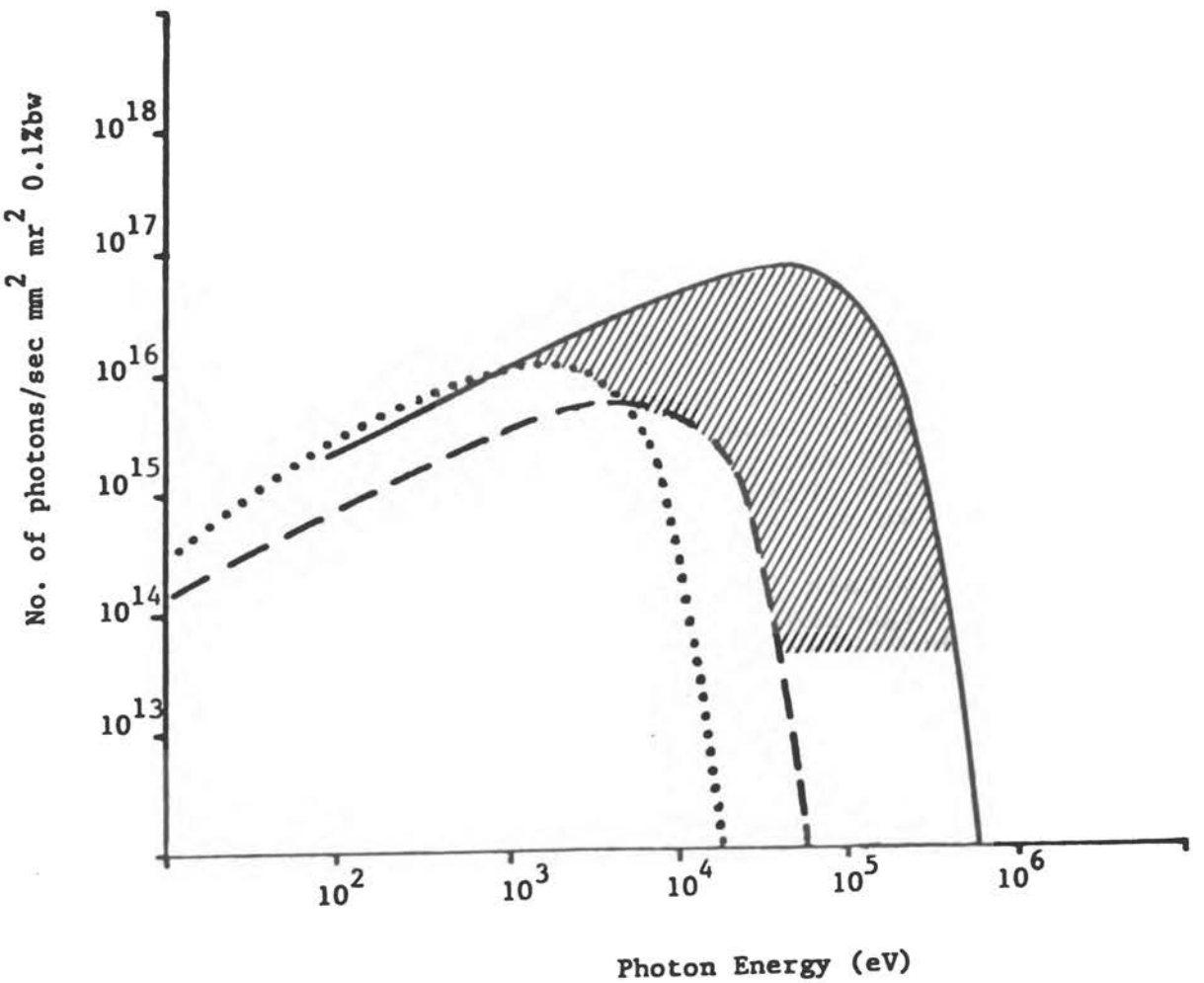


Figure 1. Photons from a Wiggler

Solid Line:	6 GeV, 200 mA, 2T, 25 periods, 10 cm/period
Dotted Line:	ALS, 1.3 GeV, 400 mA, 1.6T, 25 periods, 10 cm/period
Dashed Line:	NSLS, 2.5 GeV, 500 mA, 1.5T, 12 periods, 13.6 cm/period

ited local order, such that you need high intensity and high energies in order to be able to ascertain what is happening. In the case of plutonium, the local environment appears to be more regular so that better information can be obtained with EXAFS at present. These complex and important problems would obviously benefit from the availability of a high-energy, high-intensity source.

It is, of course, clear that effective nuclear waste storage is going to depend very much on not only what happens in the bulk, which is what I have been describing here, but also on what happens at the surface, that is, the leaching behavior. Will it be possible to examine in situ the leaching behavior with high energies, perhaps using SEXAFS? The anticipation is that it will be, although that is a question which at this moment must be considered as unanswered.

The subject of defects in ceramics emerged several times yesterday. Not a great deal has been done, but there are a large number of opportunities that one can pursue with high-energy x-rays. I am emphasizing ceramics here, structural ceramics in particular. If you want to get into the world of other structural entities, such as steels, the energies that we would have available with the systems we are talking about here are simply too low.

Let me discuss briefly the question of nondestructive evaluation of ceramics. The object here is to detect critical-size flaws in both green and fired ceramics. The amount of work that has been done in green ceramics is very small. It is a very interesting realm, where x-rays -- crude forms of x-ray microscopy are being used -- have shown microcracks, and thus demonstrated their capability for identifying the presence of critical-size flaws. The same is true in the fired state, but we have not yet gone to the point where we are able to deal with the fracture mechanics, that is, to take a real-time look at the consequences of applying stresses to these systems, watching the flaws grow to critical size, and then giving rise to fracture. The initial work that has been done with x-rays in the 40-kilovolt region does show a good bit of promise.

Even more enticing is the prospect of examining a sophisticated ceramic part, such as a turbine blade, in operation. In this case, you generally have a high-temperature oxidizing atmosphere. The thermal diffuse scattering is high. The scattering factor is reduced because of the high temperatures. Since we are addressing real systems, the parts are often not thin. As a result, you need high energy and high intensities in order to get the x-rays through and get the information out.

The initial estimates that we have come up with put these energies into the range above 50 kilovolts; some estimates have been considerably higher. Clearly, the energy depends upon the kind of system as well as the environment in which you are putting the part. In any

event, this problem would be well addressed via the opportunities afforded by a 6-GeV source, as indicated particularly by the cross-hatched region in Figure 1.

I would also like to emphasize another point that did not come up yesterday. Perhaps the world is now such that to evince imagination is to invite disaster. I think the record in science certainly has been that, when you open up new territory such as that indicated in Figure 1, progress occurs in unanticipated areas and in unanticipated ways. I really think we ought to allow for that; indeed, I think it a point of major importance.

That is not to say that this new frequency/intensity region is the only new territory that is being proposed. You have heard or are going to hear about lower-energy synchrotrons which offer similar frontiers in the world of timing. I am not trying to say this region of high frequency is a more important frontier, but rather that the very concept of a frontier is important, and one that should not be lost sight of in these deliberations.

Argonne has not been long involved in this world of synchrotron radiation, so what I would like to do now is to give you an indication of what is going on by way of source design. We have a design effort underway, and already have ideas about the kind of system that we would like to construct.

Our current plan involves a ring of eight hundred meters circumference, including 32 straight sections. The initial layout incorporates 16 wigglers (3.0 m straight sections) and 16 undulators (5.8 m straight sections). This wiggler/undulator division here is not important, because, if you look at the lattice of an accelerator of the sort that we are talking about here, it is a straight-forward matter to convert an undulator straight to a wiggler straight by merely removing a pair of quadrupole magnets; the machine must be designed so these quadrupoles are mobile. So, the important point here is that we have 32 straight sections, into which one can place insertion devices.

We show in Figure 2 a reasonable layout for an experimental hall, largely to set a scale here. A building that is 30 meters across can accommodate beam lines 80 m long, which should be enough to provide the requisite flexibility. I think it fair to say that the design of a 6-GeV ring, while requiring substantial engineering and scientific sophistication, is not going to involve great conceptual steps. We are thinking about 200-MeV injection from a microtron. A microtron, of course, affords economical construction and economical operation, so one is well advised to pursue that direction. The rest of the system is basically standard, a fast-cycling synchrotron top-loading into a 6-GeV storage ring.

One point that was discussed at some length yesterday was the

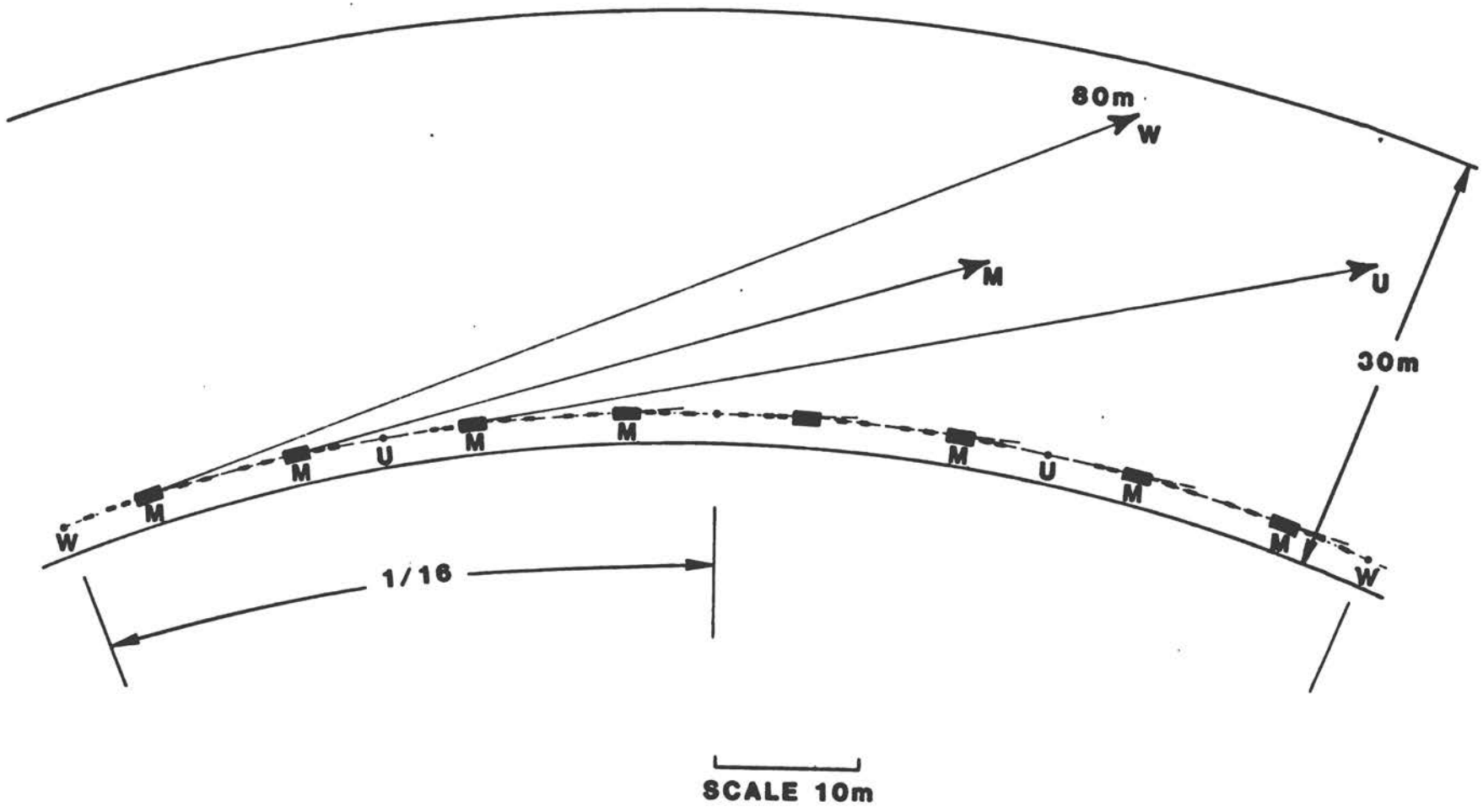


Figure 2. The layout of the experimental hall showing the ring (M=bending magnet; W=wiggler; U=undulator) and a hall width of 30 m. Note that this hall could readily accommodate an 80 m beam line.

matter of power-loading of beam line components and optical instrumentation. This is something in which the entire community, I think, is going to play a role. The Brookhaven people, with the effective cooperation of the group in Materials Science in DOE (headed by Don Stevens at that time), did something important when they started the whole PRT concept. Getting groups of interested people involved in constructing beam lines has had many beneficial consequences.

In the Eisenberger-Knotek Report it is recommended that beam lines be constructed along PRT lines, that is, interested groups submit proposals which, when accepted, provide the opportunity to generate a beam line. I strongly endorse this recommendation. For it to succeed, we must make sure that people recognize that this kind of opportunity will be there and encourage them to begin thinking about instruments and associated problems.

A concerted attack on the problems of x-ray optics at high intensity is clearly needed. There are now such efforts underway, at Berkeley and at other laboratories. I would like to see these efforts coordinated and collaborative, since the problems are common to all and the success of this venture depends upon their solution.

What time schedule for a 6-GeV source is possible? Note that I said possible and not probable, considering the many realities, political and otherwise, that enter into plans of this sort. I thought it would be worthwhile here to sketch the kind of time scale that we see as reasonable at this point, if one moves in a genuinely determined fashion; this is done in Figure 3. Somewhere about 1989, one could begin inserting all of the hardware into the building, culminating in beam available at some point toward the end of fiscal year 1990. This may be slightly optimistic, but I think this schedule realistic, even if improbable.

I want to make a couple of points here that I might call sociological. Argonne started asking questions several months ago as to whether there would be any interest in having a 6-GeV source located in our region. We found the amount of interest to be extensive on the part of currently active x-ray users, including people working actively as parts of PRTs at NSLS and people working regularly at CHESS, SSRL, and other synchrotron sources. We also found intense interest on the part of the low-energy users, the group closely associated with Tantalus and preparing to use Aladdin. I might just interject here, paranthetically, that Argonne is part of a team building a "hot" beam line at Aladdin, one that will accommodate studies of radioactive samples. So if any of you are interested in doing such work at moderate energy, there will be a beam line available before long.

In addition, we found that there were lots of people who, though not previously attacked by the synchrotron radiation bug, found the prospects of the 6-GeV source of real interest. They seemed to come

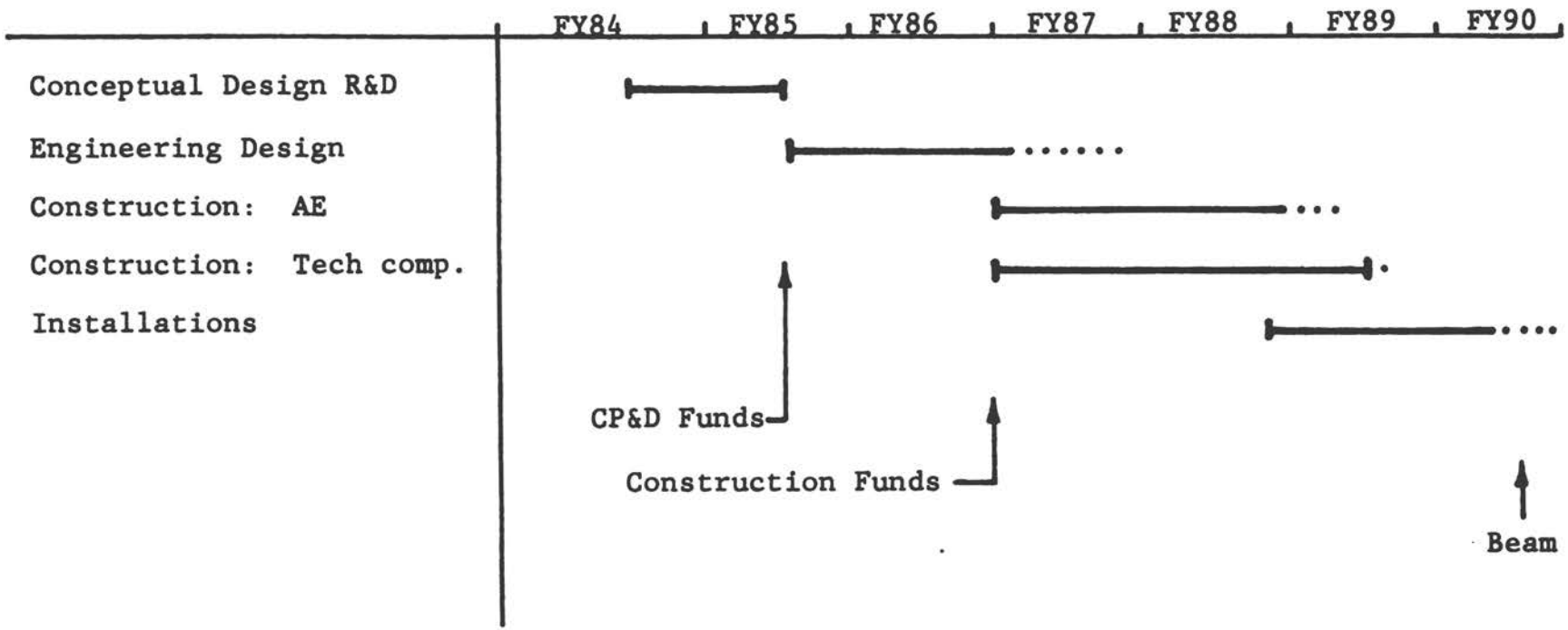


Figure 3. A possible time scale for the 6 GeV source.

from two communities, materials science/solid-state physics and biology/medicine. I think that this is going to translate into a substantial additional user community for the 6-GeV ring.

Finally, I want to emphasize a point that may not need emphasis. We found this widespread interest directed toward a 6-GeV source, not a source at a specific location.

Why should the U.S. put a 6-GeV ring at Argonne? I would just like to point out a few reasons here, focusing on materials science. The materials science effort in the region is extensive. Argonne materials programs are large. There are three regional Materials Research Laboratories, at The University of Chicago, Northwestern, and the University of Illinois at Champagne/Urbana. A point warranting particular emphasis is the major materials programs at many area universities. As most of you know, the area around Argonne includes a large number of excellent universities, many of which are large. The result is that there are a great many students in the area associated with many professors who have close connections with the synchrotron sources around the country or are interested in the 6-GeV source. A source located in this region would, thus, find itself a focal point for educational opportunity. We, and I think almost everyone, feel this of particular importance in making a move of the sort that we are contemplating here.

Industrial research in the area is strong and expanding. Highway 5, heading west out of Chicago, may not yet be Route 128, but the developments there are really quite astonishing.

I also want to pick up on the point that Brian Fender made last night: the virtue of the proximity of important and complementary user facilities. Aladdin, at the University of Wisconsin, will, it is to be hoped, soon be operating effectively. This is a 1-GeV ring which will provide VUV and soft x-ray radiation, with programs building from those at Tantalus, a system which has been so effective in establishing and promoting synchrotron radiation use in this country.

In addition, the Intense Pulsed Neutron Source (IPNS) at Argonne has demonstrated very effectively the role of pulsed neutrons in materials science. I won't say anything more about that; Gerry Lander will be addressing this facility shortly.

A very important consideration: These machines that I have referred to here are embedded in environments where there is a great sensitivity to users. This is a prime consideration. Running a user facility requires a great deal of sensitivity and a lot of resources. In order to make it work, you have to work hard at it, and I think the record in the area of having succeeded in that realm is truly exemplary.

The opportunity to construct a 6-GeV source should clearly go to an institution which warrants the confidence of the community that the job will be done well. Argonne has an excellent record in the world of accelerators, and I list some of its accomplishments here.

Argonne Successes in Accelerators

- Zero-Gradient Synchrotron (ZGS) - 12 GeV proton synchrotron
  - * User oriented - 12 simultaneous beam lines
  - * Reliability about 90% for 10 years
  - * Polarized protons
- Rapid-Cycling Synchrotron (RCS) now part of IPNS System - 500 MeV, 30 Hz protons
  - * First proton synchrotron spallation source, H^- injection.
  - * Highest current such system in the world
  - * Reliability exceeds 90%
- Argonne Tandem Linear Accelerator System (ATLAS) - 25 MeV/nucleon superconducting heavy ion accelerator
  - * Innovative superconducting technology
  - * Precision beams
- 22 MeV Electron Linac
  - * Pulses: 1000 A, 30 psec, 800 Hz
  - * Key facility of the extensive Argonne radiation chemistry program

Reliability has been specifically mentioned twice in this listing and this is a point that does warrant emphasis. In the world of high-energy physics, there seems to be a certain fatalistic acceptance of the fact that machines don't always work. In the world of condensed matter science, that fatalistic acceptance simply does not exist. When a user is called and told his experiment can run on Tuesday, April 17, at 1 o'clock, this user expects that that is going to happen. So, the matter of reliability in a machine is of extreme importance to this particular community, which has not grown up in the

sociology of high-energy physics.

In addition to these established successes, Argonne has been involved in major accelerator design efforts, some of which are:

- Argonne Super Pulsed Neutron Source (ASPUN)
  - * Extraordinary System
  - * 1500 MeV, 3.8 mA FFAG (500 MeV, 100 μA prototype)
- Synchrotron for German Pulsed Neutron Source (SNQ)
  - * 1.1 GeV, 500 μA, 50 Hz
  - * 7×10^{13} protons per 200 nsec pulse
- 4-GeV Electron Microtron
  - * Innovative
  - * Multiple, precise beams
  - * 300 μA

I would like to mention that Yanglai Cho, who is the head of our synchrotron source design effort, had the major responsibility for the design of the synchrotron for the German SNQ project. Also, our design team is not operating in isolation. Dr. Cho is now working with the University of Wisconsin group on Aladdin, and with the Fermilab people interested in accelerating electrons. Of course, Argonne's accelerator group is also involved with the SSC.

It is evident that Argonne is well located in an easily reachable place, another point of importance for a major user facility. Some additional site attributes are noted below:

- Multi-purpose, multi-disciplinary Laboratory (1550 scientific and professional staff)
- Scientific Support Systems
  - * On-site lodging (112 rooms and apartments), travel office, and cafeteria
  - * Machine shops
  - * Plastics shop

* Electronics Division
* Engineering Division - designed and built IPNS
* Graphic Arts
* Occupational Health and Safety
* Computing Services
* Libraries
* Medical Office, Paramedics, and Fire Department

It should also be noted that the 6-GeV source at Argonne could exploit a number of the resources associated with the ZGS complex, including adequate supplies of electric power and cooling water capacity, a two-electric-grid connection for additional reliability, and an extensive complement of office and laboratory buildings.

Last night, Brian Fender described the ILL dream, the location of the European high-energy synchrotron source juxtaposed with the neutron source at Grenoble. Argonne has a comparable dream, the colocation of the 6-GeV source and a new ultra-high-power spallation neutron source. Our current version of the dream is shown in Figure 4.

What we are trying to do, of course, by juxtaposing these sources is to enhance the exploitation of the complementarity between neutron scattering and photon scattering. That is, I think, a point of major importance.

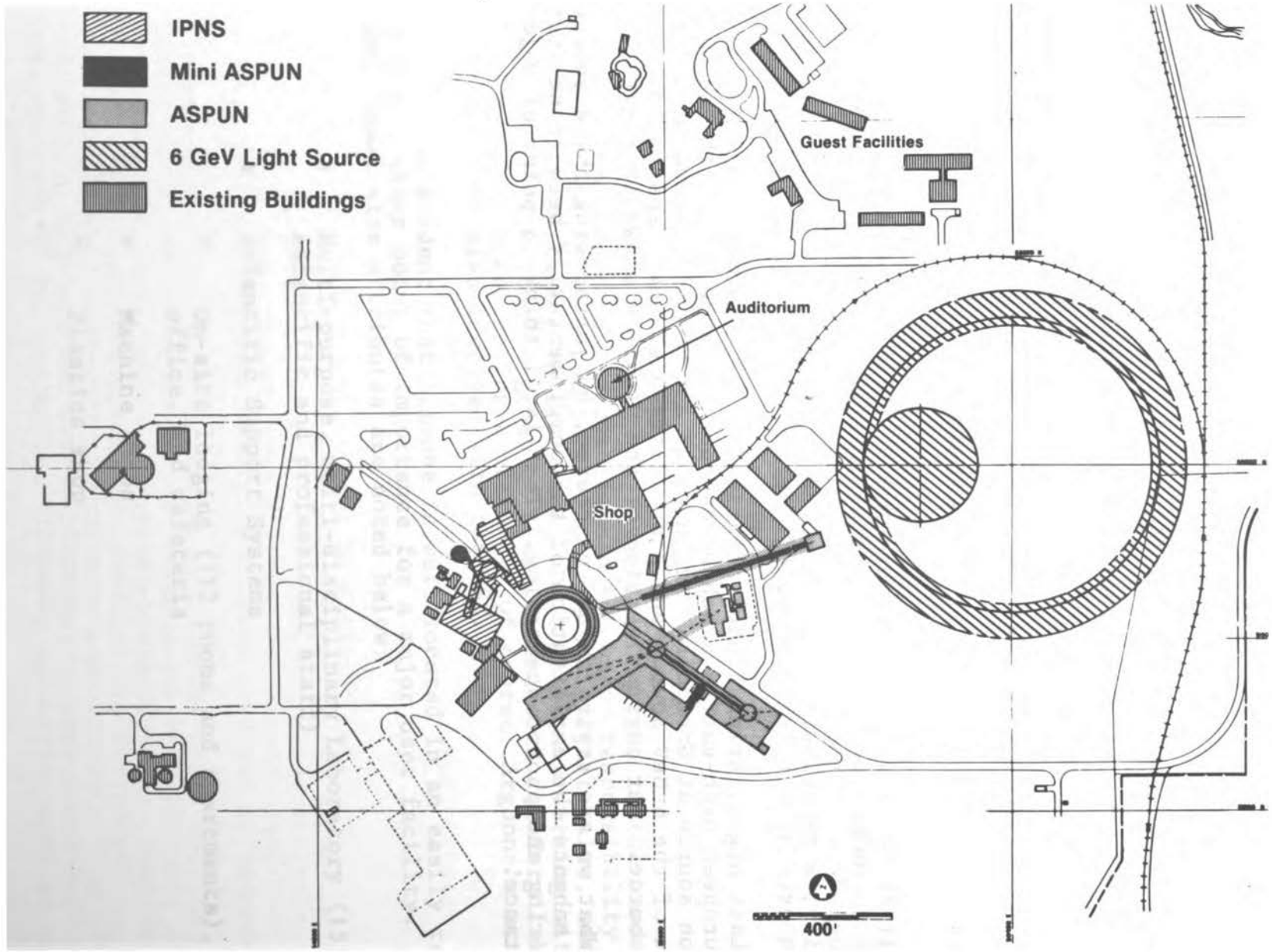


Figure 4. Proposed site of 6 GeV ring.

nsls

PLANNED EVOLUTION OF NSLS

February 1984

NATIONAL SYNCHROTRON LIGHT SOURCE

BROOKHAVEN NATIONAL LABORATORY
ASSOCIATED UNIVERSITIES, INC.
UNDER CONTRACT NO. DE-AC02-76CH00016 WITH THE
UNITED STATES DEPARTMENT OF ENERGY

PLANNED EVOLUTION OF NSLS

February 1984

NATIONAL SYNCHROTRON LIGHT SOURCE DEPARTMENT

Brookhaven National Laboratory

Associated Universities, Inc.

CONTENTS

Plan for NSLS Evolution

NSLS High Energy U/W Ring

Phase I

Phase II

PLAN FOR NSLS EVOLUTION

SUMMARY

An evolution of synchrotron radiation capabilities is proposed for the National Synchrotron Light Source at Brookhaven National Laboratory. Its purposes are:

1. To optimize the scientific return on the substantial investment of money and human effort both by PRT groups and BNL-DOE.

2. To maintain a world-leading position in forefront capabilities building on existing resources supplemented by complementary new facilities.

3. To open up new scientific and technological opportunities.

4. To increase the total number of experimental stations for a growing user community.

Specifically, full energy injection and the possiblity of operating both existing rings in top-off mode are planned. For the x-ray ring this requires construction of a new booster. This booster is planned to have ejection capability up to 6 GeV to accommodate the next generation ring, whenever it seems scientifically justified.

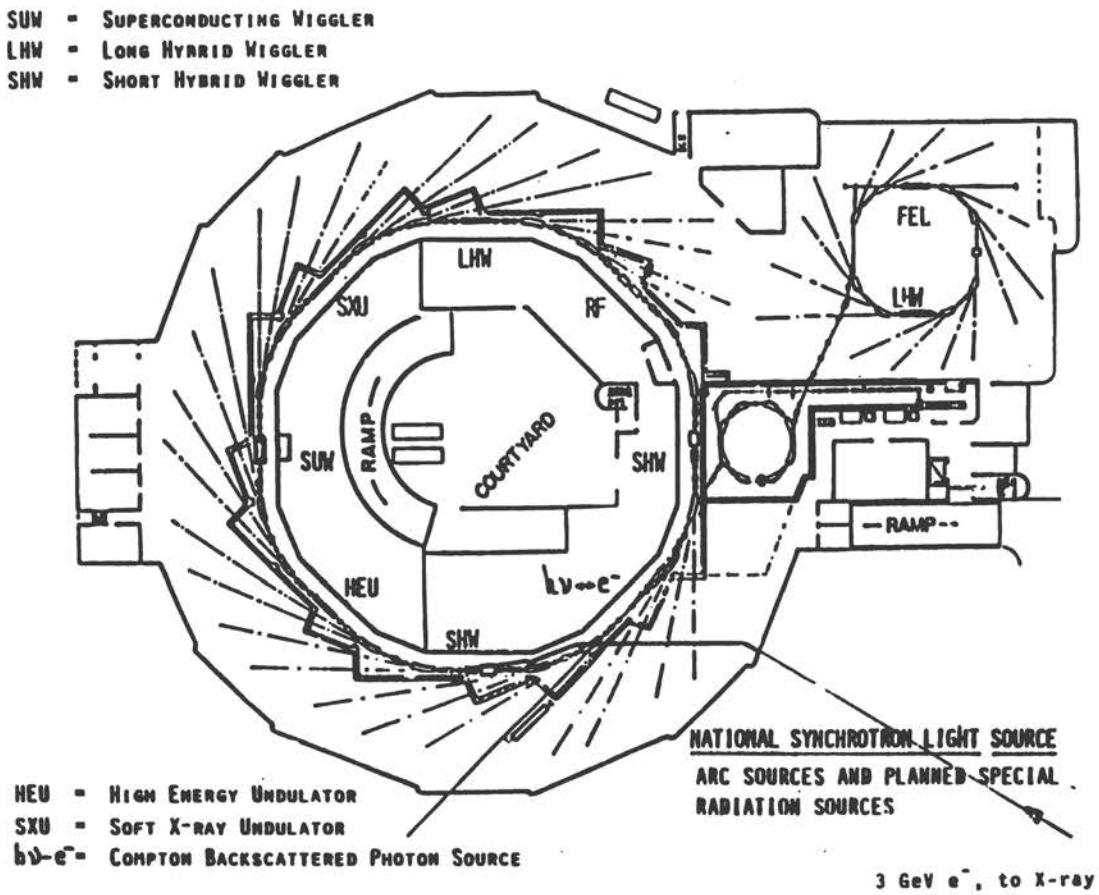

SUW = Superconducting Wiggler
LHW = Long Hybrid Wiggler
SHW = Short Hybrid Wiggler
LHW
SXU
RF
FEL
LHW
RAMP
SUW
COURTYARD
SHW
RAMP
HEU
hν-e⁻
SHW
NATIONAL SYNCHROTRON LIGHT SOURCE
ARC SOURCES AND PLANNED SPECIAL
RADIATION SOURCES
HEU = High Energy Undulator
SXU = Soft X-ray Undulator
hν-e⁻ = Compton Backscattered Photon Source
3 GeV e⁻, to X-ray

FIGURE 1

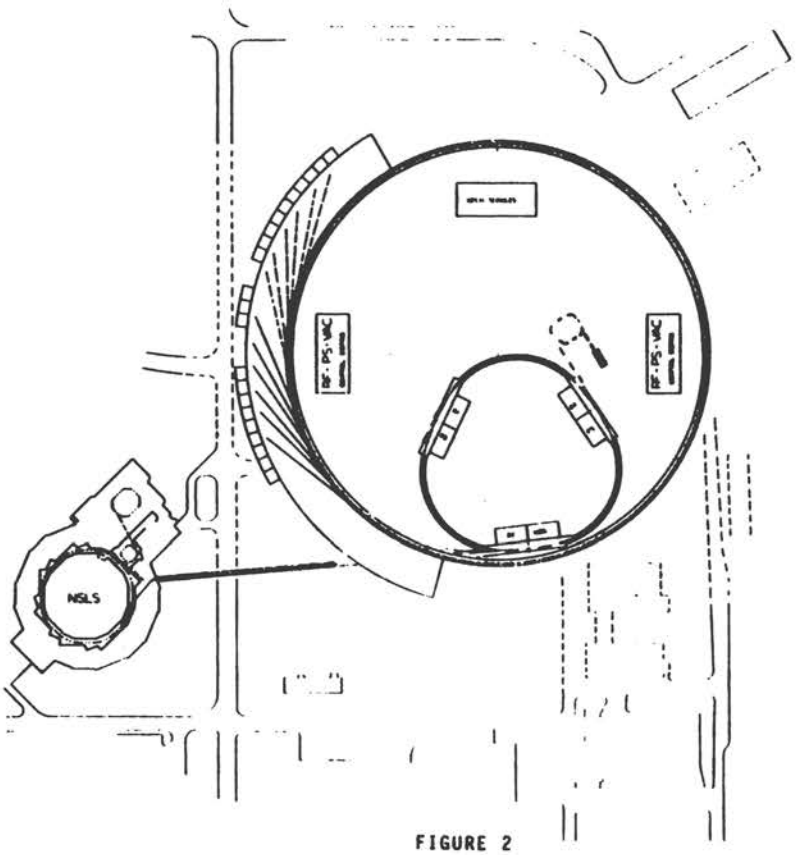


FIGURE 2
NSLS PHASE III
HIGH ENERGY U/W RING AND BOOSTER II (6 GEV)

ADVANTAGES OF NSLS EVOLUTION

1. Maximizes return on existing user investment

    a. Full energy injection maximizes beam position stability with possibility of top-off mode.

    b. Modular design minimizes disruption of ongoing activities

2. Maximizes return on existing facility investment

    50 m and 170 m storage rings, linac, 750 MeV booster, laboratories, buildings, computers, shops, etc.

3. 6 GeV ring creates new scientific opportunities

    - High energy photons
    - Ultra-bright X-ray insertion device sources

4. Maximum flexibility to respond to evolving new science and new user needs

    e.g., operation of 170 m ring as low emittance UV source; 50 m ring as FEL, TOK ring; X-ray lithography on 170 m ring; etc.

NSLS, February 1984

PLAN FOR NSLS EVOLUTION

The motivation behind the planned NSLS evolution is to maintain a world-leading position in forefront capabilities, building on existing resources supplemented by complementary new facilities. The first efforts will be to enhance the performance characteristics of both the UV and X-ray rings. A major component of this is to enable full energy injection of each ring, including the capability of injection in a top-off mode. In order to take optimal advantage of low emittance beams it is necessary to maintain beam position to a fraction of the beam size, not only for a given fill, but from fill to fill. Thus, for the UV ring, vertical stability should be maintained to better than 0.1mm. The cycling of ring dipole magnets when injection is made at an energy different from operation energy makes this very difficult to achieve. Accordingly, the booster ejection components are presently being upgraded to allow ejection at 750 MeV.

The importance of beam positional stability is at least as great in the X-ray ring, so full energy injection (up to 3 GeV) is important there too. However, there the top-off mode may play a role in optimizing experimental capability, since the high photon flux on optical elements can cause current dependent distortion.

Plans for the design, siting, and commissioning of this new booster ring have been made so that construction and commissioning will not interfere with ongoing operations. Also, the NSLS plans for the booster have been made to allow full energy injection not only of the existing 2.5-3.0 GeV ring, but for the 6 GeV one as well.

The existing X-ray ring was designed for a maximum energy of 2.5 GeV, however, easy upgradeability to 3 GeV was allowed for. The dominant component of increasing the energy to 3 GeV involves the addition of radiofrequency acceleration stations. Additional rf cavities are presently in the construction stage. With the presently installed rf power amplifiers and a complement of four rf cavities, a beam energy of 3 GeV, with a 250 mA circulating beam can be achieved.

The basic parameters of the Booster II synchrotron are as follows:

Energy	6	GeV
Circumference	340.3	m
Magnetic Radius	26.7	m
Beam Current	5	mA
Radio Frequency	370.2	MHz

With the anticipated initial 3 GeV operation, a good fraction of the rf hardware could be postponed in construction. It is desired, however, to avoid subsequent interruptions of the X-ray program, therefore, it is planned to install the full rf cavity complement at construction.

The siting and construction of the Booster II and its associated tunnels and service buildings would take into account the construction of the 6 GeV undulator/wiggler ring, which would have to be carried out with no interruption of the X-ray ring experimental program. Re-injection of the 3 GeV beam into the X-ray ring has been examined. In crossing the X-ray experimental area the charged particle beam transport would pass under a number of photon lines in a manner analogous to that done presently with the Booster I to VUV storage ring transfer line.

A preliminary study of a high electron energy, "Undulator/Wiggler" synchrotron radiation source has been carried out with the objective of potentially providing for ultimate brightness radiation sources in the hard part of the X-ray spectrum. The design parameters were guided toward the use of a 0.86 Å first order spectral peak from a state-of-the-art permanent magnet undulator source. This then led to a maximum electron energy of 6 GeV. The design of this storage ring was also optimized for minimum source emittance, following the original Green-Chasman lattice concept. This resulted in the following principal parameters:

U/W Ring Energy	6 GeV
Current	250 mA
Circumference	753 m
Magnetic Radius	33.4 m
ε_H	7×10^{-9} mrad
ε_V	7×10^{-10} mrad

With a superperiodicity of 16, this ring permits the ultimate use of (28 - N_W) undulators, N_W wiggler sources, (32 - N_{WS}) dipole sources and N_{WS} short wiggler sources.

MSLS HIGH ENERGY U/W RING

6 GeV RING

- HIGHER PHOTON ENERGY

  UNDULATORS → 5 TO 20 keV

  WIGGLERS → 20 TO 50 keV

- HIGHER PHOTON FLUX

  X 10 OVER EXISTING MACHINES

- HIGHER PHOTON BEAM BRILLIANCE

  X 10^4 AT 15 keV
  (3 GeV WIGGLER VS 6 GeV UNDULATOR)

- ANGULAR RESOLUTION

$$\frac{1}{\gamma\sqrt{N}} \sim 10^{-5} \text{ RAD} = 2 \text{ ARC SEC.}$$

- SPATIAL RESOLUTION

100 : 1 DEMAGNIFICATION ➡ $1\mu^2$ SPOT

- ENERGY RESOLUTION

$10^{10} - 10^{11}$ PHOTONS/MEV AT 15 KEV

- TEMPORAL RESOLUTION

ALSO, MORE CAPACITY

SPECIALIZED BEAMLINES

HARD X-RAY

DIFFRACTION TECHNIQUES

- CRYSTALLOGRAPHY
  - SMALL SAMPLES
  - FASTER DATA COLLECTION
  - BETTER RESOLUTION
- SURFACE SCATTERING
  - LOWER $\not{Z}$
  - CORRELATIONS TO 10μ
  - MAGNETIC SCATTERING
- INELASTIC SCATTERING
  - 1-10 MEV ΔE
- SMALL ANGLE SCATTERING
  - 10^{-5} RAD $\Rightarrow$ LENGTH >1μ
  - ISOTROPIC BEAM
- ANOMALOUS SCATTERING
- POWDER DIFFRACTION
- TOPOGRAPHY

SPECTROSCOPY TECHNIQUES

- EXAFS PARTICULARLY SEXAFS 1/1000 MONOLAYER SENSITIVITY
- NEXAFS
- MICROPROBE

GENERAL

TIME-DEPENDENT

MICROSCOPY STUDIES

SOFT X-RAY

SOFT X-RAY MICROSCOPY, HOLOGRAPHY

SPIN-DEPENDENT PHOTOEMISSION

COINCIDENCE EXPERIMENTS

GAS PHASE SPECTROSCOPY

PHOTON STIMULATED DESORPTION

EXAFS SEXAFS NEXAFS

DISCIPLINES

PHYSICS	NUCLEAR PHYSICS
BIOLOGY	EARTH SCIENCES
CHEMISTRY	METALLURGY
PLASMA PHYSICS	DEFENSE APPLICATIONS
MEDICAL APPLICATIONS	SURFACE SCIENCE

SEE PLANNING STUDY REPORT

NSLS Booster II

Parameters (general)

Energy (GeV)	6(3)*
Circumference (m)	340.34
Bending Radius (m)	26.723
ν_{RF} (MHz)	370.216
h	420
Beam Current	5
Lattice, Symmetry, N_c	FoDo, 3 fold, 27
Dipole Field, B (kG)	7.5 (3.75)*
Injection Energy (GeV)	0.8
Cycling Rate (Hz)	0.33 (0.5)*

*For X-ray Injection

NSLS HIGH ENERGY U/W RING

PRELIMINARY PARAMETERS

Energy (GeV)	6
Periodicity	16
Circumference (m)	753.58
Bending radius (m)	33.40
ν_H, ν_V	-25; -9
Momentum compaction, α_p	$4.5\ 10^{-4}$
ε_H (m.rad)	$0.7\ 10^{-8}$
ε_V (m.rad)	7.10^{-10}
Dipole field, $\hat{B}$ (kG)	7.5
Sextupole strength, B'' (kG/m^2)	-120
Number of "high β" long straights (Xp = 0)	16
Number of "low β" long straights (Xp = 0)	16
Beam current (mA)	250
Bunch Length (at I = 0) (ps)	22

HIGH ENERGY U/W RING

Radiation Sources

Undulators	$\leq (28-N_W)$
(L = 5m; λ = 2cm; N = 250)	
λ_1 (Å)	0.86
K_u	0.6
Gap (mm)	13.0
$2\hat{\theta}_{1/2}$ (mrad)	0.13
Flux at λ_1 (Ph/sec, 0.1% $\Delta\lambda/\lambda$)	$2.7\ 10^{15}$
σ_x, σ_y (mm, mm)	0.53; 0.10
σ_x', σ_y' (mrad, mrad)	0.013; 0.007
Source brightness* (ph/sec/mm^2/mrad^2/0.1% $\delta w/w$)	$2\ 10^{19}$
Short Wigglers ("Hybrids")	$\leq N_{WS}$
λ_c(Å)	0.09–0.35
Flux at λ_c (Ph/sec/0.1% $\Delta\lambda/\lambda$/mrad)	$8.8\ 10^{14}$
(L = 1 m; λ = 9.5 cm; N = 10)	

HIGH ENERGY U/W RING

Wigglers (hybrid-permanent magnet)	N_W
(L = 2.5m; λ = 9.5cm; N = 25)	
λ_c (Å)	0.35
K_w	13.3
Gap (mm)	14.0
$2\hat{\theta}_{1/2}$ (mrad)	2.2
Flux at λ_c (Ph/sec/0.1% $\Delta\lambda/\lambda$/mrad)	$2.2\ 10^{15}$
σ_x, σ_y (mm, mm), at center	0.26, 0.02
Source brightness (Ph/sec/mm^2/mrad^2/0.1% $\delta w/w$)	$3\ 10^{16}$
Dipole Sources	$\leq(32-N_{WS})$
λ_c (Å)	0.86
$\Delta\theta$ (mrad)	10
Source brightness (ph/sec/mm^2/mrad^2/0.1% $\delta w/w$)	$4.3\ 10^{15}$

PHASE I

PHASE I

The NSLS at Brookhaven National Laboratory is the first dedicated synchrotron radiation source in the U.S. with storage rings individually optimized for high brightness in the X-ray and UV regions, respectively. It is a national user facility, with user groups organized principally into Participating Research Teams (PRTs), who have committed substantial resources and personnel for the construction and operation of beam lines on which they will utilize up to 75% of the operating time. (The remaining time is available to general users.) Representation in these PRTs includes 31 universities, 12 corporations, and 9 government laboratories. Investment in beam lines to date is approximately $25 M, about equally distributed between universities, industrial laboratories, and government laboratories.

Storage Ring Characteristics

A schematic outline of the NSLS injection and storage ring system is shown in Fig. 3. Electron pulses reach an energy of 70 MeV in the linear accelerator and are accelerated to 700 MeV in the Booster synchrotron, with a cycling rate of 1 Hz. Switching enables injection into either the VUV or X-ray ring from this common system.

The VUV storage ring is a four superperiod machine of ~51 meters in circumference. Its principal design parameters are 700 MeV and 1 Ampere circulating beam current. Presently it operates at 750 MeV, has achieved peak beam current values of 400 mA and a source brightness value of about 4×10^{13} potons/sec, mm^2, $mrad^2$, 0.1% bandwidth. As such, it is the highest brightness VUV synchrotron radiation source in operation.

The four 3.2 long straight sections of the VUV storage ring are used for beam injection and a radio frequency station, plus two long straights for beam insertion devices. One of these is now used for a 38-pole permanent magnet undulator, which has been installed and operated, and is now being instrumented for usage in the 100-1000 Å range. It provides for a potential brightness increase, compared with a VUV arc source, of approximately a factor of 100.

The photon beams are transported from each VUV bending magnet, with a radiation fan of 75 mrad and 90 mrad, respectively. The fluence is approximately 10^{14} photons/sec/mrad/1%($\Delta\lambda/\lambda$) at the critical wavelength of about 25 Å (750 MeV). The VUV photon spectrum is shown in Fig. 4 for a standard arc source, the permanent magnet undulator and a future hybrid wiggler. Details on beam parameters at the source location are given in Table I. At design conditions, the maximum source brightness at approximately 1 keV photon energy is 3×10^{14} ph/sec/mm^2/$mrad^2$0.1%($\Delta\lambda/\lambda$) for the VUV arc source.

The X-ray ring is similar in optical design to the VUV storage ring. It is comprised of eight achromatic bend superperiods, thereby providing for a greater number of possible beam insertions. The maximum radiation fan in an X-ray port is 50 mrad which is typically subdivided into two or three beam lines. The maximum integrated photon flux for the X-ray ring design parameters of 2.5 GeV and 0.5 A, is ~3 x 10^{15} photons/sec/1%($\Delta\lambda/\lambda$)/(0.5 A) at the critical wavelength, for an arc source, of 2.5 A. The spectra for both an arc source and the superconducting wiggler source, shown in Fig 5, demonstrate the extent to which the spectrum is extended into the hard photon region with the incorporation of the 60 kG wiggler in the X-ray ring. At 100 keV photon energy, a flux of ~10^{14} photons/sec/mrad/1%($\Delta\lambda/\lambda$)0.5 A is achieved. Presently the X-ray ring has operated up to 2 GeV in beam energy with modest beam lifetime and beam current. A commissioning program is in progress to enhance the beam intensity and align the external photon lines with the emerging photon fans from the X-ray ring. Seventeen front ends are operational and 25 "hutches" are assembled and being outfitted with experimental equipment.

For the NSLS rings the thresholds for the various modes of instability have been calculated and correctons have been designed. Presently the dominant mode encountered in the VUV ring is the longitudinal coupled bunch instability caused by the beam in conjunction with the rf cavity parasitic mode impedances. A feedback system has permitted three bunch operation without longitudinal coupled bunch instabilities. Therefore, a one or three bunch mode of VUV ring operation has been established, which, for one bunch operation resulted in a (present) maximum current of 400 mA, but with greatly improved beam stability and source brightness. The one bunch results are summarized for the VUV ring in Table II. Inital three bunch studies have shown a doubling of beam lifetime in comparison to the one bunch mode at the same average current. Future improvements in the source emittances should result from a resurvey and realignment of storage ring magnets during the next long shutdown and the overall current values should improve after a tune-splitting cavity is installed this winter.

Experimental Facilities

During the period August, 1982 to August, 1983, which represents the first year of experimental operations on the VUV storage ring, there were 92 different users from 22 separate institutions. At the start of this period, typical beam currents were 80 mA at 600 MeV with a 30 minute lifetime. At the present time, typical beam currents are 300 mA at 750 MeV in a single bunch mode with a two hour lifetime. The VUV ring is filled three times a day with beam available from 4:00 A.M. to about 7:00 P.M. (later in the case of an extra afternoon fill). Over the last three months of this period, beam was on average, available for 47 hours out of a maximum possible of 55 hours (i.e., 85% efficiency).

When PRT proposals were first solicited in 1979, there was an overwhelming response from the scientific community which clearly perceived the advantage of having dedicated experimental facilities on what would be the worlds brightest sources of X-ray and UV radiation. The involvement of

scientists from the full spectrum of U.S institutions is clearly shown in Table III, where PRT membership is displayed according to institutional type—university, corporation, or government (Table IV lists the individual PRT members from each institution). After January 1980, at which time the majority of the present 30 PRTs were approved, there began an intensive design effort. There was considerable collaboration between the NSLS and the PRT scientists in arriving at final designs for optical components (monochromators, mirrors, slits, etc.) and many beam line components designed by the NSLS were constructed or purchased jointly with PRTs resulting in a lower unit cost for these items.

The PRT policy has made it possible to simultaneously build up scientific capability in a number of different areas. The capabilities available at the NSLS can be seen in Tables V and VI where the UV and X-ray beam lines are shown for each port (a storage ring port is divided into two to four beam lines with each beam line fully instrumented for a particular type of experiment).

In April 1983, general user UV proposals were solicited for the ten UV beam lines that were commissioned (these lines are denoted by asterisks in Table V). Approximately ten months were required to commission this first group of UV beam lines from the time that photons were first made available for alignment.

At the present time, there are 11 UV beam lines that have been commissioned and 46 beam lines (16 UV beam lines and 30 X-ray beam lines) in a design/construction phase. Approximately half of the 30 X-ray beam lines will enter an early commissioning phase this spring when the first alignment photons are provided to beam lines.

In Table VII and VIII, the different beam lines are grouped according to experimental techniques (e.g., small angle X-ray scattering) and discipline (e.g., biology), and the total number of beam lines available for each experimental technique is given. Because most of the techniques have applications in more than one discipline, collaborations between scientists from different institutions and disciplines have been promoted.

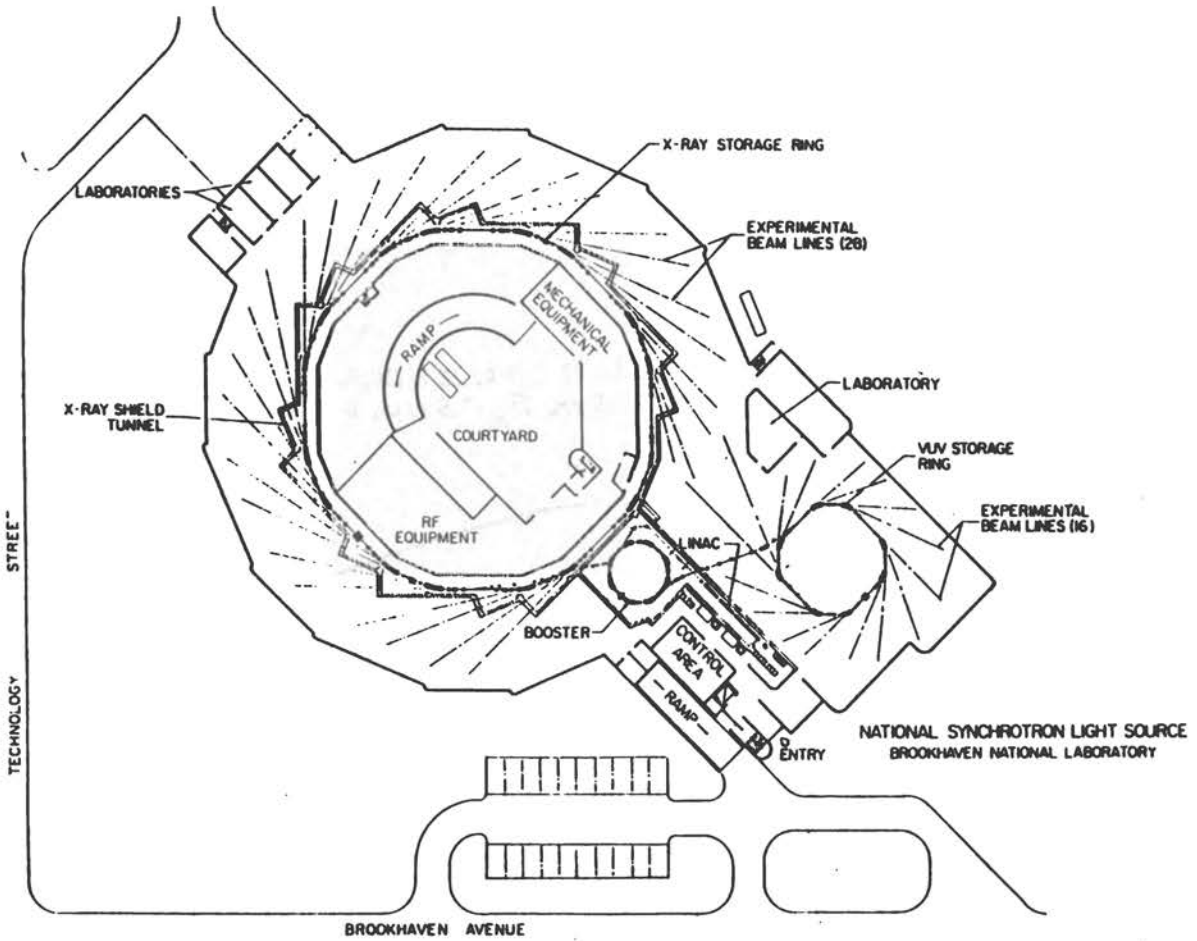

X-RAY STORAGE RING
LABORATORIES
EXPERIMENTAL BEAM LINES (28)
MECHANICAL EQUIPMENT
RAMP
LABORATORY
X-RAY SHIELD TUNNEL
COURTYARD
VUV STORAGE RING
EXPERIMENTAL BEAM LINES (16)
RF EQUIPMENT
LINAC
BOOSTER
CONTROL AREA
RAMP
ENTRY
NATIONAL SYNCHROTRON LIGHT SOURCE
BROOKHAVEN NATIONAL LABORATORY
TECHNOLOGY STREET
BROOKHAVEN AVENUE

FIGURE 3

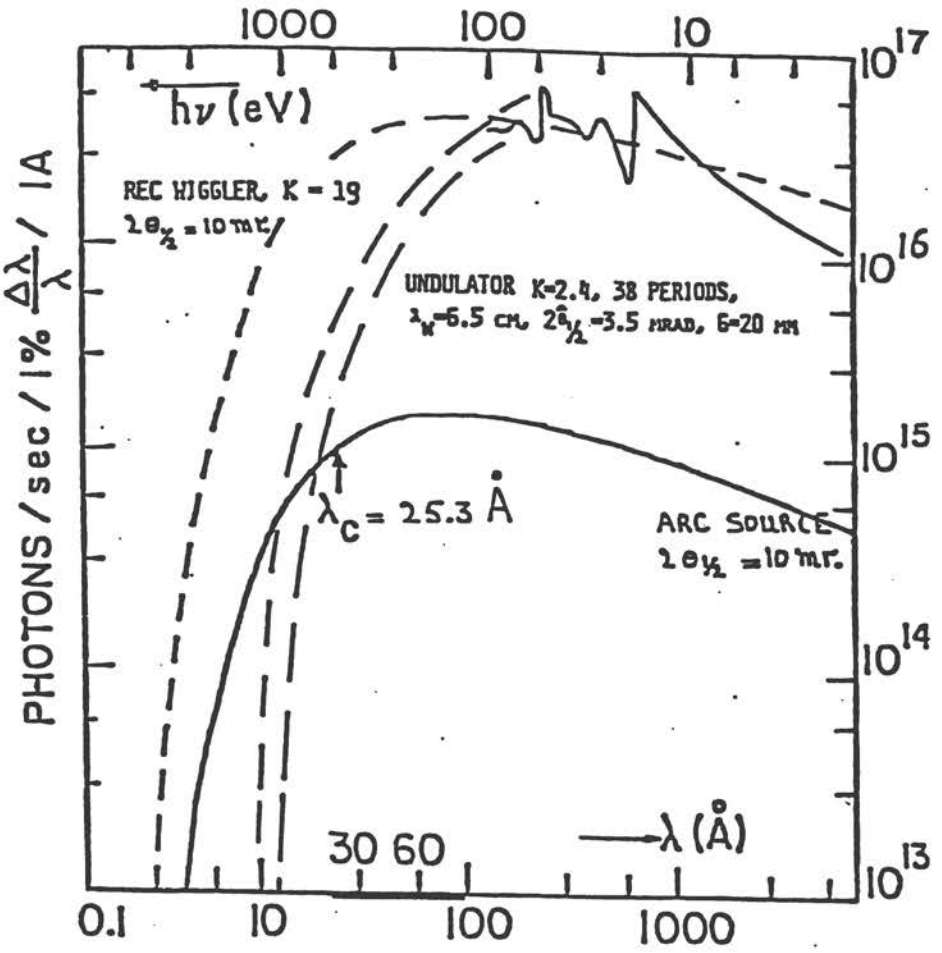


FIGURE 4
NSLS Spectrum, VUV, 0.75 GeV

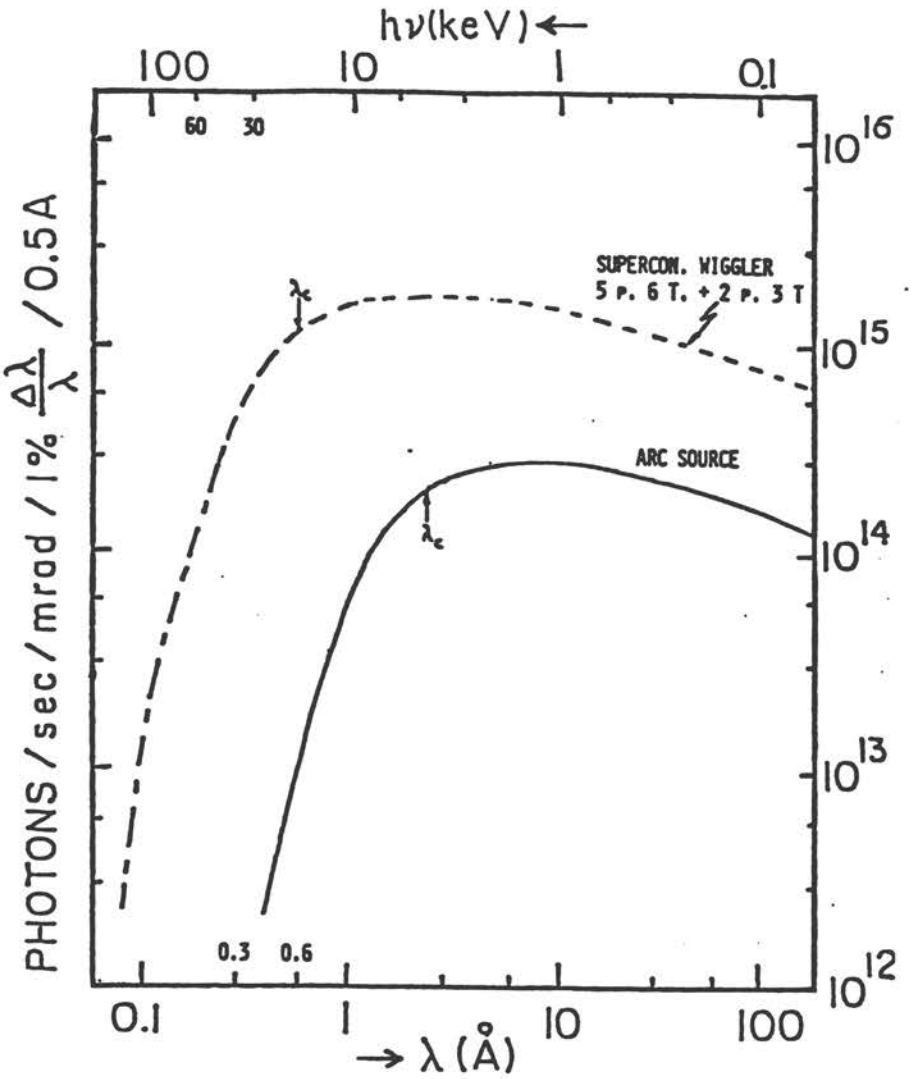


FIGURE 5

NSLS SR Spectra, X-ray Ring, 2.5 GeV

TABLE I

BEAM PARAMETERS AT THE SOURCE LOCATIONS

VUV RING (750 MEV)	**X-RAY RING (2.5 GEV)**
$\varepsilon_x = 9\ 10^{-8}$ rad.m	$\varepsilon_x = 8\ 10^{-8}$ rad.m
$\varepsilon_y = 9\ 10^{-10}$ rad.m	$\varepsilon_y = 8\ 10^{-10}$ rad.m
$\sigma_\varepsilon(\Delta p/p) = 4.4\ 10^{-4}$	$\sigma_\varepsilon(\Delta p/p) = 8.2\ 10^{-4}$
ARC Sources (ARC length $\leq$ 90 mrad.)	**ARC Sources (ARC length $\leq$ 50 mrad.)**
$\sigma_{x,t}$ = 0.3 mm; $\sigma_{x'}$ = 0.2 mrad.	$\sigma_{x,t}$ = 0.3 mm; $\sigma_{x'}$ = 0.2 mrad.
σ_y = 0.1 mm; $\sigma_{y'}$ = 0.01 mrad.	σ_y = 0.1 mm; $\sigma_{y'}$ = 0.01 mrad.
Insertion (β_x^* = 11.6 m; β_y^* = 5.5 m)	**Insertion (β_x^* = 1.4 m; β_y^* = 0.3 m)**
σ_x = 1.0 mm; $\sigma_{x'}$ = 0.09 mrad.	σ_x = 0.3 mm; $\sigma_{x'}$ = 0.24 mrad.
σ_y = 0.07mm; $\sigma_{y'}$ = 0.01 mrad.	σ_y = 0.02mm; $\sigma_{y'}$ = 0.04 mrad.

TABLE II

VUV SOURCE EMITTANCES AND SIZES

1 Bunch Mode; Tune 3.10; 1.13

Initial Currents: I(typical) = 300 mA I(max.) = 400 mA

Emittances for I = 1-30 mA	Design Emittances
$\varepsilon(V) = 3 \times 10^{-9}$ rad·m	$\varepsilon(V) = 9 \times 10^{-10}$ rad·m
$\varepsilon(H) = 15 \times 10^{-8}$ rad·m	$\varepsilon(H) = 9 \times 10^{-8}$ rad·m

(Horizontal-Vertical Coupling $\varepsilon(V)/\varepsilon(H) = 0.02$)

Source Size for I = 1-125 mA	Design Source Sites
σ Vert. = 0.2 mm	σ Vert. = 0.1 mm
σ Hor. = 0.5 mm	σ Hor. = 0.4 mm

($\beta_V = 14$ m; $\beta_H = 1.5$ m)

TABLE III

NSLS PARTICIPATING

RESEARCH TEAM MEMBERS

UNIVERSITIES

Brandeis University (X12)
Columbia University (U9)
Cornell (X26)
Georgia Institute of Technology (X14)
Harvard University (X12, X13)
Johns Hopkins University (X19)
Massachusetts Institute of Technology (X14, X20)
New York University (X9)
North Carolina State University (X11)
Northwestern University (X18)
Princeton University (X18)
Purdue University (X18)
Rensselaer Polytechnic Institute (X19)
Stanford University (X17)
State University of New York (U7, U15, X21)
Texas A & M (X26)
University of California (U3)
University of Chicago (X26)
University of Connecticut (X11)
University of Houston (X14)
University of Illinois (X18, X19)
University of Kentucky (X14)
University of North Carolina (U11)
University of Pennsylvania (U12, X9, X12, X13)
University of Pittsburgh (X13, X18)
University of Rochester (U11)
University of Tennessee (U10, X26)
University of Washington (X11)
West Virginia University (X18)
Yale University (U11, X12)
Yeshiva University (X9)

CORPORATIONS

Allied Corporation (X13)
Ashland Oil (X18)
Bell Laboratories (U4, X9, X15, X16)
Dupont (X11)
Exxon (X10)
General Electric (X11)
Gulf (X18)
IBM (U6, U8, X20)
Mobil (X11)
United Technology (U11, X11)
Universal Oil Products (X18)
Xerox (U12)

GOVERNMENT LABORATORIES

Ames Laboratory (X18)
Argonne National Laboratory (U11, X11)
Brookhaven National Laboratory (U7, U9, U11, X11, X12, X13, X22)
Lawrence Livermore Laboratory (U3)
Los Alamos National Laboratory (U3)
Nat'l Bureau of Standards (U10, X23, X24)
Naval Research Laboratory (X23, X24)
Oak Ridge National Laboratory (U11, U12, X14)
Sandia Laboratory (U3)

(2/84)

TABLE IV
NSL PRT MEMBERS

PORT U-1 & X-10 (16)

EISENBERGER, PETER, M.	EXXON RES. & ENGR'G. COMPANY
Bloch, M. J.	Exxon Res. & Engr'g. Company
Chianelli,	Exxon Res. & Engr'g. Company
Cramer, S.	Exxon Res. & Engr'g. Company
deNeufville, J.	Exxon Res. & Engr'g. Company
Eberhardt, W.	Exxon Res. & Engr'g. Company
Hoffman, F.	Exxon Res. & Engr'g. Company
Kaldor, A.	Exxon Res. & Engr'g. Company
Kim, K. S.	Exxon Res. & Engr'g. Company
Liang, K.	Exxon Res. & Engr'g. Company
Moser, H. R.	Exxon Res. & Engr'g. Company
Safinya, C. R.	Exxon Res. & Engr'g. Company
Sette, F.	Exxon Res. & Engr'g. Company
Sinfelt, J.	Exxon Res. & Engr'g. Company
Stöhr, J.	Exxon Res. & Engr'g. Company
Via. G.	Exxon Res. & Engr'g. Company

PORT U-3 (36)

DAY, R. H.	LOS ALAMOS NATIONAL LABORATORY
KNOTEK, M. L.	SANDIA NATIONAL LABORATORY
GRUNER, G.	UNIVERSITY OF CALIFORNIA/SAN DIEGO
MULTHAUF, L.	LAWRENCE LIVERMORE LABORATORY
Bartlett, R. J.	Los Alamos National Laboratory
Baughcum, S. L.	Los Alamos National Laboratory
Berzins, G.	Los Alamos National Laboratory
Blais, N. C.	Los Alamos National Laboratory
Burginyon, G.	Lawrence Livermore Nat'l. Laboratory
Ceglio, N. M.	Lawrence Livermore Nat'l. Laboratory
Christoph, G. G.	Los Alamos National Laboratory
Cox, L. E.	Los Alamos National Laboratory
Cromer, D. T.	Los Alamos National Laboratory
Del Grande, N. K.	Lawrence Livermore Nat'l. Laboratory
Eisenberg, D.	UCLA-Molecular Biology & Chemistry
Eller, P. G.	Los Alamos National Laboratory
Ellis, W. P.	Los Alamos National Laboratory
Fenimore, E. E.	Los Alamos National Laboratory
Gruber, D. E.	University of California/San Diego
Jones, C. R.	Los Alamos National Laboratory
Jones, L. A.	Los Alamos National Laboratory
Kania, D. R.	Los Alamos National Laboratory
Kaufmann, R. L.	Lawrence Livermore Nat'l. Laboratory

Loge, G. W.	Los Alamos National Laboratory
Loubriel, G. M.	Sandia National Laboratory
Quick, C. R. Jr.	Los Alamos National Laboratory
Rothschild, R. E.	University of California/San Diego
Ryan, R. R.	Los Alamos National Laboratory
Rye, R. R.	Sandia NationalLaboratory
Stulen, R. S.	Sandia National Laboratory
Thompson, K. A.	Los Alamos National Laboratory
Tiee, J. J.	Los Alamos National Laboratory
Tirsell, K. G.	Lawrence Livermore Nat'l. Laboratory
Wang, C.	Lawrence Livermore Nat'l. Laboratory
Williams, A.	Los Alamos National Laboratory
Williams, R. S.	UCLA - Dept. of Chemistry

PORT U4 (4)

SMITH, N.	BELL LABORATORIES
Kevan, S.	Bell Laboratories
Sette, F.	Bell Laboratories
Stoffel, N.	Bell Laboratories

PORT U6 (9)

WILSON, A.	IBM
Acosta, R.	IBM
Conte, J.	IBM
Costas, D.	IBM
Flavin, R.	IBM
Hofer, D.	IBM
Maldonado, J.	IBM
Silverman, J.	IBM
Warlaumont, J.	IBM

PORT U7 (9)

STRONGIN, M.	DEPARTMENT OF PHYSICS - BNL
COLBERT, S.	DEPARTMENT OF PHYSICS - BNL
Garret, R.	Department of Physics - BNL
Johnson, P.	Department of Physics - BNL
Jona, F.	SUNY, Stony Brook
Murgai, V.	Department of Physics - BNL
Raaen,S.	Department of Physics - BNL
Ruckman, M.W.	Department of Physics - BNL
Sham, T. K.	Department of Physics - BNL

PORT U8 (8)

HIMPSEL, F.	**IBM**
Freeof,	IBM
Hofer, D.	IBM
Jordan, J.	IBM
Ludeke, R.	IBM
Morar, J.	IBM
Pollack, R.	IBM
Spiller, E.	IBM

PORT U9A (15)

WESTON, RALPH E.	**Chemistry Department - BNL**
Flynn, G. W.	Columbia University
Bersohn, R.	Columbia University
Bondybey, V. E.	Bell Laboratories
Braun, C. L.	Dartmouth College
Cantor, C. R.	Columbia University
Hochstrasser, R. M.	University of Pennsylvania
Holroyd, R. A.	Chemistry Department - BNL
Innes, K. K.	SUNY, Binghampton, NY
Longworth, J. W.	ORNL
Okabe, H.	National Bureau of Standards
Premuzic, E. T.	Energy & Environment - BNL
Preses, J.	Chemistry Dept. - BNL
Testa, A. C.	St. John's University
Ware, W. R.	University of Western Ontario

PORT U-9B (15)

SUTHERLAND, J. C.	**BIOLOGY DEPARTMENT - BNL**
Coohill, T.	Western Kentucky University
Gray, D.	University of Texas/Dallas
Hind, G.	Biology Department - BNL
Keck, P. C.	Biology Department - BNL
Keiderling, T.	University of Illinois/Chicago
Lang, D.	University of Texas/Dallas
Laws, W. R.	Biology Department - BNL
McGlynn, S. P.	Louisana State University
Nafie, L. A.	Syracuse University
Snyder, P. A.	Florida Atlantic University
Stephens, P. J.	SUNY, Binghampton
Sutherland, B. M.	Biology Department - BNL
Turner, D. H.	University of Rochester
Wu, C. W.	A. Einstein College of Medicine

PORT U10 (3)

CALLCOTT, T.A.	UNIVERSITY OF TENNESSEE
Arakawa, E.T.	ORNL
Ederer, D.L.	National Bureau of Standards

PORT U11 (13)

GROVER, R. J.	CHEMISTRY DEPARTMENT - BNL
Baer, T.	University of North Carolina
Berkowitz, J.	Argonne National Laboratory
Chupka, W. A.	Yale University
Farrar, J. M.	University of Rochester
Jones, K. W.	Department of Physics - BNL
Klemm, R. B.	Energy & Environment - BNL
Krause, M. O.	ORNL
Ng, C-Y.	University of Iowa
Seery, D. J.	United Technology Research Center
White, M. G.	Department of Chemistry - BNL
Walters, Edw.	University of New Mexico

PORT U-12 (10)

PLUMMER, E. W.	UNIVERSITY OF PENNSYLVANIA
Burstein, E.	University of Pennsylvania
Fischer, J.	University of Pennsylvania
Graham, W.	University of Pennsylvania
Gustafsson, T.	University of Pennsylvania
Heeger, A.	University of Pennsylvania
Jenkins, L.	ORNL
Jensen, E.	University of Pennsylvania
Thomas, R.	Xerox
Zehner, D.	ORNL

PORT U-15 (6)

KIRZ, J.	SUNY, STONY BROOK
Howells, M.	NSLS - BNL
Kenney, J.	Suny, Stony Brook
Pine, J.	California Institute of Technology
Rarback, H.	SUNY, Stony Brook

PORT X-5 (7)

SANDORFI, A. M.	PHYSICS DEPARTMENT - BNL
Giordano, G.	INFN - Frascati (Italy)
LeVine, M. J.	Physics Department - BNL
Matone, G.	INFN - Frascati (Italy)
Nathan, A. M.	University of Illinois
Thorn, C. E.	Physics Department - BNL
Scharf, C.	University of Rome

PORT X-9 (79)

CHANCE, B.	JOHNSON FOUNDATION
Asakura, T.	University of Pennsylvania
Averill, B.	Michigan State University
Barlow, C.	Evergreen State College
Berman, H.	Institute for Cancer Research
Bickar, D.	Duke University Marine Laboratory
Blackwell, J.	Case Western University
Blasie, J. K.	University of Pennsylvania
Blumberg, W.	Bell Laboratories
Buhks, E.	Solar Energy Systems, Inc.
Capaldi, R.	University of Oregon
Chang, C.	Michigan State University
Cheung, W. Y.	St. Jude's Children's Hospital
Ching, Y.	Bell Laboratories
Cooperman, B. S.	University of Pennsylvania
Debrunner, P.	Univ. of Illinois/Urbana-Champaign
Deluca, H.	University of Wisconsin-Madison
Dutton, P. L.	Johnson Foundation
Egami, T.	University of Pennsylvania
Elam, T.	Naval Research Laboratories
Elliott, M.	University of Vermont
Englander, S. W.	University of Pennsylvania
Erecinska, M.	University of Pennsylvania
Fee, J.	University of Michigan
Frauenfelder, H.	University of Ill./Urbana-Champaign
Glusker, J.	Institute for Cancer Research
Gruner, S.	Princeton University
Gunsalus, I. C.	University of Ill./Urbana-Champaign
Haselgrove, J. C.	Johnson Foundation
Hastings, W.	Harvard University
Heiney, P. A.	MIT
Herbette, L.	University of Connecticut
Ho, C.	Carnegie-Mellon University
Hurych, C.	Northern Illinois University
Kalid S.	Institute for Structural & Functional Studies

King, T.	State University of New York/Albany
Korszun, Z. R.	Institute for Structural & Functional Studies
Kretsinger, R. H.	University of Virginia
Krueger, R.	MIT
Lehninger, A. L.	Johns Hopkins University
Leigh, J. S.	Johnson Foundation
Lobrutto, R.	Johnson Foundation
Marcus, R. A.	California Institute of Technology
Mason, H.	Oregon Health Science Center
McWhan, D.	Bell Laboratories
Mildvan, A.S.	Institute for Cancer Research
Miller, C.	National Institute of Health
Moffat, K.	Cornell University
Mortenson, L.	Exxon Research & Engineering
Mueller, P.	University of Pennsylvania
Muhoberac, B.	University of Texas Heal Sciences
Ohnishi, T.	University of Pennsylvania
Orme-Johnson, W.	MIT
Peisach, J.	A. Einstein Medical College
Plummer, W.	University of Pennsylvania
Potter, J.	University of Cincinnati Medical Center
Powers, L. S.	Bell Laboratories
Prendergast, F.	MAYO Clinic
Reed, G.	Johnson Foundation
Reynolds, G.	Princeton University
Rosenbaum, G.	Inst. for Structural and Functional Studies
Rothschild, K.	Boston Univ. School of Medicine
Scarpa, A.	University of Pennsylvania
Schultz, J.	Papanicolaou Cancer Research Inst.
Smith, J.	Georgia State
Solomon, E.	University of Pennsylvania
Somlyo, A. P.	University of Pennsylvania
Spiro, T.	Princeton University
Stiefel, E.	Exxon Research and Engineering
Stoeckenius, W.	San Francisco Medical Center
Turnbull, D.	Harvard University
Valentine, J.	UCLA
Vallee, B. L.	Harvard Medical School
Wharton, D. C.	Northeastern University
White, D.	University of Pennsylvania
Worthington, C. R.	Carnegie Mellon University
Yonetani, T.	Johnson Foundation
Zhow, Y. H.	Johnson Foundation

PORT X-11 (17)

SAYERS, D.	UNIVERSITY OF NORTH CAROLINA
Altman, L.	Mobil Research & Development
Budnick, J.	University of Connecticut
Fajer, J.	Energy & Environment - BNL
Hanson, L.	Energy & Environment - BNL
Heald, S.	Energy & Environment - BNL
Issacs, H.	Energy & Environment - BNL
Katzer, J.	University of Delaware
Kendig, M.	Energy & Environment - BNL
LaPierre, R.	Mobil Research & Development
Morrison, T.	Argonne National Laboratory
O'Grady, W. E.	Energy & Environment - BNL
Pick, M.	Energy & Environment - BNL
Shenoy, G. K.	Argonne National Laboratory
Stern, E.	University of Washington
Stucky, G. D.	E. I. DuPont
Wong, J.	G. E. Research & Development

PORT X-12 (9)

SCHOENBORN, B.	DEPARTMENT OF BIOLOGY - BNL
Caspar, D. L. D.	Brandeis University
Greer, J.	Columbia University
Harrison, S.	Harvard University
Huxley, H.	Med. Resrch. Council, Cambridge, UK
Moore, P. B.	Yale University
Stamatoff, J.	Celanese Research Company
Sweet, R.	Department of Biology - BNL
Wise, D.	Department of Biology - BNL

PORT X-13 (10)

KOETZLE, T.	DEPARTMENT OF CHEMISTRY - BNL
Abola, J. E.	University of Pittsburgh
Craven, B. M.	University of Pittsburgh
Jeffrey, G. A.	University of Pittsburgh
Kvick, A.	Department of Chemistry - BNL
Lipscomb, W. N.	Harvard University
McClure, R. J.	University of Pittsburgh
McMullen, R. K.	Department of Chemistry - BNL
Stout, C. D.	University of Pittsburgh

PORT X-13 (24)

COX, D. E.	DEPARTMENT OF PHYSICS - BNL
Bell, P.	Geophysical Laboratory, Washington
Brown, N.	University of Pennsylvania
Chien, C. L.	Johns Hopkins University
Egami, T.	University of Pennsylvania
Finger, L.	Geophysical Laboratory, Washington
Fish, G.	Allied Chemical Corporation
Gaskell, D. R.	University of Pennsylvania
Hasegawa, R.	Allied Chemical Corporation
Hastings, J. B.	NSLS - BNL
Hazen, R.	Geophysical Laboratory, Washington
Heeger, A. J.	University of Pennsylvania
Mao, D.	Geophysical Laboratory, Washington
Nagel, S. R.	University of Chicago
Piermarini, G.	National Bureau of Standards
Prewitt, C. T.	SUNY, Stony Brook
Schiferl, D.	LANL
Sleight, A. W.	DuPont Chemical Corporation
Stuckey, G. D.	E. I. DuPont
Sweedler, A. R.	California State Univ./Fullerton
Takahashi, S.	Lamont-Doherty Geological Lab., NY
Weaver, S.	Lamont-Doherty Geological Lab., NY
Worrell, W. L.	University of Pennsylvania
Young, R. A.	Georgia Institute of Technology

PORT X-14 (23)

SPARKS, C. J.	OAK RIDGE NATIONAL LABORATORY
Angell, A.	Purdue University
Blum, L.	University of Puerto Rico
Borie, B. S.	ORNL
Byrne, J. G.	University of Utah
DeAngelis, R. J.	University of Kentucky
Halder, N. C.	University of Southern California
Houska, C. R.	Virginia Polytechnic Institute
Huang, H.	Rice University
Ice, G.	ORNL
Kaplow, R.	M.I.T.
Kay, M. I.	University of Puerto Rico
Krawitz, A.	University of Missouri
Larson, B. C.	ORNL
Lawless, K. R.	University of Virginia

Mackie, P.	Georgia Institute of Technology
Moss, S. C.	University of Houston
Narten, A. H.	ORNL
Ryba, E. R.	Pennsylvania State University
Spruiell, J. E.	University of Tennessee

PORT X-15 (10)

FREEMAN, R.	BELL LABORATORIES
Blumberg, W. L.	Bell Laboratories
Citrin, P.	Bell Laboratories
Golovchenko J.	Bell Laboratories
Kincaid, B.	Bell Laboratories
Levesque, R.	Bell Laboratories
McWhan, D.	Bell Laboratories
Meixner, A.	Bell Laboratories
Powers, L	Bell Laboratories
Robinson, I.	Bell Laboratories

PORT X-17 (4)

HOFSTADTER, R.	STANFORD UNIVERSITY
Rubenstein, E.	Stanford University
Hughes, E. B.	Stanford University
Zeman, H. D.	Stanford University

PORT X-18 (4)

HERCULES, D. M.	UNIVERSITY OF PITTSBURGH
Hoggins, J. T.	Ashland Chemical Co.
Lester, G. R.	UOP, Inc.
Lester, J. E.	Gulf Research & Devlp'mt.
Montano, P. A.	West Virginia University

PORT X-18 (16)

LIEDL, G. L.	PURDUE UNIVERSITY
Chapman, D.	Purdue University
Chen, H. H.	University of Illinois
Cohen, J. B.	Northwestern University
Colella, R.	Purdue University
Delgass, W. N.	Purdue University
Epperson, J. E.	Argonne National Laboratory
Faber, J.	Argonne National Laboratory
Georgopoulous, P.	Argonne National Laboratory
Iton, L.	Argonne National Laboratory
Karim, D.	Argonne National Laboratory
Knapp, G.	Argonne National Laboratory
Mikkola, D.	Michigan Technological University
Mueller, M.	Argonne National Laboratory
Rundman, K.	Michigan Technological University
Staudenmann, J. L.	Iowa State University

PORT X-19 (11)

BILELLO, J.	SUNY, STONY BROOK
Birnbaum, H. K.	University of Illinois
Chen, H.	University of Illinois
Green, R. E.	Johns Hopkins University
Herley, P.	SUNY, Stony Brook
Herman, H.	SUNY, Stony Brook
Liu, J.	SUNY, Stony Brook
MacCrone, R.	Rensselaer Polytechnic Institute
Pope, D.	University of Pennsylvania
Suenaga, M.	Energy & Environment - BNL
Patel, J. R.	Bell Laboratories

PORT X-20 (6)

HORN, P. M.	IBM
Birgeneau, R.	M.I.T.
Cargill, S.	IBM
Litster, D.	M.I.T.
Morar, J.	M.I.T.
Wuensch, B.	M.I.T.

PORT X-21 (19)

BIGELEISON, J.	SUNY, STONY BROOK
Brady, G.	SUNY, Stony Brook
Chu, B.	SUNY, Buffalo
Coppens, P.	SUNY, Albany
Gibson, W. M.	SUNY, Albany
Chaturvedi, R.	SUNY, Cortland
Herman, H.	SUNY, Stony Brook
Kao, Y. H.	SUNY, Albany
Karlin, K.	SUNY, Albany
Kartha, G.	Roswell Park Memorial Institute
King, T. E.	SUNY, Buffalo
Phillips, J.	SUNY, Buffalo
Prewitt, C. T.	SUNY, Stony Brook
Seeman, N.	SUNY, Albany
Snyder, R.	SUNY, Cortland
Stephens, P.	SUNY, Buffalo
Stevens, E.	SUNY, Buffalo
Yencha, A.	SUNY, Albany
Zubietta, J.	SUNY, Albany

PORT X-22 (10)

MONCTON, D.	DEPARTMENT OF PHYSICS - BNL
Axe, J. D.	Department of Physics - BNL
Birgeneau, R.	M.I.T.
D'Amico,	Department of Physics - BNL
Gibbs, R. J.	Accelerator Department- BNL
Hastings, J. B.	NSLS - BNL
Passell, L.	Department of Physics - BNL
Shapiro, S. M.	Department of Physics - BNL
Shirane, G.	Department of Physics - BNL
Stephens, P. W.	SUNY, Stony Brook

PORT X-24 (36)

MADDEN, R.	NATIONAL BUREAU OF STANDARDS
Bleach, R. D.	Naval Research Laboratory
Block, S.	National Bureau of Standards
Boettinger, W. J.	National Bureau of Standards
Burdette, H. E.	National Bureau of Standards
Cohen, G. G.	National Bureau of Standards
Cowan, P.	National Bureau of Standards
Cruddace, R.	Naval Research Laboratory
Deslattes, R.	National Bureau of Standards

Dick, C.	National Bureau of Standards
Dobbyn, R. C.	National Bureau of Standards
Gilfrich, J. V.	Naval Research Laboratory
Hendrikson, W. A.	Naval Research Laboratory
Hubbard, C. R.	National Bureau of Standards
Hunter, W. R.	Naval Research Laboratory
Kabler, M.	Naval Research Laboratory
Kruger, J.	National Bureau of Standards
Kuriyama, M.	National Bureau of Standards
LaVilla, R. E.	National Bureau of Standards
McLaughlin, W. L.	National Bureau of Standards
Mauer, F.	National Bureau of Standards
Nagel, D.	Naval Research Laboratory
Newbury, D.	National Bureau of Standards
Palik, E. D.	Naval Research Laboratory
Patterson, D. O.	Naval Research Laboratory
Peterlin, A.	National Bureau of Standards
Reneker, D. H.	National Bureau of Standards
Rife, J.	Naval Research Laboratory
Roth, R. S.	Naval Research Laboratory
Schnur, J.	Naval Rsearch Laboratory
Skelton, E. F.	Naval Research Laboratory
Smardzewski, R. R.	Naval Research Laboratory
Taylor, C.	Naval Research Laboratory
Thomson, R. M.	National Bureau of Standards
Whitlock, R. R.	Naval Research Laboratory
Williams, R. T.	Naval Research Laboratory

PORT X26 (13)

SMITH, J.	UNIVERSITY OF CHICAGO
Bence, E.	SUNY, Stony Brook
Drake, M.	University of Arizona
Gordon, B.	Energy & Environment - BNL
Gordon, G.	University of Maryland
Grodzins, L.	M.I.T.
Hanson, G.	SUNY, Stony Brook
Hillman, M.	Energy & Environment-BNL
Jones, K. W.	Physics Department-BNL
Kraner, H.	Instrumentation Department-BNL
Ogilvie, R.	M.I.T.
Somolyo, A.	University of Pennsylvania
Wood, J.	Smithsonian Institution

(PORT X26) (5)

JONES, K. W. — DEPARTMENT OF PHYSICS - BNL

Church	Texas A&M
Herzog, G.	Rutgers University
Johnson, B.	Department of Physics - BNL
Kostroun, V.	Cornell University
Kruse, T.	Rutgers University
Sellin, I.	University of Tennessee

(2/84)

TABLE V

NSLS UV BEAM LINES

			λ(A)	
U 1.	EXXON (Eberhardt, Hoffman, Kaldor, Kim, Stöhr, Via)	SEXAFS, ARUPS, XPS INFRA-RED VIBR'TNL. SPECT.	20-2000 10^4-10^6	ERG NIM
U 2.	NSLS Diagnostics			
U 3.	LANL/SANDIA/U.CALIF/ LAWRENCE LIVERMORE (Day, Knotek, Gruner, Multhauf)	SPECTROSCOPY RADIOMETRY	12-1500 6-100	ERG
U 4.	BELL LABS (Smith, Kevan, Sette)	*A) SEXAFS/ARUPS/XPS *B) ARUPS C) ARUPS/ABS/REFL.	12-1200 80-5000 400-6000	PGM TGM NIM
U 5.	NSLS Free Electron Laser			
U 6.	IBM (Wilson, Warlaumont, Silverman)	*LITHOGRAPHY	White	
U 7.	BNL/SUNY (Strongin, Johnson, Sham, Weng, Williams, Jona)	*A) ARUPS/XPS/SEXAFS B) GAS SOLIDS	15-1200	PGM TGM
U 8.	IBM (Himpsel, Spiller)	A) ARUPS *B) ARUPS C) EXAFS/SEXAFS D) MICROSCOPY	18-2000 80-2500 8-100	TGM TGM Fresnel Zone Plate
U 9.	NSLS/BNL-CHEM. (Weston, Holroyd, Preses) NSLS/BNL-BIO. (Sutherland)	*A) FLUORESCENCE LIFETIME *B) DICHROISM/FLUORESCENCE	1050-12,000 1200-300,000	NIM NIM
U10.	TENN/NBS/ORNL (Calcott, Ederer Arakawa)	X-RAY FLUORESCENCE	12-120	SXES
U11.	NSLS/BNL-CHEM. (Grover, White)	*GAS PHASE SPECTROSCOPY	300-2000	NIM
U12.	PENN/ORNL/XEROX (Plummer, Jenkins, Zehner, Salaneck)	A) ARUPS B) ARUPS C) INFRA-RED VIBR'TNL. SPECT.	15-1200 80-2500 10^4-10^6	TGM TGM NIM
U13.	-			
U14.	NSLS (Howells, Williams, Klaffky) NSLS (Hastings)	*A) ARUPS/XPS/SEXAFS B) Optics R&D	15-1200 8 -100	PGM DCM
U15.	NSLS/SUNY (Howells, Kirz)	*TGM MONOCHROMATOR/MICROSCOPE	12-50	TGM
U16.	-			

* = Commissioned beam lines, ARUPS = angle-resolved ultraviolet photoemission spectroscopy, XPS = X-ray photoemission spectroscopy, EXAFS = extended X-ray absorption fine structure, SEXAFS = surface EXAFS, ERG = extended range grasshopper, PGM = plane grating monochromator, TGM = toroidal grating monochromator, NIM = normal incidence monochromator, SXES = soft x-ray emission spectrometer.

(2/84)

TABLE VI
NSLS X-RAY BEAM LINES

X 5.	BNL PHYSICS (Sandorfi)	Compton Backscattering - Nuclear Physics
X 9.	JOHNSON RES. FOUND. (Chance)	A) EXAFS (Biology) B) Scattering
X10.	EXXON (Eisenberger)	A) Scattering B) EXAFS C) Crystallography
X11.	N.C. STATE/CONN./BNL/G.E./U.WASH./MOBIL/ DuPONT/ARGONNE (Sayers, Budnick, Heald, Wong, Stern, LaPierre, Stucky, Shenoy)	EXAFS
X12.	NSLS/BNL-BIO. (Schoenborn)	A) Small Angle Scattering B) Protein Crystallography
X13.	NSLS/BNL-CHEM. (Koetzle, Kvick, Thomlinson) NSLS/BNL PHYSICS/PENN/SUNY/ALLIED CHEM/DuPONT (Cox, Egami, Prewitt, Hasegawa, Stuckey)	Crystallography/Diffuse Scattering Energy Dispersive Diffraction
X14.	ORNL (Sparks)	A) Diffuse Scattering B) Microprobe C) Topography
X15. X16.	BELL LABS (Freeman, Citrin, Golovchenko, Kincaid, BELL LABS McWhan, Powers, Robinson)	A) Scattering B) Interferometry C) EXAFS/Scattering D) Spectroscopy
X17.	(Reserved for Wiggler)	
X18.	PURDUE/MIDWEST (Liedl) W.VA/PITT./GULF/ASHLAND/UOP (Montano, Hercules, Lester, Boggins, Lester)	Diffraction EXAFS
X19.	NSLS (Hastings) NSLS/SUNY (Bilello)	EXAFS/SEXAFS/XPS Topography
X20.	IBM/MIT (Horn, Birgeneau)	A) Scattering [Low Q Resolution] B) Scattering [High Q Resolution]
X21.	SUNY (Coppens)	Scattering
X22.	BNL PHYSICS (Moncton, Shirane)	A) Scattering [High Q Resolution] B) Scattering [High E Resolution]
X23. X24.	NRL/NBS NRL/NBS (Kabler, Nagel;Madden, Deslattes, Kuriyama)	A) Topography B) Small Angle Scattering C) EXAFS/SEXAFS D) Crystallography E) XPS/UPS
X25.	Wiggler Test	
X26.	U. CHICAGO/BNL (Smith, Jones, Gordon) BNL PHYSICS/CORNELL/TEXAS A&M/U. TENN. (Jones, Kostroun, Church, Sellin)	Microprobe Atomic Physics

EXAFS = extended X-ray absorption fine structure, SEXAFS = surface EXAFS, UPS = ultraviolet photoemission spectroscopy, XPS = X-ray photoemission spectroscopy

(1/84)

TABLE VII
EXPERIMENTS ON VUV STORAGE RING

	Solid State Physics/Materials Science	Chemistry	Biology	Advanced Technology	Earth and Space Science	Number of Beam Lines Available*
UV Photoemission	U1, U3, U4(2), U5, U7(2), U8(3), U12, U14, X1	U3, U11	—	—	—	13
Gas Phase Spectroscopy	U7	U11	—	—	—	2
Fluorescence Studies	U10	U9	U9	—	—	2
Circular Dichroism	—	U9	U9	—	—	2
Soft X-ray Lithography	—	—	—	U6	—	1
Infrared Spectroscopy	U1, U12	U1, U12	—	—	—	2
Radiometry	—	—	—	U3	U3	1
Soft X-ray Microscopy	—	—	U8, U15, X1	—	—	1
Holography	—	—	U15	U15	—	1

*These include commissioned lines and lines presently in a design/construction phase. Commissioned lines are indicated in Table V.

TABLE VIII
EXPERIMENTS ON X-RAY STORAGE RING

	Solid State Physics/Materials Science	Chemistry	Biology	Earth and Space Science	Nuclear Physics	Number of Beam Lines Available*
Scattering	X10, X14, X15, X18, X20(2) X21, X22(2)	X10, X21				9
Absorption Spectroscopy	X10, X11(2) X15, X18, X19	X10, X11, X18	X9, X15			7
Elastic Diffraction	X10, X13, X18 X21, X22, X24	X13, X21	X12	X13		6
Small Angle Scattering	X12, X23		X12			2
Topography	X19, X23					2
Interferometry	X16, X21					2
Microprobe	X26	X26	X26	X26		1
Gamma Ray Spectroscopy					X5	1
Gas Phase Spectroscopy		X26				1
Photoemission Spectroscopy	X16, X24					2

*These beam lines are presently in either a design/construction phase or a commissioning phase.

PHASE II

PHASE II

The NSLS Phase II Construction Project is made up of two basic components: (1) beam line construction, involving the development and installation of at least six additional beam lines and associated insertions; and (2) conventional construction, involving expansion of the existing NSLS building. Briefly, the objectives of the project are to:

- o Design and build six state-of-the-art beam lines with emphasis on wiggler and undulator insertions.
- o Provide laboratory and experimental support areas to accomodate up to 80 beam lines.
- o Provide integrated work and office space for 128 NSLS personnel.

The Phase II project began October 1983 and will be completed in 36 months at a total project cost of $19.7 million.

Proposed Insertion devices and Experimental Beam Lines

Six beam lines and three insertions[1] will be designed and built as part of the Phase II construction program (Table IX). Their locations on X-ray and VUV storage rings are shown in Fig. 6 and noted in the Table. The first three beam lines in the Table were proposed to the scientific community as pertinent to the community's current needs and have been endorsed by the Users' Executive Committee. The NSLS Department Chairman has approved them for early construction. The remaining three beam lines will be reviewed by user groups, then approved for construction by the NSLS Department Chairman no later than July 1984.

TABLE IX
EXPERIMENTAL BEAM LINES AND INSERTIONS
NSLS PHASE II CONSTRUCTION

Beam Line	Port Number	Insertion Device
Superconducting Wiggler	X17	Superconducting Wiggler
High Q Resolution X-ray	X21	Hybrid Wiggler
X-ray Microscopy & Holography	X1	Soft X-ray Undulator
Infrared	U3	None
Tranverse Optical Klystron (TOK) Soft X-ray	U13	Multipole Wiggler
High Energy Resolution Inelastic X-ray Scattering	X13	Hybrid Wiggler

[1]The superconducting wiggler has already been constructed. The TOK insertion magnet will be built with non-NSLS II funds.

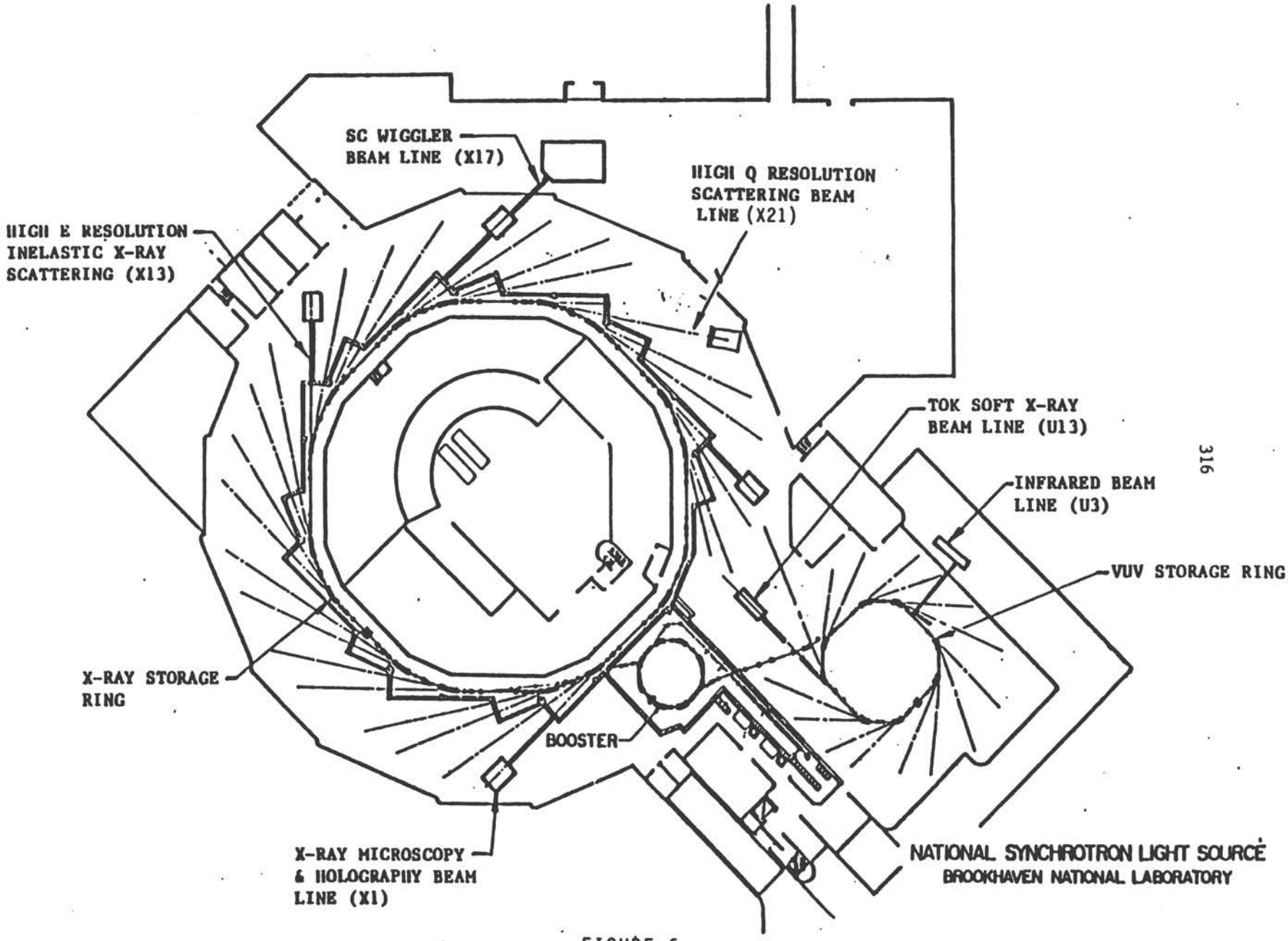

SC WIGGLER
BEAM LINE (X17)
HIGH Q RESOLUTION
SCATTERING BEAM
LINE (X21)
HIGH E RESOLUTION
INELASTIC X-RAY
SCATTERING (X13)
TOK SOFT X-RAY
BEAM LINE (U13)
INFRARED BEAM
LINE (U3)
VUV STORAGE RING
X-RAY STORAGE
RING
BOOSTER
X-RAY MICROSCOPY
& HOLOGRAPHY BEAM
LINE (X1)
NATIONAL SYNCHROTRON LIGHT SOURCE
BROOKHAVEN NATIONAL LABORATORY

FIGURE 6

A Prospectus for a
6 GeV Dedicated Synchrotron Radiation Facility
at Cornell University

In recognition of the need for a dedicated high energy synchrotron radiation facility, it is proposed that a 6 GeV dedicated electron storage ring for synchrotron radiation be constructed on the Cornell University campus in conjunction with the existing facilities at the Wilson Synchrotron Laboratory. In 1968 the Laboratory of Nuclear Studies placed into operation a 12 GeV electron synchrotron for particle physics experiments. Then in 1977 a program was initiated to add an electron storage ring to the facility to perform electron-positron colliding beam experiments with beam energies extending up to 8 GeV per beam. This facility called CESR (Cornell Electron Storage Ring) was placed in operation in less than two years after construction was begun. It has played the leadership role in the study of the upsilon family of resonances and the study of the "bottom" quark. The CESR facility is supported by the National Science Foundation.

At the time that CESR was being designed it was decided to provide a modest synchrotron radiation facility. Working together with members of the School of Applied and Engineering Physics and the Laboratory of Atomic and Solid State Physics, the CHESS (Cornell High Energy Synchrotron Source) facility was established. CHESS was planned to operate in a parasitic mode with three beam lines and several stations per beam line. The management of the facility was provided through the establishment of a center under the leadership of Prof. Boris Batterman as Director. The total construction

cost of the facility was $1.3 M and it has now been serving the user community for about 4 years. Currently CHESS has 100 active proposals. Of these, 44 percent come from outside universities, 33 percent from industrial and national laboratories, and 23 percent from Cornell investigators. A total of 30 institutions are represented. The most recent operating budget covered a three-year period at an annual level of about $700,000. The CHESS facility is supported by the National Science Foundation.

CHESS is the only synchrotron radiation source in the U.S. which receives radiation from a storage ring running at energies which correspond closely to that of the proposed next generation dedicated synchrotron radiation source (5 to 6 GeV). This experience, coupled with Cornell's long and distinguished history in accelerator construction and in x-ray physics, provides a unique background for fulfilling the need for a new 6 GeV dedicated synchrotron source.

The CESR and CHESS facilities are located near the center of the Cornell campus in a tunnel under one of the playing fields as shown in the cutaway view in Fig. 1. The synchrotron and storage ring are mounted in a tunnel of approximately one-half mile perimeter at a depth of about 50 feet below the surface of the fields. The Laboratory itself is located on the side of the gorge as shown. Fig. 2 shows the layout on the campus and Fig. 3 shows a view of the tunnel with the synchrotron located on the left side and CESR on the right.

It is proposed that a new 6 GeV dedicated storage ring be built for synchrotron radiation which would make use of the existing synchrotron as a positron injector. As shown in Fig. 4 and Fig. 5, this ring would be mounted in a tunnel located near the surface of the field in an enclosure placed in a cut-and-cover excavation. The beam from the synchrotron would

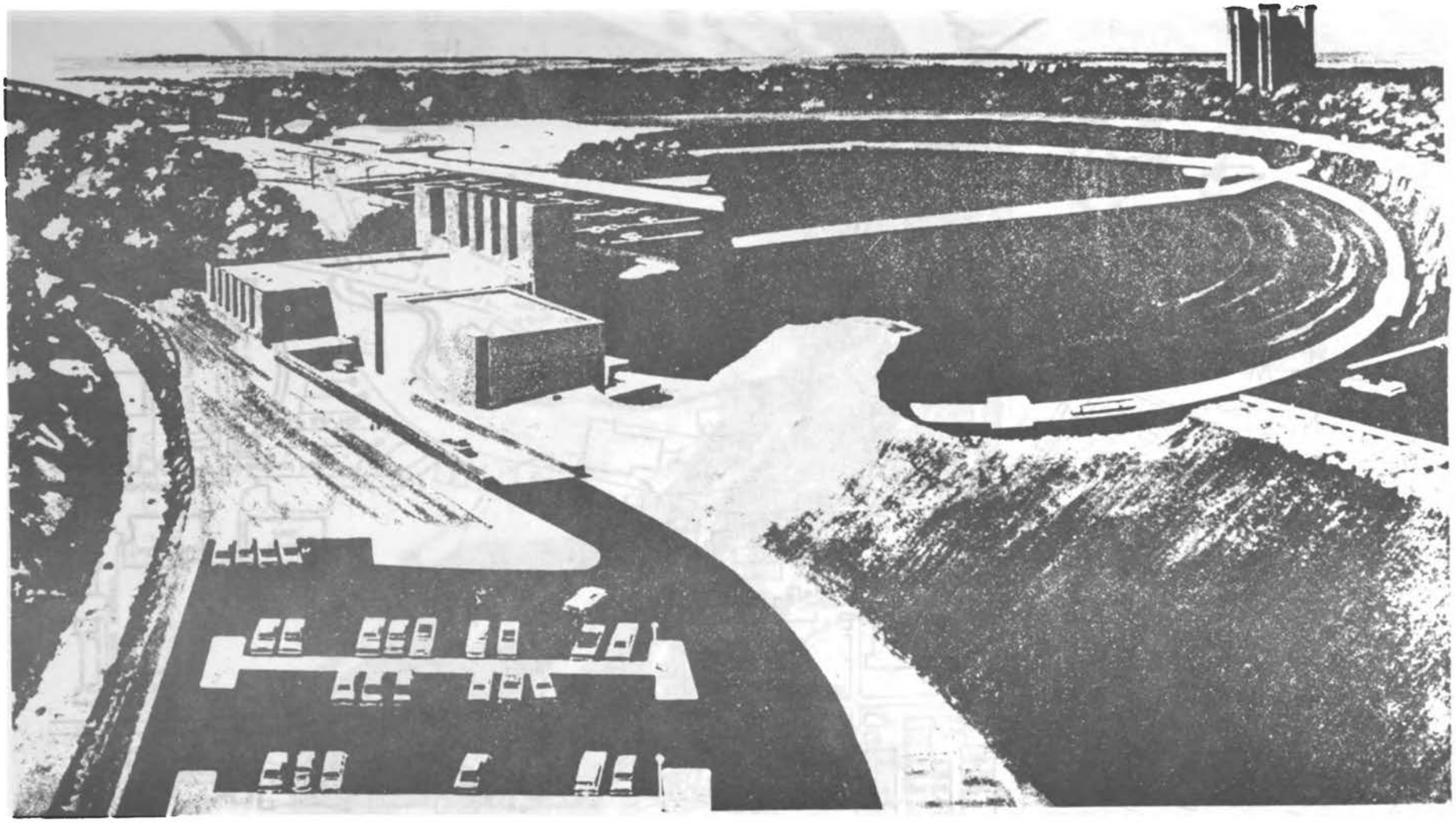


Fig. 1. Cutaway view of the synchrotron and CESR facility.

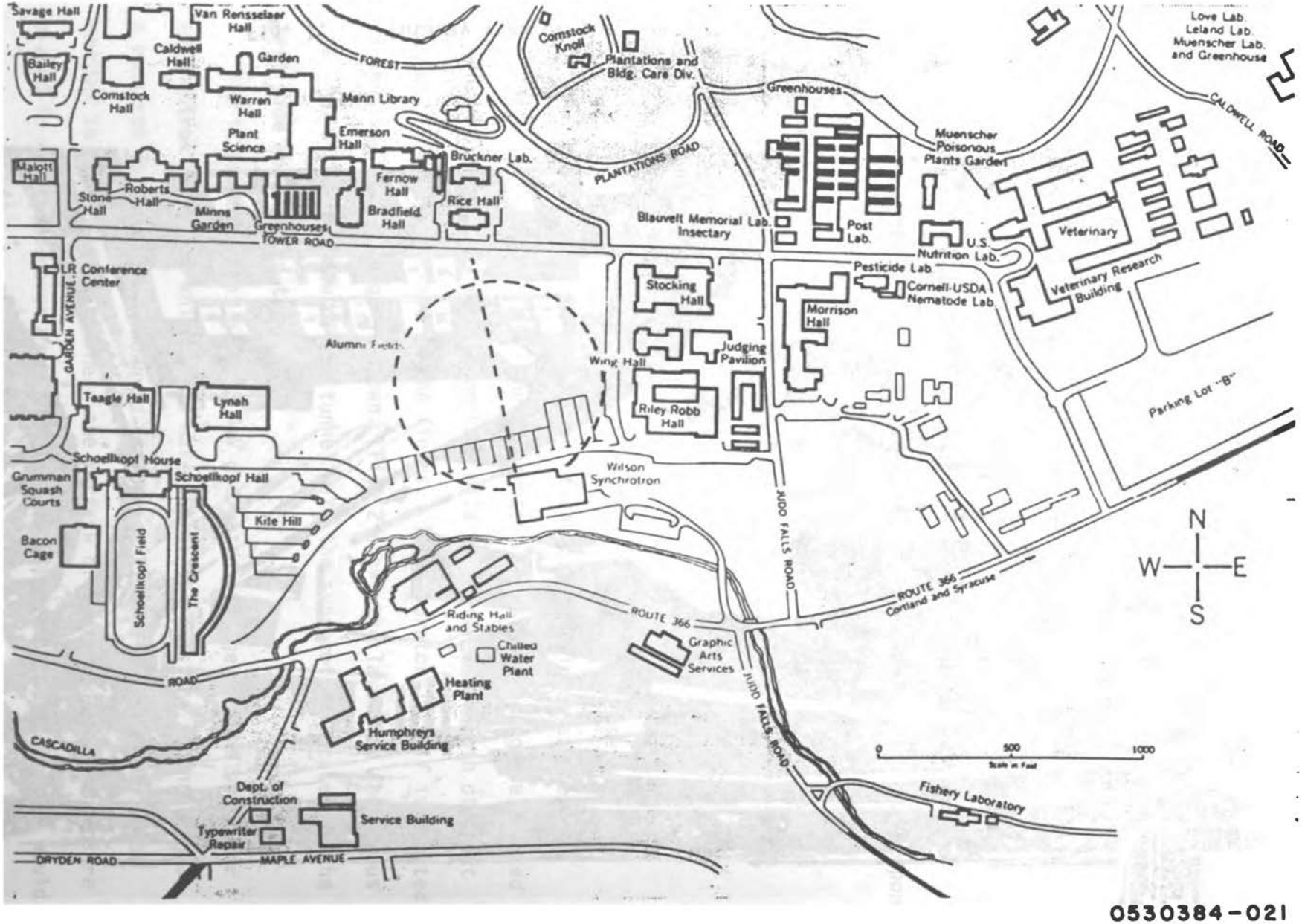


Fig. 2. Campus map showing the Wilson Synchrotron Laboratory and the CESR tunnel.

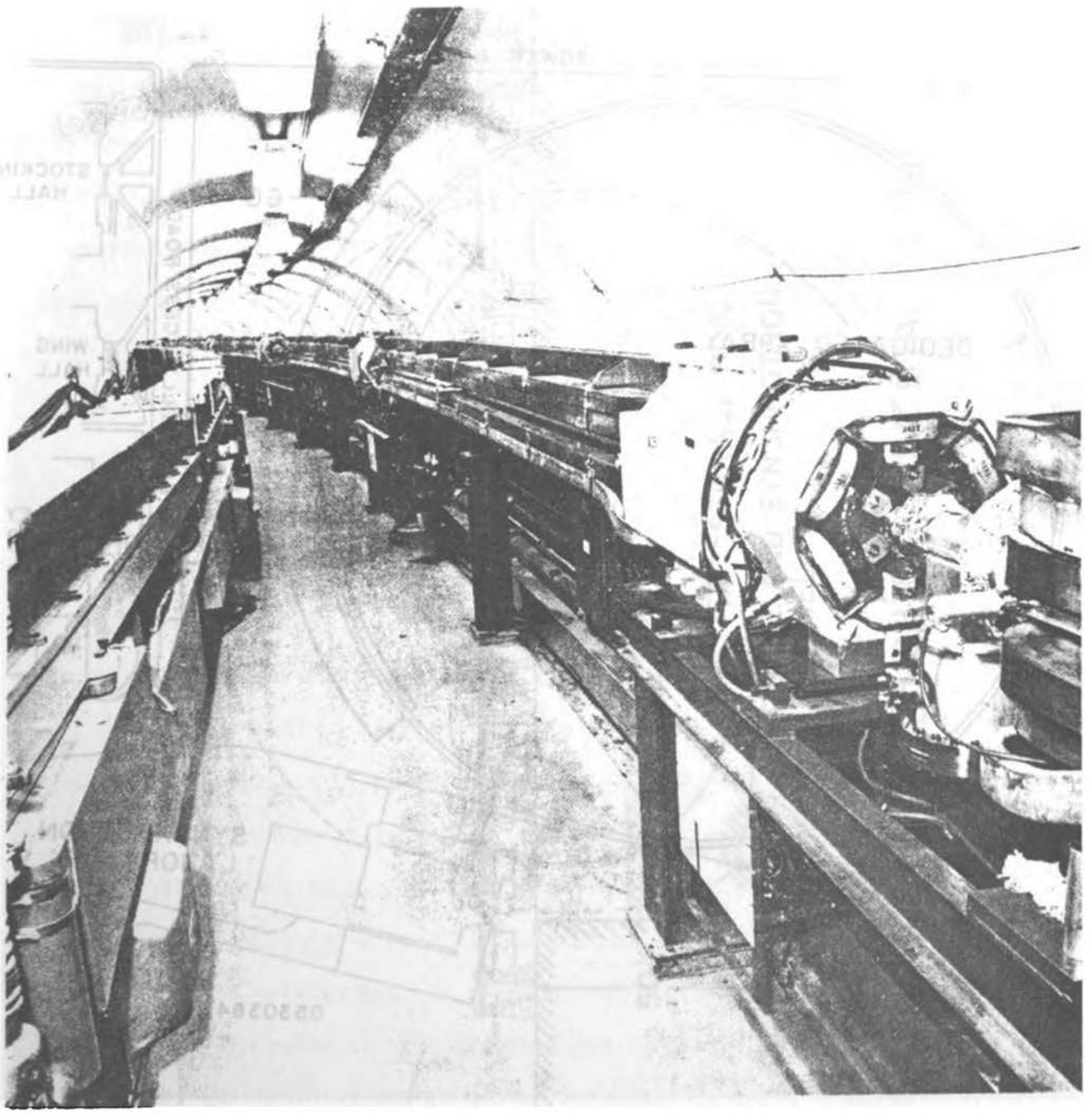


Fig. 3. Photograph of tunnel showing the synchrotron on the left and the CESR ring on the right.

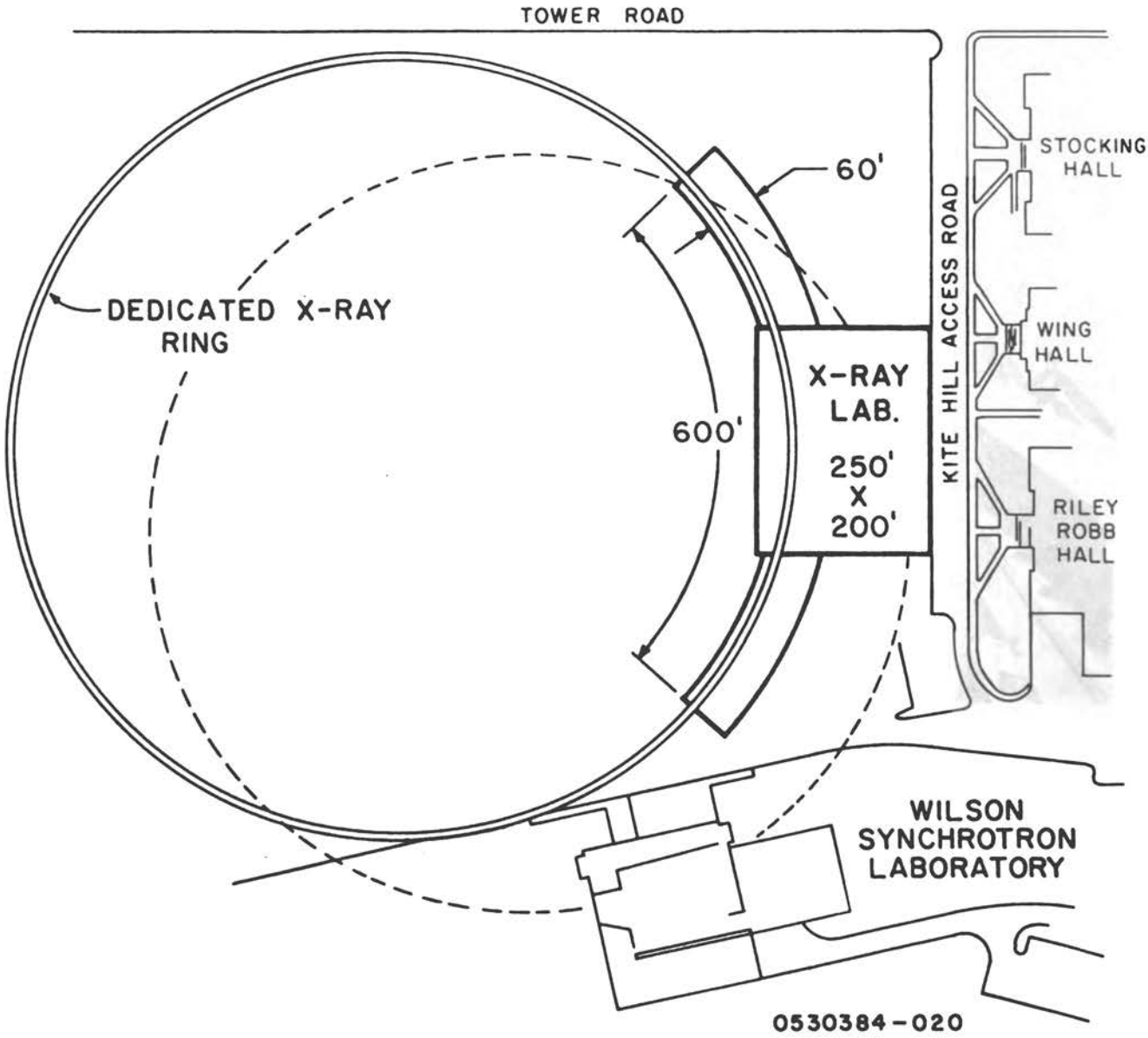
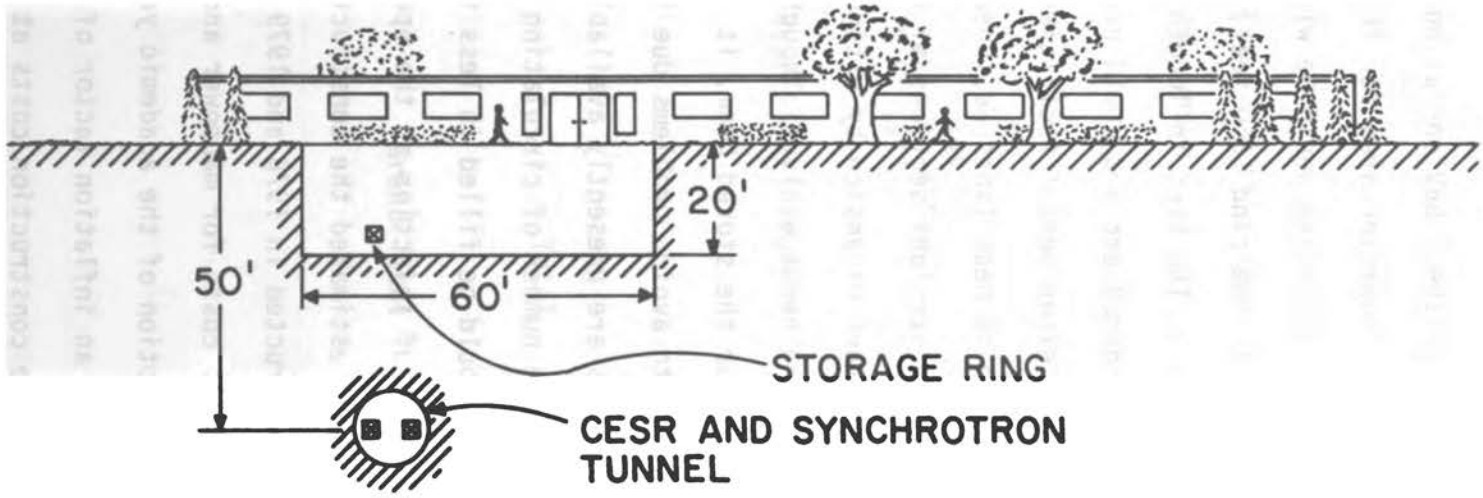


Fig. 4. Plan view of the Dedicated X-ray Ring superimposed on the existing CESR/CHESS Facility.



SECTION THROUGH EXPERIMENTAL FLOOR

0530384-019

Fig. 5.

be carried in a slanting tunnel from the synchrotron below to be injected into the dedicated ring at the 6 GeV operating energy.

In order to provide a working area for the synchrotron radiation research activities, the enclosure would be widened to about 60 feet over approximately one-third of the ring (650 feet), a space which will provide tangential beam lines up to 150 feet in length. A building would be constructed above the widened arc and would provide office and laboratory space in support of the experimental facilities. The proposed working area would easily accommodate 10 beam lines designed to receive radiation from insertion devices in the straight sections of the ring. The design could readily provide for further expansion by extending additional beam lines around the ring as future needs evolve. Though either positrons or electrons could be chosen for the stored beam, it is expected that positrons would be used in order to avoid problems due to ion trapping. High positron injection rates are presently available in the multibunch mode (10 ma/min). A variable number of circulating beam bunches could be selected and the ring could be filled in less than 10 minutes, making use of the topping-off mode of injection at the operating energy.

In Table I we have estimated the construction cost for the facility. The CESR ring was constructed in 1978 and 1979 at a <u>total</u> cost of $12.5 M. This figure included all costs for manpower and supervision for the construction with the exception of the academic year salaries of five Cornell faculty members. Using an inflation factor of two extrapolated to FY 84 dollars, we estimate the construction costs at $25 M. This should be quite a secure estimate. Since the existing synchrotron will supply the beam at energy, no new injector is required. We have estimated the cost of civil construction including the ring enclosure and the 50,000 sq. ft. building

Table I

Construction Cost Estimates

($ Millions FY 84)

Storage Ring Equipment		$ 25 M
All labor costs and installation included. Estimate based on actual CESR costs of $12.5 M FY 1977-78 inflated by factor of 2		
Ring Enclosure, Experimental Floor, and Support Areas		10 M
Experimental Beam Lines		20 M
10 @ $2 M each		
	Total	$ 55 M
Contingency (20%)		11 M
	Grand Total	$ 66 M

SCHEDULE
TIME AND COSTS

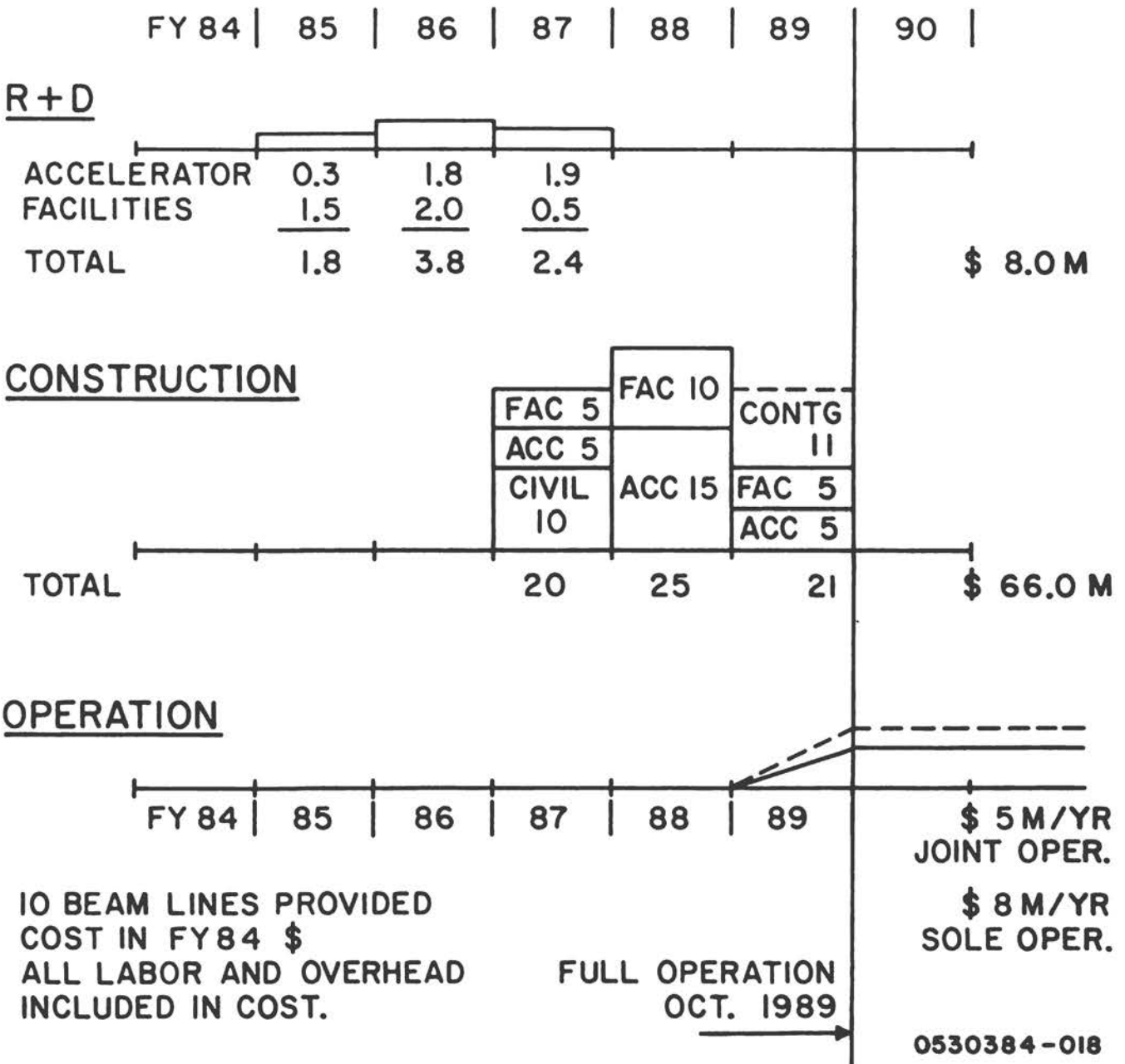


Fig. 6.

at $10 M. The 10 beam lines are estimated at $2 M/line for a total of $20 M. The total estimated cost in FY 84 dollars is thus $55 M. Adding a 20% contingency brings the grand total to $66 M for the construction.

In Fig. 6 we show the proposed time schedule and costs including Research and Development prior to construction, the construction, and an estimate of operating costs.

We would imagine serious R/D work to begin at a low level by mid FY 85, with the intent to provide a basic plan for the facility in enough detail so that the plans for the civil construction could be drawn up in FY 86. In order to ensure that the design features of the new facility will be optimized for its intended use, a series of meetings and workshops would be conducted to obtain full input from the synchrotron radiation community. The R/D effort would extend over three years and would include work both for the storage ring and for the experimental facilities. A total of $8 M is estimated for this effort. The construction would begin in FY 87 with the largest item being the civil construction. The construction costs would peak in FY 88 and be completed in FY 89 with full operation beginning in October 1989.

It is estimated that if the facility is operated jointly with the existing CESR operation, then the cost for operating the dedicated radiation facility would be about $5 M/year. This includes the personnel costs for the scientific and support staff of the dedicated storage ring. This estimate is based on our experience with our existing operation at CESR and CHESS. If, at some date in the future, the high energy physics operation at CESR is terminated and the synchrotron radiation facility then assumes the full cost of the operation of the synchrotron facility, the annual cost of the operation may rise to $8 M per year. It should be pointed out

that even though the CESR storage ring is operated in parallel with the new facility, with simple care in scheduling of filling periods, there should be no interference between the use of the synchrotron as an injector for the dedicated ring and for the filling of CESR. The synchrotron itself can be appropriately shielded so that access to the high energy phsyics detector of CESR can be achieved and still maintain injection capability from the synchrotron. The normal schedule for the synchrotron facility would provide for beam at least 11 months per year with the remaining time distributed as required for maintenance of the facility.

It should be strongly emphasized that the designs of the existing CESR ring and CHESS facility fortuitously already strongly resemble the new proposed dedicated x-ray ring. The CHESS beam line apparatus (beam stops, crotches, and general beam monitoring and handling devices) have been designed for photon beams produced by an 8 GeV, 100 ma electron beam. The heat loading capabilities of our existing designs are directly adaptable to the new machine. We thus will save considerable time and expense by incorporating many of these existing designs; but, more importantly, because of the experience already obtained, the reliability of these devices will be assured.

The existing CESR storage ring has operated in a trouble-free mode for more than four years. This ring has extremely flexible control of the beam optics as a result of being the first of its generation to provide separate excitation for each of its quadrupoles. This feature together with the associated computer control system provides a unique ability to operate the ring with a wide range of lattice structures. All the hardware, fundamental aspects of the control system, and the software support can be directly applied to the new machine to provide exceptional flexibility of operation.

It is proposed that the construction and operation of the facility be a joint effort of the existing CHESS center and the Laboratory of Nuclear Studies. A Director would be appointed to manage the construction and operation of the Laboratory. An Associate Director from the LNS staff would be in charge of the design and construction of the storage ring and the civil construction. A corresponding Associate Director from the CHESS organization would be responsible for the development of insertion devices, beam lines and the organization and management of the continuing experimental program. The staffs of both Associate Directors would jointly develop the configuration of the storage ring to meet the special needs of the synchrotron radiation community. When the facility is placed in operation, it is envisioned that the CESR staff would be responsible for the maintenance and upkeep of the dedicated ring, but that in normal operation the CHESS staff would be responsible for the actual operation of the ring including injection, control of the beams in the ring, and safety. This dedicated synchrotron radiation facility would be nationally available to users and operate with the guidance of the appropriate policy and program committees advisory to the Director.

It is anticipated that the construction of the ring and accelerating equipment could be accomplished with only modest increases in the CESR staff. In order to operate the facility, serve the users, and provide an administrative structure for the operating of the facility, a relatively large increase in the CHESS staff would be required. This expansion would necessarily include additional senior professorial staff and an in-house professional research staff to interact with the user community. It is estimated that about 40 employees would be required to operate the facility in the joint mode of operation with CESR. If the high energy physics

program were discontinued, a total of 80 to 100 employees might be needed to operate the entire facility.

The University administration has given strong encouragement to develop a proposal of this type. Because of the broad interest on the campus in synchrotron radiation, we expect strong support from the administration for faculty appointments which will be necessary to construct, operate and utilize a facility of the highest quality with strong local scientific guidance, support, and management.

In summary, we wish to emphasize the following points:

1. The injector for the dedicated storage ring facility exists and has worked reliably for 15 years. It can provide either e^+ or e^- and is capable of injection at the approximately 6 GeV operating energy of the ring.

2. Cornell accelerator construction has always been highly regarded in the field. It has a good track record for delivery and cost effectiveness.

3. CHESS is a synchrotron radiation laboratory with direct experience in high energy x-ray production and scientific use.

4. The unique design features of CESR and CHESS are particularly appropriate for the proposed 6 GeV ring. Much of the past engineering design is directly adaptable to the new ring.

5. If design and construction begins within a year or so, the dedicated 6 GeV storage ring for synchrotron radiation can be in operation by the end of the decade.

6. The University administration, in preliminary discussions, is enthusiastic about the possibilities of having a dedicated ring on campus and will commit faculty positions to support its operation.

7. The proposed facility design lends itself to evolving national needs. The facility can be expanded to include more beam lines as such need develops.

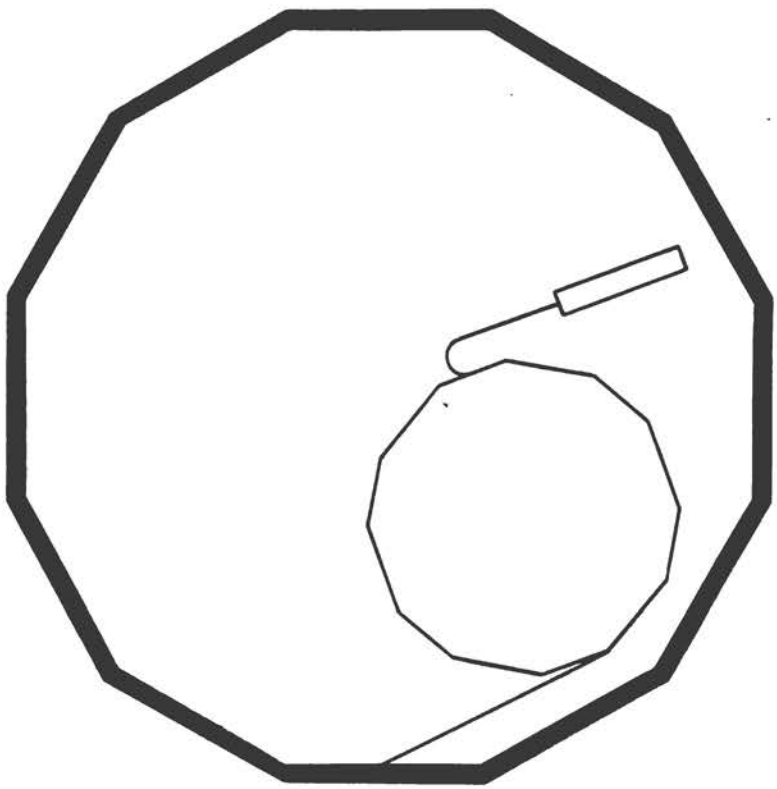
Boris Batterman
Director, CHESS; Professor of Applied & Engineering Physics

B. D. McDaniel
Director, Laboratory of Nuclear Studies; Professor of Physics

April 26, 1984

Pub-5111

The Advanced Light Source: Scientific Opportunities



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Prepared for the U.S. Department of Energy
under Contract DE-AC03-76SF00098

Pub-5111

THE ADVANCED LIGHT SOURCE: SCIENTIFIC OPPORTUNITIES

April 16, 1984

Scientific Editors

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Prepared for the U.S. Department of Energy
under Contract DE-AC03-76SF00098

Foreword

The National Academy of Sciences has been asked by the President's Science Advisor, George A. Keyworth, II, for Assistance in establishing priorities for major facilities in the materials sciences. A Major Materials Facilities Committee has been established under the aegis of the Commission on Physical Sciences, Mathematics, and Resources of the National Research Council. The Committee Chairman is Frederick Seitz of Rockefeller University.

Synchrotron radiation is one major area of research that the Seitz Committee is examining. A Synchrotron Radiation Subpanel, chaired by David W. Lynch of Iowa State University, was established with responsibility for conducting an in-depth review of synchrotron radiation opportunities and facilities to enable the Committee to set priorities for future generic facilities.

This document was prepared at the request of the Committee to provide a concise summary of the Lawrence Berkeley Laboratory's proposed Advanced Light Source. In keeping with the Committee's request, particular emphasis has been given to "the important future scientific and technological opportunities in synchrotron radiation especially as they relate to capabilities of (the) proposed facility."

The first draft of this report was distributed to the Synchrotron Radiation Subpanel for its executive meeting on February 28, 1984 at the University of California, Los Angeles. A second draft was distributed to the entire panel for comments. This final version is to be incorporated as an appendix to the final Seitz Committee report.

This report draws on the ideas of many scientists, whose letters are reprinted along with a technical description of the Advanced Light Source in a companion document. *The Advanced Light Source: Machine Description and Background Material* Pub-5111 Appendix. It is available upon request from the Lawrence Berkeley Laboratory.

Contents

Summary vii

1. Introduction 1-1

2. The Advanced Light Source 2-1

   Photon Beam Characteristics 2-3
   ALS Operations 2-7
   ALS Costs 2-8

3. Scientific Opportunities at the ALS 3-1

   Introduction 3-1
   Biology, Biochemistry and Biophysics 3-1
   Atomic and Molecular Physics 3-3
   Chemical Reactivity 3-4
   Materials Science 3-6
   Coherent Power and Mixed Beam Experiments 3-9
   National Defense Programs 3-10
   Medical Applications 3-11
   Industrial Applications 3-11

4. Institutional Setting 4-1

Summary

The Advanced Light Source (ALS) is the first dedicated synchrotron radiation source optimized to generate vacuum ultraviolet and soft x-ray (XUV) light using magnetic insertion devices. A research tool of unparalleled range and power, it will enable U.S. scientists to remain world leaders in the rapidly moving fields that rely increasingly on synchrotron radiation as a probe. Qualified investigators from industry, universities, and national laboratories will be able to take advantage of the ALS's unique capabilities—high spectral brilliance, high spatial resolution, controllable polarization, and very short pulse length (on the order of picoseconds). Many-pole undulators in this optimized storage ring will provide spatially and longitudinally coherent radiation that is broadly tunable across the XUV region of the spectrum. In addition, with frequency-domain techniques it will be possible to make measurements in this spectral region on a time scale of femtoseconds.

A source with these new capabilities will allow unprecedented studies in both basic and applied science. In the **biological sciences**, for example, the unparalleled photon flux to small samples together with the capability for wavelength tuning will enhance imaging and scattering techniques available with XUV radiation. With picosecond-length pulses and the ability to match soft x-rays to the absorption features of major structural biological elements, such as carbon, nitrogen, and oxygen, it will be possible to make dynamical response studies of specimens without the need for dehydration, fixing, or staining. Variable polarization and high photon fluxes will permit new life science studies, including studies of DNA conformation. The coherence properties of undulator radiation will extend the use of synchrotron radiation into the phase-sensitive world of x-ray interferometry and biological microholography.

In **atomic and molecular physics**, very high photon fluxes are needed for spectroscopic studies of free atoms and molecules in the gas phase; only with radiation from undulators and wigglers is the signal-to-noise ratio for many experiments in the x-ray region becoming acceptable. The ALS will set new standards for spectral resolution, and will make possible picosecond dynamical studies of phenomena such as atomic inner-shell transitions, quantum interference effects, and photoemission.

In **chemistry**, the ALS output in the vacuum ultraviolet region will be sufficient to open new areas of research in the study of chemical reactivity. Its high spectral brilliance and picosecond time structure will permit high-spectral-resolution dynamical studies of reaction kinetics, intramolecular transfer processes, excited state proton and electron

transfer, and molecular photodissociation and photoionization. In addition, it will dramatically expand opportunities for research in condensed-phase chemistry—for instance, extending hydrodynamical studies of rotational motion and diffusion to much smaller solute molecules than can now be treated, and permitting real-time studies of "cage effects" in solution with systems of sufficient simplicity to be related to the microscopic parameters of a molecular dynamics theory.

In **materials and surface science**, the capabilities of the ALS will permit new investigations of bulk materials as well as surfaces and interfaces. Time-resolved studies in catalysis will be possible with XUV radiation of extremely high brilliance and picosecond time structure. For instance, it will be possible to study the dynamics of surface contamination and interface formation and to verify microscopic models for catalysis, oxidation, corrosion, and interface growth.

Industrial utilization of XUV radiation will be increased by the availability of appropriate radiation sources and a focal point for industrial-academic collaboration. One industrial application of the undulator radiation at the ALS will be to improve mask fabrication in the micro-electronics industry. By utilizing the full potential of synchrotron radiation for x-ray lithography, it will be possible to achieve significantly finer feature sizes at less demanding aspect ratios while maintaining competitive writing speeds.

In the area of **national security**, scientists at several national defense laboratories have expressed the need for access to a modern soft x-ray synchrotron radiation facility like the ALS. They have emphasized dependable access to high-flux, high-brilliance facilities for program-related research.

The scientific opportunities outlined above are a sampling of the potential for state-of-the-art synchrotron radiation research with the ALS. In addition, the ALS will add to this country's heavily used synchrotron radiation facilities and, even more important, will provide opportunities for student research and training in an area where a lack of qualified personnel is already being felt.

Lawrence Berkeley Laboratory (LBL) is an appropriate site for the ALS. Its strengths in accelerator physics and instrument design are well known. It has played a pioneering role in the development of permanent-magnet insertion devices, and the team that designed the ALS has participated in designing accelerators, accelerator devices, and particle detectors around the world. The laboratory is experienced in operating national research facilities, notably the Bevalac complex, the 88-Inch Cyclotron, the Neutral Beam Engineering Test Facility, and the National Center for Electron Microscopy. The Center for X-Ray Optics, established at LBL in 1983, is designed to accelerate the application of XUV radiation in pure and applied science through the development of new optical techniques. Finally, LBL is unique among national laboratories in being a major research partner of an outstanding research and teaching institution, the University of California at Berkeley; research programs at the ALS will be able to draw on the combined resources of the laboratory and the university and will attract students from many disciplines that are critical to this country's scientific and technological future.

The design for the ALS is complete. It has been reviewed by a technical review committee of synchrotron radiation and accelerator experts. The committee's recommendations have been incorporated in the design, and no insoluble design problems have surfaced. Three construction-readiness reviews have been carried out by the Department of Energy's Office of Management; the review team concluded that the ALS is ready to be built and that its cost estimate is comprehensive and realistic.

1 Introduction

Synchrotron radiation (SR) is becoming an important tool in many branches of science. Current sources provide radiation that is continuously tunable across a broad region of the electromagnetic spectrum. It is also highly polarized and directed into an extremely narrow beam. With these features, SR provides a powerful probe of atomic and molecular resonances (Figure 1–1). Probing techniques can provide significant information on the structure and dynamics of atomic, chemical, material, and biological assemblies (Figure 1–2).

The recent development of magnetic insertion devices is enabling extraordinary improvements in the potential of SR as a scientific and technological tool. As stated in the report of the DOE Planning Study for Advanced National Synchrotron-Radiation Facilities (February, 1984), insertion-device-based SR sources will offer "gains in photon-beam brilliance as large as the gains present-day synchrotron sources provided over conventional sources." The study panel further recognized that there would be an explosion of new scientific opportunities accessible with SR sources specially optimized for these long, alternating-magnetic-field undulators and wigglers. Moreover, two new low-emittance electron storage rings are required to access both the vacuum ultraviolet/soft x-ray region (referred to here collectively as the XUV) and the hard x-ray region. Only in the XUV case, however, are the technical issues sufficiently well understood to permit a construction start in the near future.

Historically, SR has been obtained in a parasitic mode from bending magnet stations at high-energy physics facilities (electron-positron storage rings, for example). More recently, some storage rings dedicated to SR generation have become available. Even at these sources, bending magnets remain the dominant source for SR experiments.

During the past five years, there has been considerable development of specialized periodic magnetic structures—wigglers and undulators. Figure 1–3 compares the properties of radiation from insertion devices and bending magnets. Insertion devices are now technically well developed and their radiation is superior to that from bending magnets for most applications. Lawrence Berkeley Laboratory (LBL) has played a leading role in the development of these new devices and has contributed to the strong position of the U.S. in SR technology. Permanent magnet technology for insertion devices pioneered at LBL made possible the shifted spectrum achieved at Stanford's SSRL with LBL's 54 pole wiggler, the world's most powerful source of SR when commissioned in late 1983 (Figure 1–4).

To date, undulators and wigglers have been retrofitted in existing storage rings. Consequently the best match between rings and undulator characteristics has not been possible, and the undulators have been unable to achieve their spectral brilliance limits (see discussion of spectral brilliance, Chapter 2). In particular, the large electron beam emittance of existing storage rings broadens the central radiation cone, and reduces the spectral brilliance by a factor of N (N is the number of undulator periods).

The next step in the evolution of SR sources is to design an electron storage ring and its insertion devices to optimize their spectral performance. This integrated design approach lies at the heart of the Advanced Light Source. The storage ring emittance, length of straight sections, undulators, optical power loading capabilities, and desired XUV spectral brilliance have all been designed in a self-consistent manner. Additional attributes that become available with a moderate-energy ring such as the ALS, specifically optimized for applications in the XUV.

In the next chapter, the characteristics of the Advanced Light Source are described, especially as they relate to the use of undulators to provide high spectral brilliance XUV radiation, coherent power, and complete polarization control. Chapter 3 outlines the scientific opportunities available at the Advanced Light Source. Chapter 4 addresses the institutional context of the proposed facility.

Molecular, Atomic, and Electronic Processes

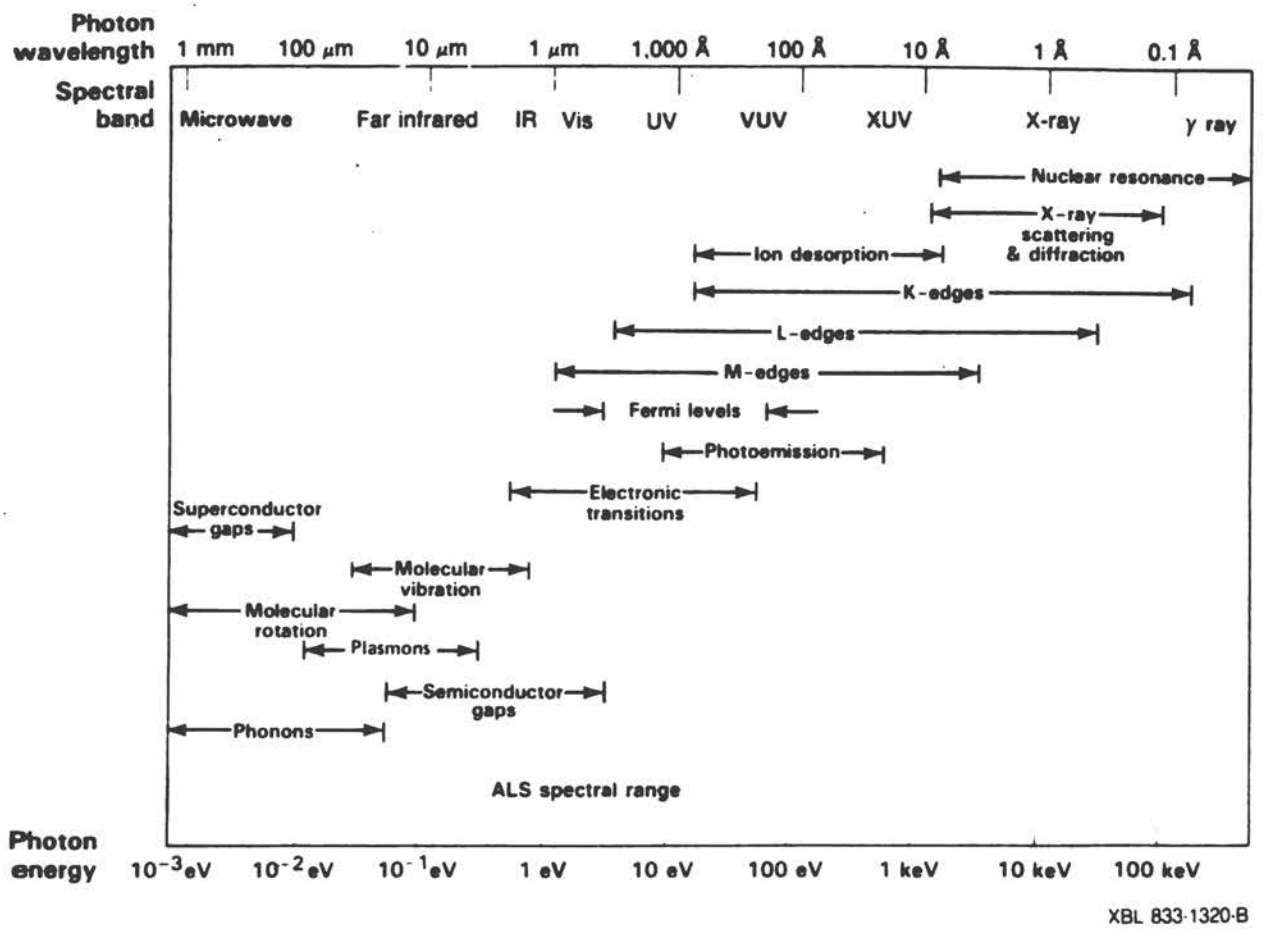


Figure 1–1.

Characterization Techniques Using Synchrotron Light

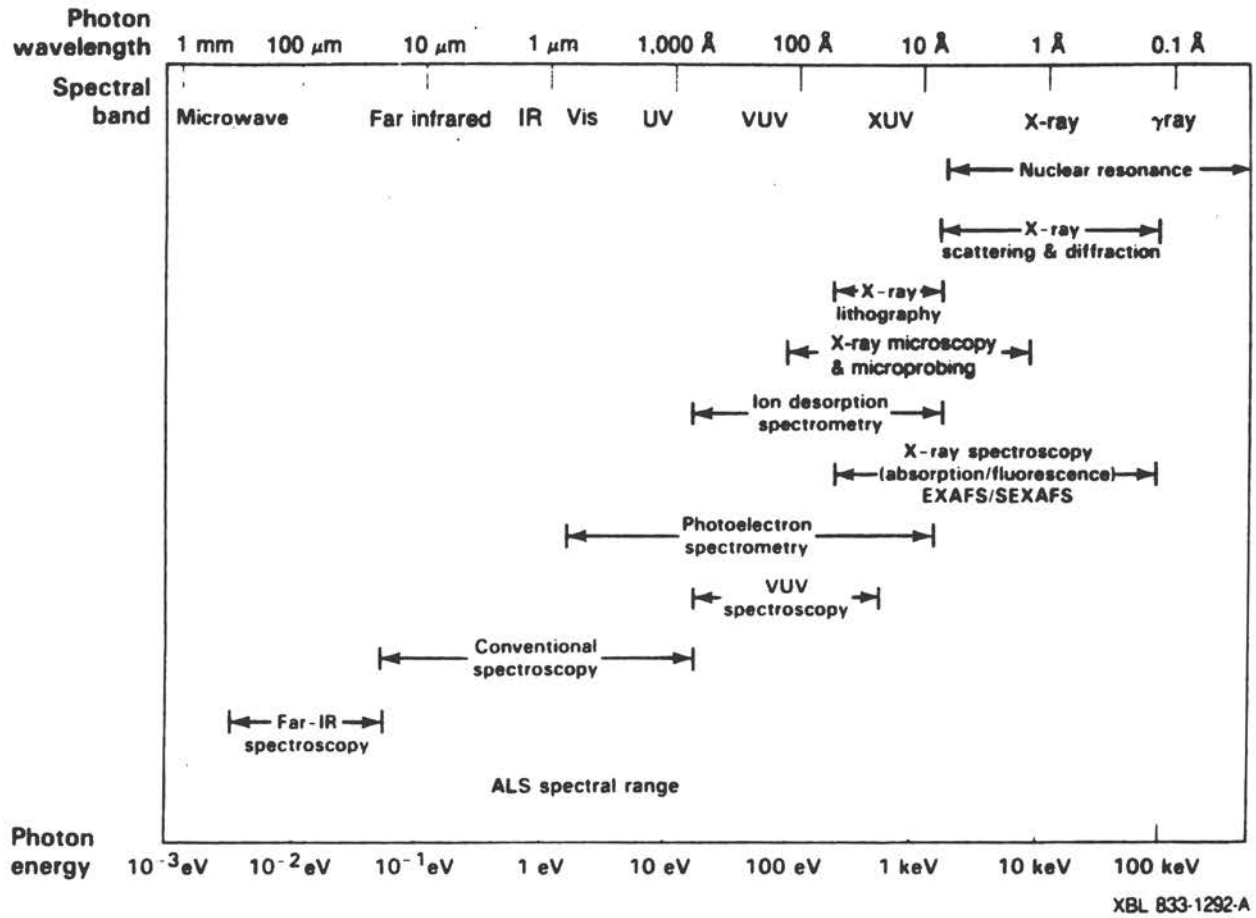
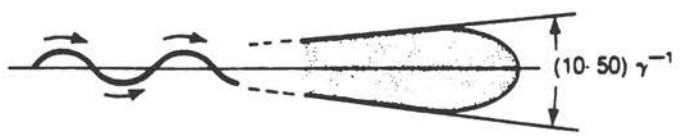


Figure 1–2.

Synchrotron Radiation Sources

Bending Magnet — A "Sweeping Searchlight"



Wiggler — Incoherent Superposition

$$\frac{dP}{d\Omega} \propto N$$

Undulator—Coherent Interference

$$\frac{dP}{d\Omega} \propto N^2$$

$$\Omega \propto \frac{1}{N}$$

$$P \propto N$$

N = number of magnetic periods (~100)

$$\gamma^{-1} = \frac{m_o c^2}{E_e} = \frac{0.511}{E_e(\text{GeV})} \text{ mrad}$$

XBL 8311-4541

Figure 1-3.

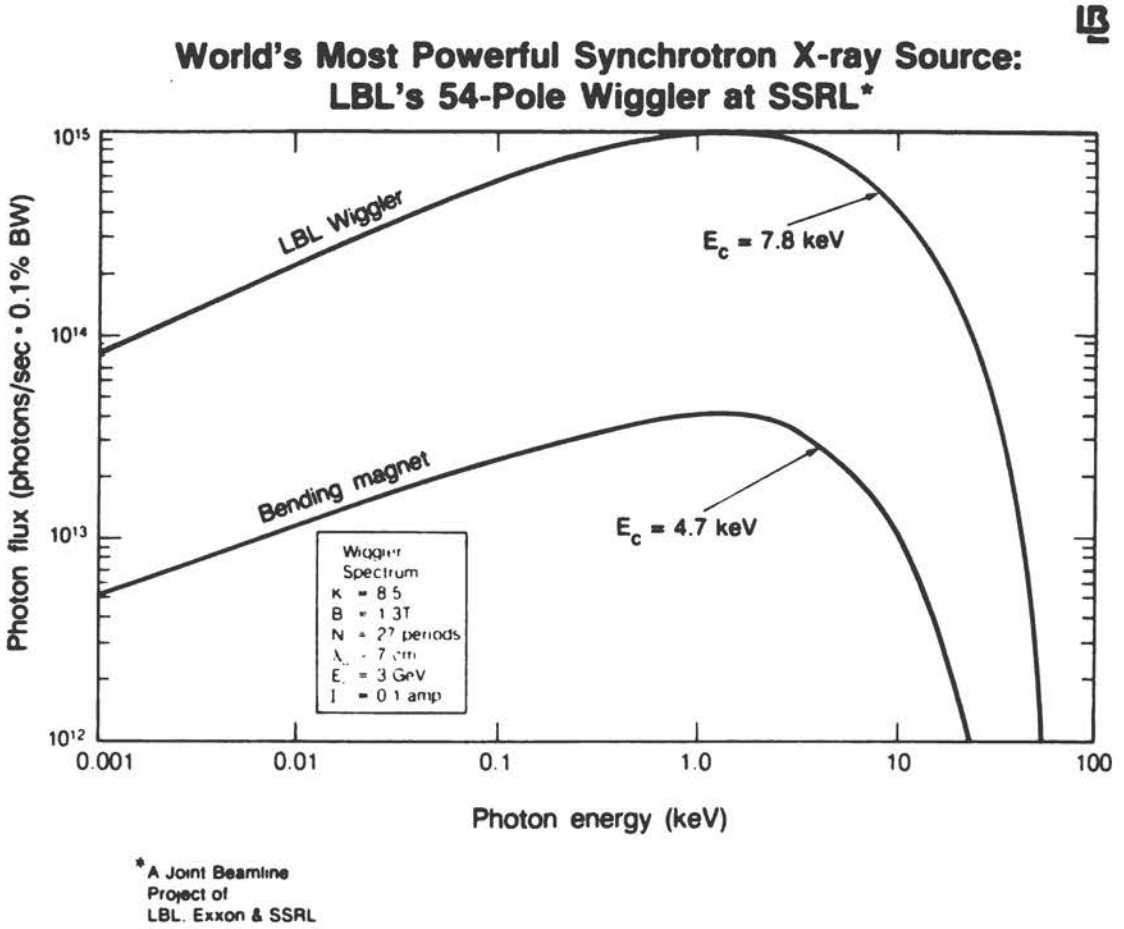

World's Most Powerful Synchrotron X-ray Source:
LBL's 54-Pole Wiggler at SSRL*
Photon flux (photons/sec • 0.1% BW)
10^15
10^14
10^13
10^12
LBL Wiggler
Bending magnet
E_c = 7.8 keV
E_c = 4.7 keV
Wiggler Spectrum
K = 8.5
B = 1.3T
N = 27 periods
λ_w = 7 cm
E_e = 3 GeV
I = 0.1 amp
0.001
0.01
0.1
1.0
10
100
Photon energy (keV)
*A Joint Beamline Project of LBL, Exxon & SSRL
XBL 8311 656 A

Figure 1–4.

2 The Advanced Light Source

The Advanced Light Source is a 1.3-GeV electron storage ring optimized to produce broadly tunable XUV synchrotron radiation from magnetic insertion devices. Goals for the design include

- High spectral brilliance
- Picosecond time structure
- Variable polarization characteristics
- Broadly tunable coherent radiation
- Long beam lifetime (> 8 hours)
- Beam stability (fractional beam width)
- Efficient use of radiation with nondegrading optics

The technical features incorporated in the ALS to achieve these goals are described in detail in Appendix A, contained in a companion volume (LBL Pub. 511 Appendix). Table 2–1 summarizes the design parameters. Additional factors considered very important for the ALS as a national user facility were user friendliness and the availability of beam lines for both individual users and participating research teams (ALS Affiliates) (Figure 2–1). The funding request includes full activation of the six general-user straight sections, including four specially designed undulators and two wigglers driving 14 branch lines. The additional six straight sections, driving a similar number of branch lines, are available for development by Affiliates.

Table 2–1.
Advanced Light Source design parameters.

Injector	
Linac energy	50 MeV
Linac current	20 mA
Booster energy	1.3 GeV
Booster current	10 mA
Booster pulse rate	$1\ s^{-1}$
Storage Ring	
Nominal energy	1.3 GeV
Peak energy	1.9 GeV
Circumference	182.4 m
Maximum current	400 mA
Beam lifetime	8 hours
Horizontal emittance	$7 \times 10^{-9}\ \pi$ m-rad
No. of straight sections	12
Length of straight sections	6 m

Layouts of the first six beam lines for general users were reviewed in detail by some 200 scientists attending the ALS/SSRL Users Workshop in May 1983. Features of the initially proposed general-user beam lines are listed in Table 2–2, while the spectral brilliance curves for three of the insertion devices are shown in Figure 2–2, with the spectrum of the LBL/SSRL/Exxon wiggler (Figure 1–4) included for reference. Figures 2–3 and 2–4 show possible layouts of the beam lines driven by wiggler E and undulator D, and indicate scientific techniques appropriate to these spectral ranges.

Table 2-2.
ALS general user beam lines.

Source	Energy range (eV)	Branch line angle (Degrees)	Proposed monochromators (eV)
U_A	5–700	0	Grating (5–700)
		13.9°	Grating (5–700)
U_B	25–1,500	0	Grating (25–1,500)
		5.4°	Grating (15–1,500)
		5.4°	Grating (25–1,800)
U_C	75–3,000	0	Crystal (800–3,000)
		3.2°	Grating (75–1,500)
		3.2°	Grating (75–5,000)
U_D	200–10,000	0	Crystal (200–20,000)
		1.9e	Grating (75–1,500)
W_E	0.1–14,000	0	Crystal (200–10,000)
		3.2°	Crystal (500–3,000)
		19.4°	Grating (10–500)
		30°	IR (0.1–1)
W_F	500–40,000	0	Crystal (3–40 keV)
		0.8°	Crystal (5.0–10 keV)
		0.8°	Crystal (3–40 keV)
		1.4°	Crystal (3–40 keV)
		1.4°	Crystal (3–40 keV)

Photon Beam Characteristics

Spectral Brilliance. Spectral brilliance is the property of radiation that permits experiments requiring many photons to be performed at high spectral resolution on very small samples. It has technical advantages as well. For example, spectrally brilliant beams place modest demands on optics and monochromators. Undulators are the current state of the art in spectrally brilliant sources as they produce strongly collimated beams of radiation concentrated spectrally in several, harmonically related bands (Figure 2–5).

For many researchers, undulators will simply be a source of greatly intensified radiation of prescribed spectral content, which can be concentrated on ever smaller samples. These features not only will improve the signal-to-noise ratio in many applications, but will also shorten required exposure times and provide qualitative improvements in the effectiveness of measurement techniques and spectrometers.

Currently, the most challenging spectroscopic applications require high spectral resolution. In most cases, the optical system is overfilled both spatially and spectrally, i.e.

photons are being wasted because they do not strike the sample or are not the right energy. A high-brilliance source—one with the largest possible fraction of photons originating from a near-diffraction-limited phase space volume—has a real advantage for such applications. The emittance and undulator designs for the next generation machines achieve spectral brilliances within a factor of ten of diffraction limits. Bending magnet sources are generally seven orders of magnitude from these limits, and thus often incur enormous waste of photons.

To appreciate the full value of a high-spectral-brilliance source, we must consider, along with the source, the optical system that condenses the beam, monochromatizes it, and finally delivers it to the sample under investigation. At each stage of this process there is a limit to the radiation width and angular spread that the optics can accept. For example, a monochromator with both slits set for a desired spectral resolution has finite spatial acceptance (slit width) and angular limits due to grating geometry and angle subtended by the slit. More subtle acceptance widths are incurred through overly large acceptance angles (low F numbers) in aberrated optical systems. Overall system limits are often described by the two-dimensional product of spatial width and angular acceptance $(W\Delta\theta)_x(W\Delta\theta)_y$. In essence this is a phase space acceptance volume. If the incoming beam originates from a larger phase space, the system is overfilled and the surplus photons are wasted. The emission phase space for SR is set in large part by the storage ring "emittance"—the beam size $\times$ angular spread product which characterizes the highly relativistic electron beam. At a given wavelength, there is a lower limit to the emission phase space volume set by diffraction. When the full photon beam originates from a diffraction-limited space $\times$ angle product it is said to be spatially coherent. This is the condition of maximum possible brightness for that source, in units of photons per second, per area, per unit solid angle. Spectral brilliance additionally accounts for spectral content (bandwidth), and is directly proportional to longitudinal (or temporal) coherence properties.

High Flux and Picosecond Time Structure. Of great importance for many modern applications of SR are the combinations of high flux and picosecond time structure. For the first time, dynamical studies of chemical and molecular phenomena, resolved at picosecond and sub-picosecond time scales, will be studied with intense, tunable VUV and soft x-ray radiation. Available bunch lengths are shown in Figure 2–6, as a function of beam current. The ALS, with its smooth walls, will permit researchers to achieve fractional bunch-length time resolution, possibly in the sub-picosecond regime. Figure 2–7 shows how such sub-picosecond measurements might be achieved using frequency-domain techniques in a sufficiently stable ring. Uses of the technique are discussed in Chapter 3.

Coherence. The coherent nature of XUV radiation available from undulators is particularly noteworthy. These unique sources will provide new XUV opportunities in many scientific fields, much as lasers have for applications of visible (and near-visible) light. Many-pole undulators in optimized storage rings will provide spatially and longitudinally (temporally) coherent radiation that is broadly tunable across the XUV. Researchers will thus have unprecedented control (pointing, focusing, brightness, etc.) of radiation in this region of the spectrum, as well as opportunities to utilize sophisticated coherent phase techniques previously available only with longer-wavelength radiation sources such as lasers, masers, and klystrons.

Undulator radiation is largely coherent in nature because both the emission area and the radiation cone are small, providing a near diffraction-limited source. The radiation

cone is small because the emitting electrons are highly relativistic, and the effective emission area is small because modern storage rings achieve "low emittance," that is, the electron beam is contained within a small area × solid angle product. Longitudinal coherence is achieved through the small-angle interaction of radiation from the many (N) magnetic periods. Participation of all N periods of the magnetic structure produces a spectral line width $\lambda/\Delta\lambda \approx N$.

Although quasi-coherent radiation is also potentially available in the coming decade or so with imaginable x-ray laser schemes, the earliest and only assured route to broadly tunable coherent soft x-rays is with undulators in newly designed storage rings (Figure 2–8). The outstanding coherence properties of XUV radiation from next generation storage rings arise, in large part, because the emittance of a spatially coherent XUV beam is similar to the achievable electron beam emittance. Optimum performance with modern storage rings occurs at about 25 Å (500 eV photons). Shorter wavelength facilities produce radiation with spatial coherence decreasing as λ^2. Longitudinal (temporal) coherence of undulator radiation is also wavelength related, since coherence length is defined by $l_c = \lambda^2/\Delta\lambda \simeq N\lambda$. Thus, while XUV radiation enjoys a privileged, near diffraction-limited position vis à vis present storage ring capabilities, shorter wavelength radiation facilities have coherence properties decreasing as $N\lambda^3$. These arguments are summarized in Figure 2–9 and indicate that a substantial fraction (~1%) of the 25 Å undulator radiation from the ALS will be spatially coherent and of 1 μm coherence length. For comparison, at a 6-GeV machine of identical emittance, the fraction of 1 Å radiation having identical coherence properties will be reduced by more than four orders of magnitude to less than 10^{-6}. We thus conclude that SR in the XUV region has unique advantages in the area of coherent applications.

One manifestation of the coherence properties is the spatial interference pattern illustrated in Figure 2–10 for the third harmonic of undulator D at 500 eV. Emanating from the interaction region, a flux of approximately 10^{16} photons per second radiates into a central cone of 40 × 100 μrad full (2σ) angle, from a blur circle (ellipse) of about 160 × 400 μm. Produced by the coherent interaction of radiation from 142 undulator periods, the radiation is naturally emitted with less than a 1% bandwidth. Because of the small phase space and limited spectral content, the radiated power is not only of high spectral brilliance but also largely coherent in nature.

The coherence properties of the ALS are sufficient to extend SR capabilities to perform x-ray interferometry, holography, and other interference techniques, on the modest-sized samples of interest to materials scientists, biologists, and others. Indeed, there is no other generation scheme in sight that provides an assured path to the scientific opportunities accessible only with coherent XUV radiation.

Other XUV Beam Characteristics. Complete polarization control is necessary for many studies of anisotropic sample properties, and can now be achieved in a storage ring of sufficiently low emittance with the crossed-undulator concept illustrated in Figure 2–11. Designed at LBL, the device consists of two crossed undulators in series, separated by a variable electron path phase delay. Circular, linear (including bi-stable flipping), and elliptical polarizations are all available with appropriate electron phase delay modulation. Table 2–3 shows how the crossed undulators would provide arbitrarily polarized first-harmonic radiation at 26 eV using Brookhaven's VUV ring, or first-harmonic radiation of higher spectral purity at 260 eV with the ALS. The capability to produce polarized radiation of wavelengths throughout the soft x-ray regime will be available at the ALS.

Table 2–3.
Two future sources of variable polarization radiation.

Ring	NSLS (VUV)	ALS
Electron energy	750 MeV	1.3 GeV
Emission angle	9×10^{-2} mr	2×10^{-2} mr
Number of periods	5	30
Undulator period	10 cm	4 cm
Fundamental wavelength	470 Å (26 eV)	47 Å (260 eV)
Spectral purity	4%	0.14%
Polarization Purity	86%	84%
Flux at sample (1% optical eff.)	10^{12} photons/s	10^{12} photons/s

In recent years the power densities to which SR optics have been subjected have increased to the point where photon-induced surface distortions have begun to degrade the function of the optics. Moreover, the growing use of insertion devices greatly increases the power density in SR beams at all photon energies, and will aggravate this problem. Table 2–4 gives some revealing data for existing and planned SR sources. The 54 pole LBL/Exxon/SSRL wiggler has broken new ground in the present generation of sources, and as yet no optical system has been exposed to its full power beam. By contrast, the power problems posed by the 1 Å undulator radiation on a hard-X-ray ring appear to be beyond existing technology. The Center for X-Ray Optics at LBL is presently engaged in an R&D program to achieve the best exploitation of an intense beam. We believe that new design concepts, coupled with frontier technology, will be needed to exploit fully the photon beams from next-generation sources.

Table 2–4.
Power loading demands with different synchrotron radiation sources.

Radiation Source	kW/cm^2 (at 10 m)[a]
Bending Magnet (NSLS/X-Ray Ring)	4×10^{-2}
Wiggler (SSRL/LBL 54 Pole)	3 (not yet achieved)
Undulator (NSLS/X-1, 500 eV)	1
Undulator (ALS/UD, 500 eV)	1
Undulator (6 GeV/15 keV)[b]	200

[a]Equivalent units are $kW/(mrad)^2$.

[b]Eisenberger-Knotek Report (2/84), DOE's Planning Study for Advanced National Synchrotron Radiation Facilities. Electron Energy—6 GeV, Current—400 ma, $\epsilon = 7\pi\times10^{-9}$ m·rad, N = 230.

ALS Operations

The Advanced Light Source will be operated as a national research facility open to qualified scientists throughout the United States. To accommodate the demands of researchers with diverse interests and a broad range of technical expertise, skilled support will be available to users at all stages of use—from proposal submission through the running of experiments. Dedicated technical staff, in the form of a core group of scientists, technicians, and computer specialists, will have primary responsibility for assisting experimenters, thereby increasing their research productivity. Duties of these personnel will include designing or modifying beam lines to achieve specific performance characteristics, designing and interfacing data acquisition systems, and installing and maintaining sophisticated research equipment. In addition, an Accelerator Operations Group (scientists, operators, engineers, and technicians) will be devoted to facility operations. The staff of the Center for X-Ray Optics will provide long term assistance to users through the development of new insertion devices, beam-line optics, and instrumentation necessary to keep the ALS at the technological forefront, providing the highest quality photon beams to users. All told, about 80 people will staff the ALS, split approximately 1/3–2/3 between dedicated support to users and accelerator operations.

Other features that make the ALS a "user-friendly" facility from initial design include ample experimental space around the ring, overhead cranes to service the entire experimental floor, abundant staging areas, and expandable construction. Stable alignment of the beam lines will be assured by proper design and careful attention to decoupling of vibrations. Finally, the ALS will be available essentially all year, especially during the summer months when university-based researchers are less heavily involved with teaching.

Three different types of arrangements will be available for researchers interested in using the ALS:

Individual researchers will submit proposals to the ALS Program Advisory Committee for the use of certain beam lines for specific experiments. Received proposals will be considered by the Program Advisory Committee, a group comprising synchrotron radiation researchers from industry, universities, and national laboratories (similar groups at LBL's present national facilities typically have one LBL representative out of six members). This committee will make recommendations, based solely on merit, on the allotment of beam lines and machine time to various users.

ALS Affiliates are participating research teams composed of companies, national laboratories, and academic groups, or combinations of these researchers, who want to have a specially designed and equipped ALS beam line. They will submit proposals for the design, construction, and funding of beam lines. Affiliates will make substantial intellectual and financial commitments to the beam line development. The Program Advisory Committee (or ad-hoc peer review panel if the ALS is not yet running) will review such proposals. If the proposal is accepted, the ALS technical staff and the Affiliate will then design and build the beam line in partnership.

Special Beam Line Groups formed of University and industry researchers who lack the resources necessary to become Affiliates could contribute significantly to the development of beam lines for the ALS and obtain, in exchange, a specified amount of dedicated time on the beam line. LBL welcomes proposals from such groups to design and build optics and instrumentation in collaboration with ALS technical staff. The proposals would be reviewed and selected by the Program Advisory Committee on the basis of scientific and technical excellence and for complementarity with other general beam lines. An ALS Beam Line Workshop, to be held soon after the ALS is approved for construction, will provide an excellent opportunity for these groups to form.

ALS Costs

The design for the Advanced Light Source is complete (see Appendix A). It was fully reviewed by a technical review committee, including SR experts from the United States and abroad, in January 1983. The design team has incorporated recommendations of this committee and other reviewers. In this process, no insoluble design problems surfaced. In addition, three construction-readiness reviews have been carried out by DOE's Office of Management, looking into technical, cost, schedule, and other management concerns. The review team concluded that the ALS is ready to build and that its cost estimate (Table 2–5) is both comprehensive and realistic.

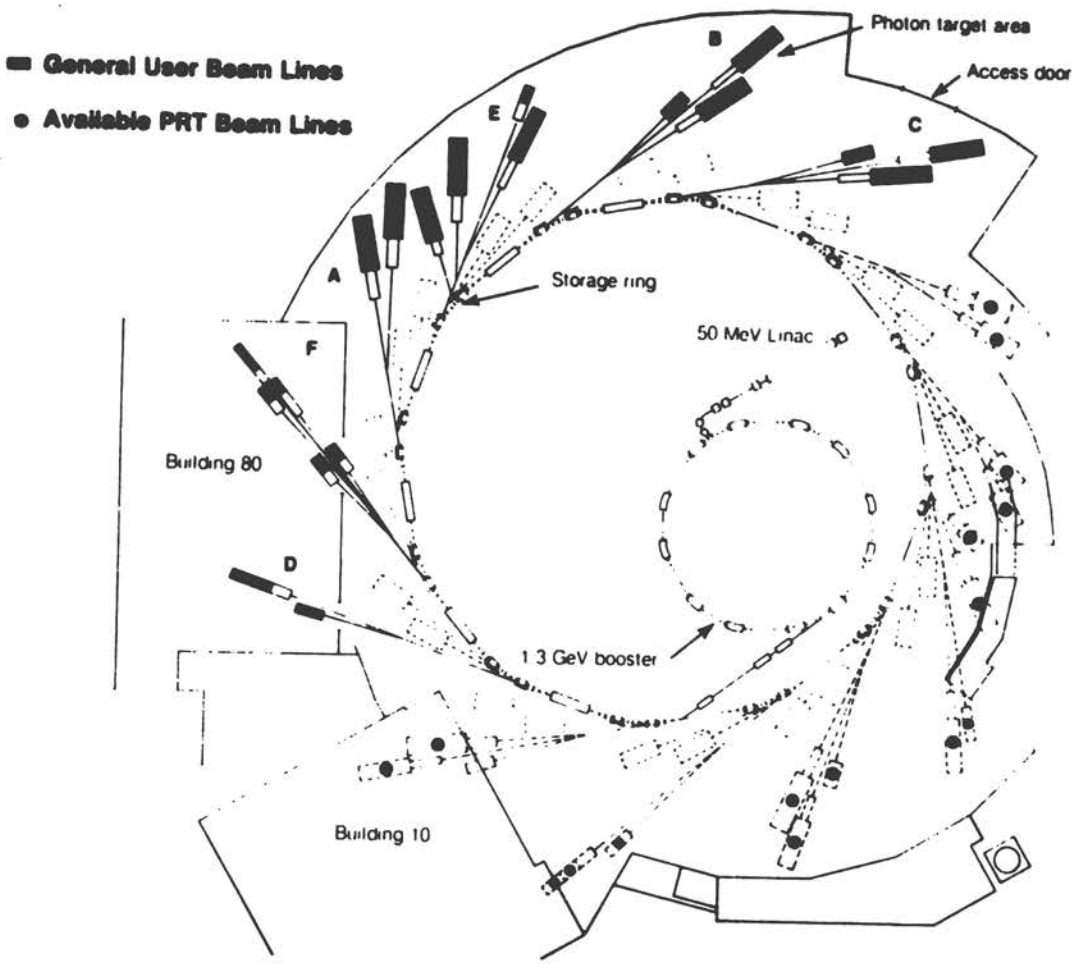
Table 2–5.
ALS construction cost[a] (FY 85 M$).[b]

Accelerator Systems		30.5
Storage Ring	13.5	
Injector System	8.3	
Control System	3.0	
Contingency	5.7	
Beamline System		30.4
Insertion Devices	8.3	
Photon Beamlines	16.4	
Contingency	5.7	
Conventional Facilities		11.7
Removals and Site Preparations	2.5	
Building Addition	3.0	
Shielding	2.0	
Utilities	2.7	
Contingency	1.5	
Total		72.6

[a]Including project management. engineering. design.

[b]Escalated to 85$ from FY83 detailed cost estimate.

The ALS will Have Both General User and PRT Beam Lines



XBL 8311-4523

Figure 2–1.

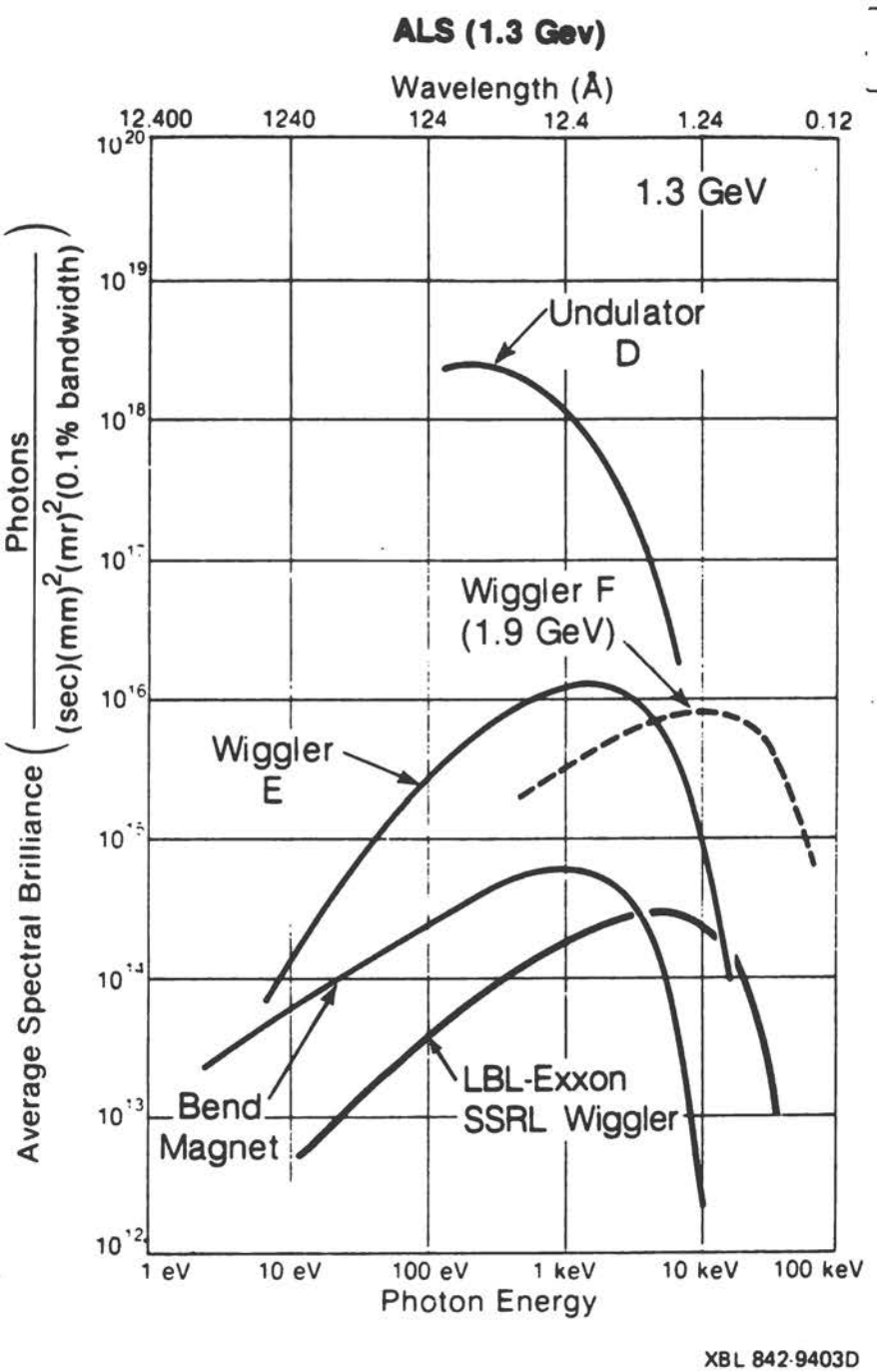

ALS (1.3 Gev)
Wavelength (Å)
12.400
1240
124
12.4
1.24
0.12
1.3 GeV
Undulator
D
Wiggler F
(1.9 GeV)
Wiggler
E
Bend
Magnet
LBL-Exxon
SSRL Wiggler
Average Spectral Brilliance (Photons / (sec)(mm)²(mr)²(0.1% bandwidth))
1 eV
10 eV
100 eV
1 keV
10 keV
100 keV
Photon Energy
XBL 842-9403D

Figure 2–2.

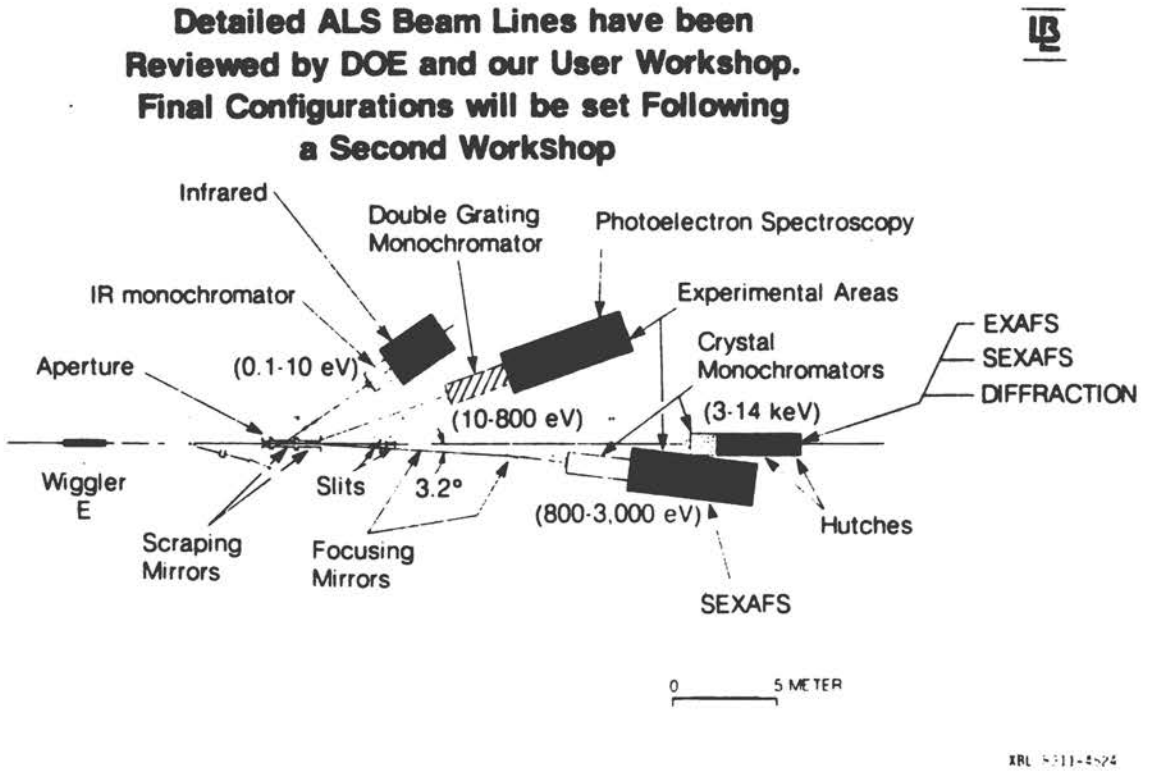


Figure 2–3.

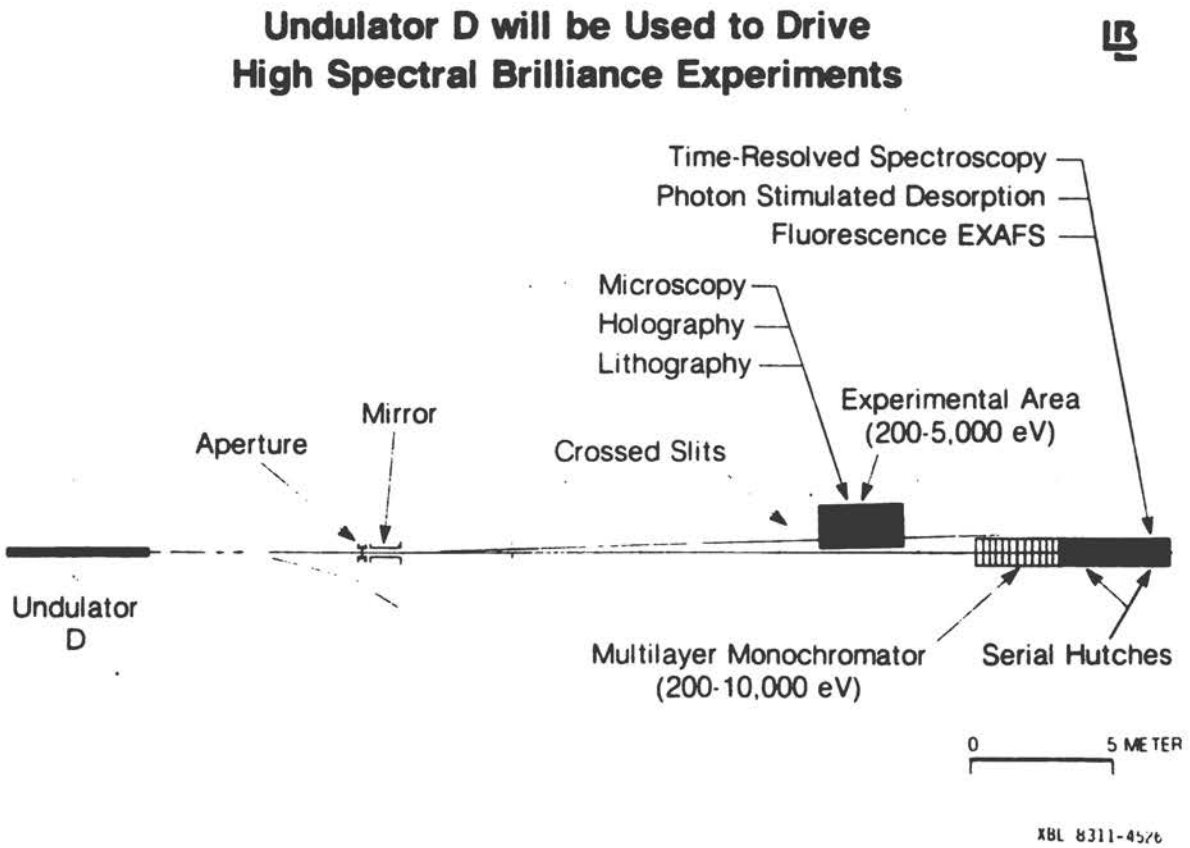


Figure 2–4.

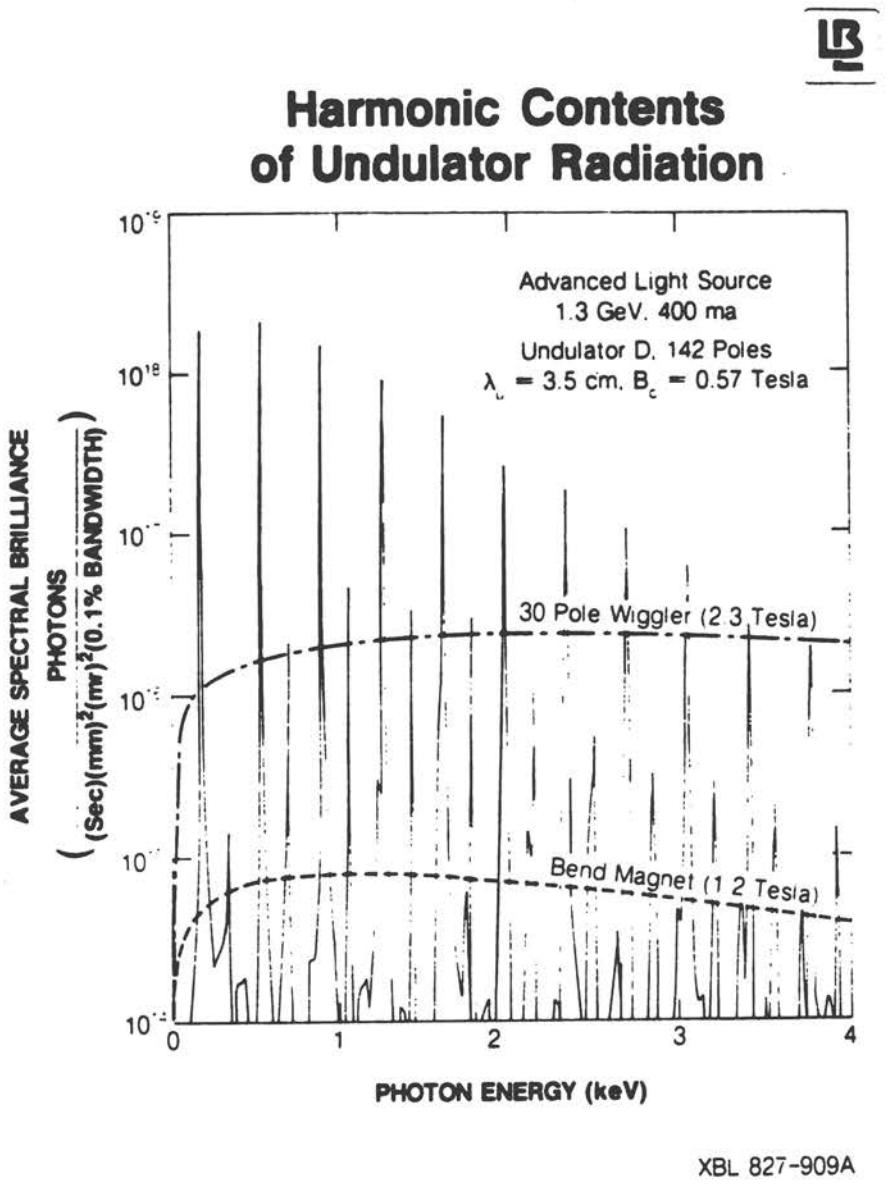

Harmonic Contents
of Undulator Radiation
Advanced Light Source
1.3 GeV. 400 ma
Undulator D. 142 Poles
λu = 3.5 cm. Bc = 0.57 Tesla
30 Pole Wiggler (2.3 Tesla)
Bend Magnet (1.2 Tesla)
AVERAGE SPECTRAL BRILLIANCE
PHOTONS
(Sec)(mm)²(mr)²(0.1% BANDWIDTH)
10¹⁸
10¹⁷
10¹⁶
10¹⁵
10¹⁴
0
1
2
3
4
PHOTON ENERGY (keV)
XBL 827-909A

Figure 2–5.

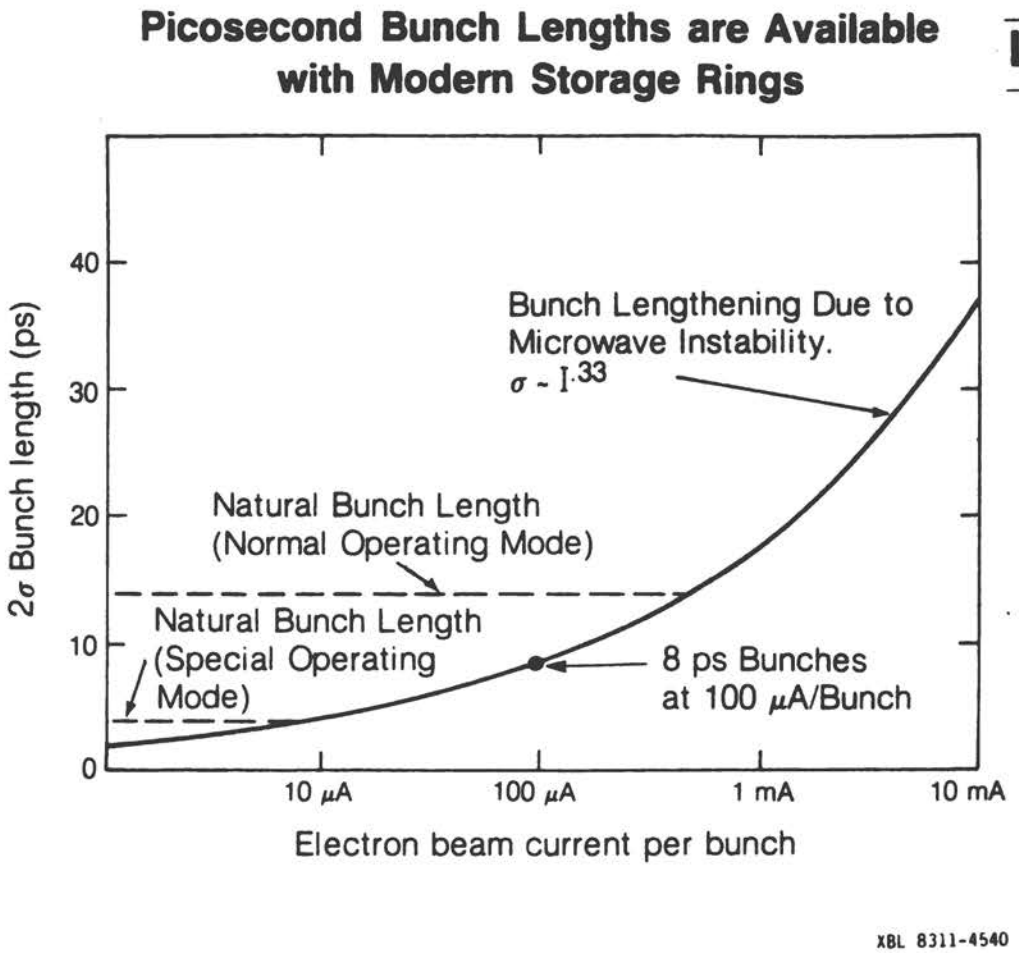

Picosecond Bunch Lengths are Available with Modern Storage Rings
2σ Bunch length (ps)
40
30
20
10
0
Bunch Lengthening Due to Microwave Instability.
σ ~ I^.33
Natural Bunch Length (Normal Operating Mode)
Natural Bunch Length (Special Operating Mode)
8 ps Bunches at 100 μA/Bunch
10 μA
100 μA
1 mA
10 mA
Electron beam current per bunch
XBL 8311-4540

Figure 2–6.

357

Frequency Domain Time Measurements with Time Resolution of (10^{-1} to 10^{-2}) of Bunch Length

(Storage Rings Have Inherently Stable Circulating Beams)

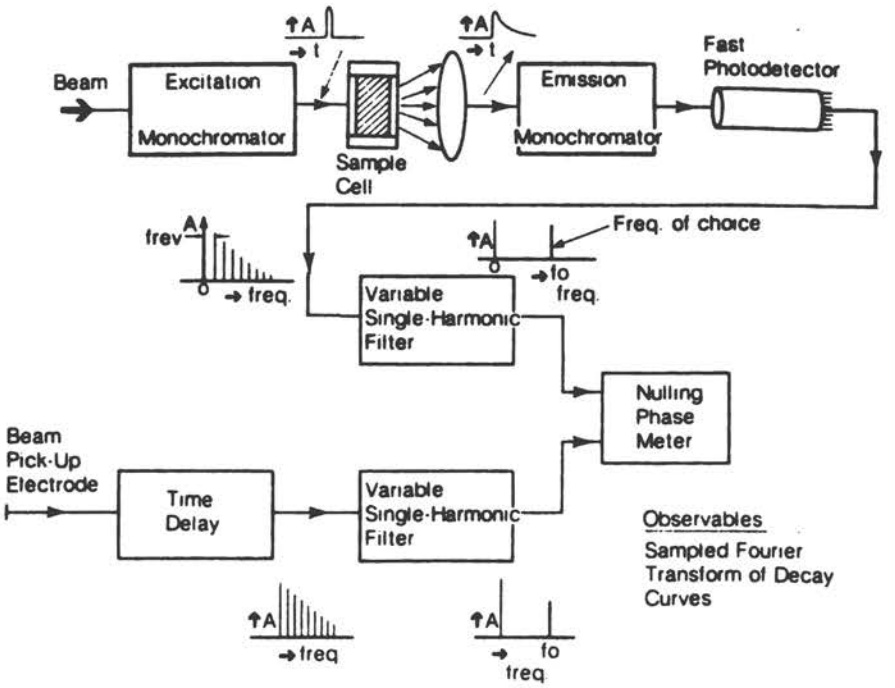
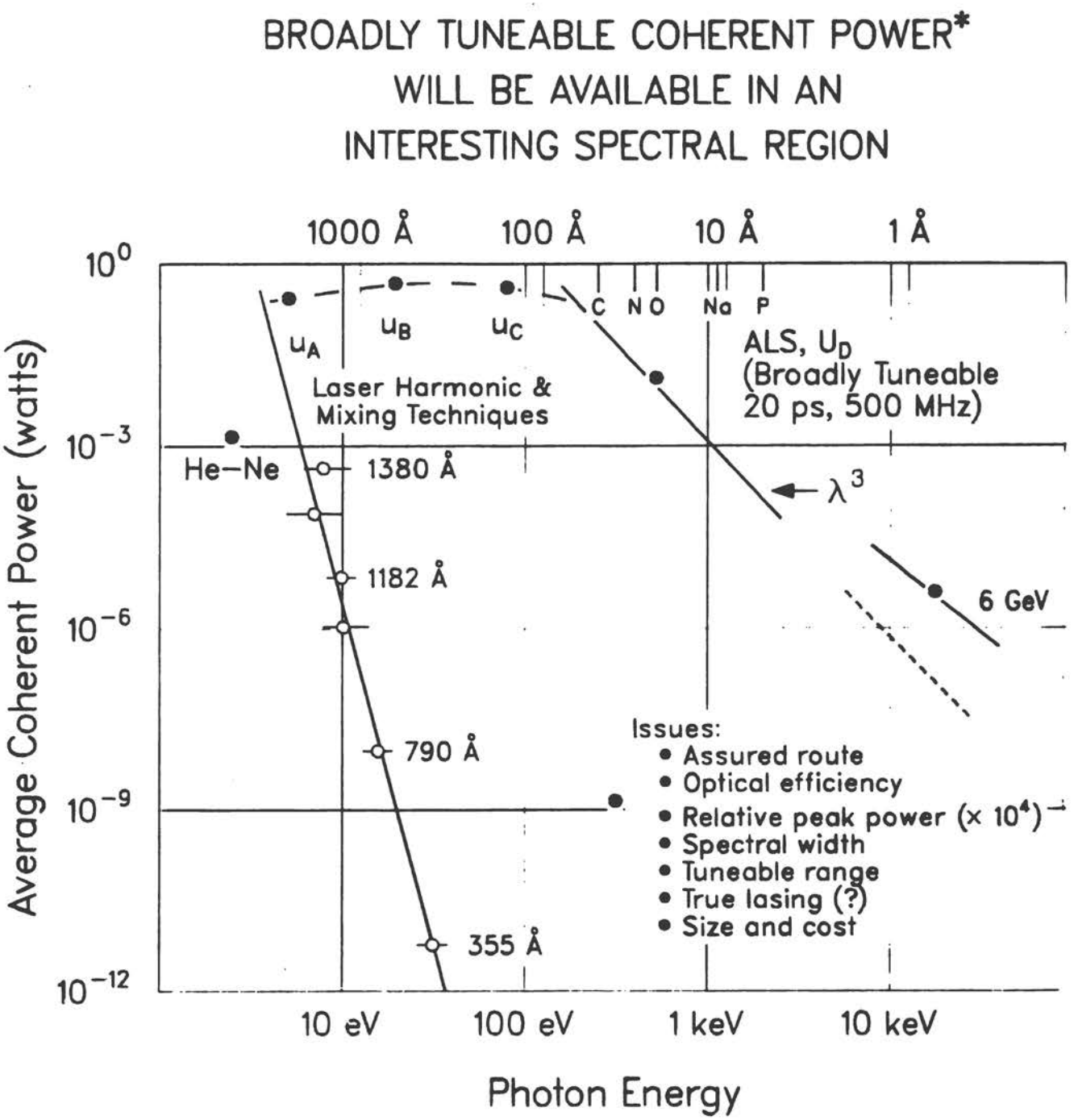


Figure 2–7.



*Full spatial coherence; longitudinal coherence ≧ 1μm

XCG 843-13016

Figure 2–8.

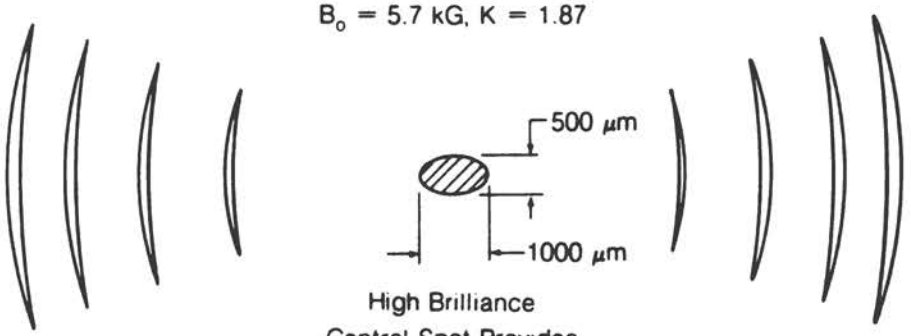
Coherent Radiation From Undulators Is Near Optimum At Soft X-Ray Wavelengths

- Achievable electron beam emittances: ϵ_x, ϵ_y (μm-mrad)
- Diffraction limited phase space (spatial, coherence) set by $d \cdot (2\theta) \simeq 2.4\ \lambda$
- For soft x-rays $\epsilon_x \epsilon_y \simeq (2.4\ \lambda)^2$
- Longitudinal (temporal) coherence, $\ell_c \simeq \frac{\lambda^2}{\Delta\lambda}$, for an undulator $\ell_c \simeq N\lambda$
- Coherent power fraction is proportional to $N\lambda^3$
- ALS/U_D generates 10 milliwatt of tuneable coherent radiation

Figure 2-9

Spatial Distribution of Radiation from ALS Undulator D at 500 eV

142 Periods, λ_u = 3.5 cm
B_o = 5.7 kG, K = 1.87



High Brilliance
Central Spot Provides
10^{16} Photons/(sec)(1% BW)

Central Cone at Source:

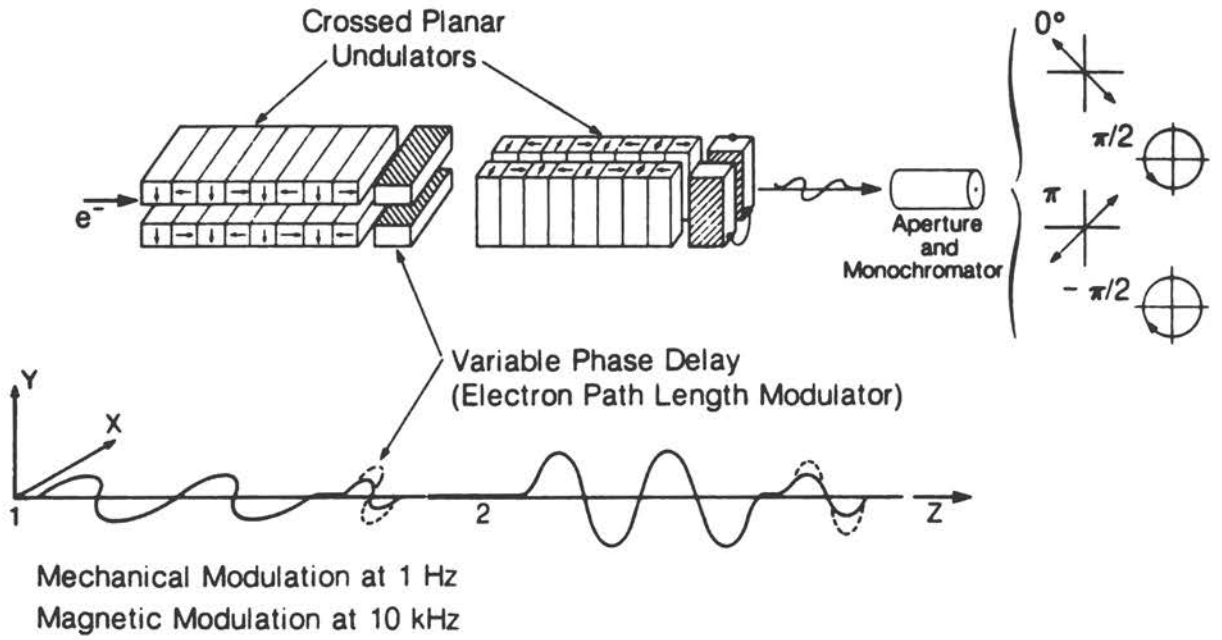
160 μm x 400 μm
40 μr x 100 μr

1.3 GeV, 400 ma
3rd Harmonic
100 Watts/cm^2 at 10 m

XBL [illegible]

Figure 2-10

Variably Polarized Radiation can be Generated with Crossed Undulators in Low Emittance Storage Rings



Mechanical Modulation at 1 Hz
Magnetic Modulation at 10 kHz

XBL 8311 65.4

Figure 2-11

3 Scientific Opportunities at the ALS

Introduction

Synchrotron radiation (SR) sources in which essentially all the radiation is generated by the interaction of high-brightness relativistic electron beams with long, many-period magnetic insertion devices, will create and enhance numerous opportunities in pure and applied science. These sources are characterized by high spectral brilliance and controllable polarization. As such, they are well suited for very high resolution monochromators, and high spatial resolution x-ray microprobe and imaging systems. In addition, new XUV facilities will offer very short pulse lengths, on the order of 20 picoseconds, and sufficient stability to permit extension of fast-timing experiments to fractional bunch-length resolutions with frequency domain measurement techniques. This section summarizes some important scientific and technological opportunities that are appropriately matched to the spectral and timing characteristics of the ALS. They are based on suggestions made by a large cross section of scientists in letters (see Appendix B) and at the ALS/SSRL Users Workshop. For more complete coverage of the science that can be performed with insertion-device-based SR sources, please refer to the report of the DOE Planning Study for Advanced National Synchrotron Radiation Facilities.

Biology, Biochemistry and Biophysics

The next-generation XUV sources will provide new capabilities for dynamical, high-spatial-resolution, element-specific studies of subcellular and intracellular processes (including mutations), as well as studies of biological microstructures. Specific advantages accrue to the soft x-ray probe because it is less damaging to tissue than electrons or hard x-rays are, it can provide spatial resolution better than 100 Å, it can be element specific, and it can be used to image thick, whole-cell specimens.

Various imaging and scattering techniques available with XUV radiation will be enhanced by the unparalleled photon flux available to study to small samples, together with the capability for tuning the x-ray wavelength to absorption edges of dominant elements, diffusible ions, and trace amounts of metals. For example, by using soft x-rays well

matched to absorption features of major structural biological elements such as carbon (283 eV), nitrogen (399 eV), and oxygen (531 eV) and other low Z elements of biological importance, such as Na, Mg, P, S, Cl, K, and Ca, with K-edges in the 1 to 4 keV range, it will be possible to accomplish dynamical response studies of specimens without the need for dehydration, fixing, or staining. Three-dimensional imaging data, obtained by utilizing the semicoherent nature of undulator sources and x-ray holographic techniques, will complement the information available from high-spatial-resolution electron microscopes.

To obtain diffraction or scattering data that are well resolved in time for dynamical studies, sources with very high flux densities are required so that the data per time interval have good statistics. Examples of the classes of problems suggested for study with such sources are the photodissociation and reassociation of carbon monoxyhemoglobin or myoglobin and the cycling of rhodopsin in the retinal membrane upon photoexcitation. Moreover, self-assembly dynamics of higher-order structures could be studied. For example, the formation of microtubules from tubulin dimers, or the assembly of viral coat proteins, could be studied by time-resolved, small-angle scattering with sufficiently bright beams.

Very intense x-rays and light in pulses short enough that motion or change of state will not distort the phenomena studied will also be useful for fundamental studies of the effects of radiation on living cells. Mechanisms of soft x-ray damage to cells can be studied in detail heretofore impossible, permitting new classes of questions to be asked. For example, if cellular components can be radiated selectively, one can study the difference in sensitivity to radiation among components, thereby clarifying the mechanisms of radiation damage. The tracks of short-range photoelectrons produced by absorption of x-rays in the 0.5–1.5 keV range should provide a unique probe for analyzing radiobiological events of dimensions approaching those of a DNA molecule. The availability of continuously tunable soft x-rays should provide new information for critical analysis of models of the action of radiation, that is, of assumptions concerning effects on cellular genetic material and effects of cellular repair mechanisms.

Still other classes of problems will become accessible through the new polarization capabilities of the ALS. Alternate left- and right-polarized radiation in the XUV can be produced by colinear undulators of orthogonal orientation, as was shown schematically in Figure 2–10. With the high photon fluxes available from a source designed for high brilliance, it will be possible to study the structures of condensed chromatin in cell nuclei. Only the first stages of folding of chromatin have been determined to date. Crystals and films of chromatin in different stages of condensation can be studied to determine the steps of folding. A related problem is the folding of DNA in viruses.

Additional information obtained from far-UV measurements with circularly polarized light would make it possible to distinguish nucleic acid sequences that cannot be distinguished on the basis of their near-UV bands. Unusual base-pair arrangements could be identified easily with far-UV measurements, as could changes in DNA conformation with ligand binding and in protein conformation with DNA binding.

A conference to discuss the new life-science studies that will become possible with arbitrarily polarized soft x-ray and VUV radiation is scheduled for May 1984 at the University of New Mexico.

Figures 3–1 to 3–6 show soft x-ray microprobe and imaging developments, which have currently achieved spatial resolutions down to 600 Å. Utilization of Fresnel zone plates for further intensification (Figure 3–3) is limited by availability and thermal loading

constraints, issues typical of those being considered by Berkeley's new Center for X-Ray Optics. Biological images (Figure 3–4) and x-ray holograms (Figure 3–5) will be achievable at the ALS with exposure times reduced to less than a millisecond.

Atomic and Molecular Physics

In the two decades since the value of SR for atomic spectroscopy was demonstrated through the discovery of the autoionizing states of helium, the use of radiation from storage rings has provided new techniques for absorption and photoemission spectroscopy, and for scattering experiments. Measurements of Auger and photoelectron angular distributions, as well as spin polarization are providing new insights into many-electron phenomena. Complete characterization of initial and final states has become increasingly possible for atoms as well as molecules. Researchers have been able to study the inner shells of heavy atoms, where relativistic and quantum electrodynamic effects play a major role. The dynamics of excitation and deexcitation of deep-hole states have become accessible to exploration, as have processes that link these two stages.

However, experimental difficulties and the limitations of present sources have prevented SR from being used to full advantage in atomic and molecular physics, according to B. Crasemann of the University of Oregon. Gas-phase targets must be used for the study of free atoms and molecules and thus elaborate differential-pumping arrangements are required to keep the targets from contaminating the ultrahigh vacuum of storage rings, unless the photon energy exceeds the 3-keV cutoff of beryllium windows. The tenuity of the gaseous targets requires very high-flux photon beams, and the demands of the experiments require higher spectral resolution than can be achieved readily with bending magnet sources. Only with the use of undulators and wigglers is the signal-to-noise ratio for many experiments in the x-ray region becoming acceptable.

These difficulties will be resolved with the next generation of SR facilities. With the high flux and high spectral resolution of these sources it will be possible to study the breakdown of the traditional separation between excitation and deexcitation of deep-lying atomic hole states. It has been demonstrated that the two phases blend together at threshold, resulting in the resonant-Raman effect, in which both excitation and deexcitation are expressed by a single second-order matrix element. In both x-ray and Auger resonant Raman transitions, the emitted radiation exhibits linear dispersion with exciting x-ray energy, and the line width of the emitted photons or electrons at resonance falls below the natural lifetime width of the hole state. It is tantalizing to contemplate exploring the fine details of the resonant Raman effect as a function of excitation well within the width of the intermediate state, and to study the influence that surrounding atoms may have on the process. Just above threshold, the Auger resonant Raman effect smoothly blends into postcollision interaction; the receding photoelectron transfers energy to the Auger electron—a process that bridges the gap between excitation and deexcitation and promises to lend exceptional insight into the dynamics of atomic inner-shell transitions.

Another important use of the ALS would be in photoelectron spectroscopy of those transuranium elements available in only very small quantities (plutonium through einsteinium). The primary interest in these elements is in developing an understanding of relativistic effects in this high-Z region, and in determining the role of interactions between

5f electrons and s and d electrons in actinide metals and compounds. Metallic vapors, pure metals, and easily vaporizable organometallic compounds would be especially valuable for such studies.

According to O.L. Keller at Oak Ridge National Laboratory, studies of metallic vapors of Ag, Ga, and Pb at the Tantalus photon source in Wisconsin suggest that to obtain the most important information on electronic structure and dynamics for the chemically significant 5f, 6d, and 7s electrons, about 1 gram of a transuranium element would be needed at Tantalus. The limited availability of the heavier actinides, not to mention their high specific activity, imposes a materials limit of a few tens of milligrams to a few milligrams per experiment, through californium, and a few tens of micrograms per experiment for einsteinium. These materials limits indicate the need for a flux at least 100 times higher than presently available to carry out successful systematic studies of the actinide series through californium, and a flux perhaps 10^4 higher to go to einstenium. M. Krause of Oak Ridge National Laboratory estimates that a brilliance of 10^{15} photons/(s $mm^2 mr^2$ 0.1% BW) is required in the energy range between 20 eV and 600 eV to accomplish these experiments. Even allowing for beam line optical inefficiencies, the ALS should provide this brilliance easily. Furthermore, Berkeley would be a good place to set up a special transuranium laboratory at a synchrotron because it has long experience with these elements from their discovery onward, and a number of researchers at Berkeley are performing research in the transuranium area that would allow collaboration in preparing metals and organometallic compounds, as well as in the SR studies. Such collaborative efforts, and the convenience of preparation facilities is particularly critical when dealing with elements that have short half-lives, are sensitive to air and moisture, and require extraordinary precautions.

Chemical Reactivity

The ALS will provide great opportunities for investigating chemical reactivity, one of the three areas of chemical research identified as most promising by the Committee to Survey Opportunities in the Chemical Sciences (National Academy of Sciences, National Research Council, G. Pimentel, Chairman). By providing intense, brilliant, and tunable VUV radiation, the ALS will access a chemically interesting wavelength range where tunable lasers currently do not operate. One important advantage of working in the VUV region is that the photon energies are often sufficient to induce chemical reactions leading directly to the production of electronically excited states and/or ions. Since such products can be detected with high sensitivity, the ALS output is sufficient to open new horizons in research on the chemistry of highly excited molecules.

An area in which the ALS is unique is its ability to produce picosecond pulses of continuously tunable UV, VUV, and soft x-ray radiation. The use and development of picosecond laser spectroscopic techniques for the direct real-time observation of the ultrafast relaxations and reactions that often typify condensed-phase chemistry have opened new horizons in chemical research. The availability of the ALS will dramatically expand opportunities for research in this area (Figure 3–7).

Condensed-phase reactions are typically treated using either continuum theories, such as hydrodynamics, or by complete molecular dynamics simulations. Hydrodynamic theories are computationally straightforward and are accurate at long time scales. However,

they break down for processes that are sufficiently rapid that motional averaging cannot occur. The limitations of continuum mechanics in the modeling of condensed-phase reaction dynamics have yet to be determined. A clear goal for picosecond spectroscopy is to define the regions of applicability of hydrodynamics.

Rotational motion and diffusion are determining factors in the dynamics of condensed-phase reactions. Such processes have been followed using picosecond time-resolved fluorescence depolarization spectroscopy. Limitations of current picosecond sources and techniques cause present experiments to involve typically the excitation of large dye molecules in simple solutions. Perhaps not surprisingly, the rotational reorientation dynamics of a dye, such as Rhodamine 6G, in an ethanolic solution is accurately described by a hydrodynamic treatment. The availability of tunable picosecond UV pulses from the ALS would allow similar measurements to be performed using much smaller solute molecules where one may expect the dynamics of rotational reorientation to be much more strongly influenced by the microscopic structure of the liquid.

Another area in which the microscopic structure of the liquid can be expected to be a controlling factor in the reaction dynamics is in the geminate recombination of reactive fragments in solution, the so-called "cage effect." Once again the technical limitations imposed by existing picosecond sources have prevented the direct observation of the dynamics of this fundamental process. The ALS will provide a photon source of sufficient intensity to both initiate and follow caging dynamics in real time. The broadly tunable photons from the ALS will enable studies of the cage effect to be carried out in systems of sufficient simplicity (e.g., H atoms in supercritical rare-gas fluids) to permit a direct coupling with the microscopic parameters of a molecular dynamics theory.

The availability of a picosecond pulsed vacuum light source is extremely useful in the study of time-resolved intramolecular dynamics of polyatomic molecules. For example, using a pulsed laser as an excitation source for local mode overtone excitation of polyatomic molecules and using picosecond SR VUV photon pulses for real-time ionization detection of the dissociation products, it would be possible to obtain urgently needed detailed information on the intramolecular energy transfer of isolated molecules.

Another aspect of the potential for opening new and important areas of chemical research with the ALS may be put into perspective by comparing the product of photon fluence (photons/cm^2 $\times$ sec) and a typical VUV absorption cross section (cm^2). Taking the average absorption cross section of 10^{-18} cm^2 for the dissociation and ionization of polyatomic molecules, the 10^{12} photons/cm^2 $\times$ sec from existing SR sources will only affect one millionth of those molecules exposed to the light. With a light source providing 10^{16} photons/cm^2 $\times$ sec, one percent of the molecules in the irradiated region can be photoionized or photodissociated. This degree of dissociation or ionization will allow many new, exciting experiments to be performed, and allow study, for example, of primary VUV photodissociation of polyatomic molecules, of nascent radicals in kinetics studies and IR absorption spectroscopy, of the energetics and dynamics of ion chemistry, and of the heat of formation of polyatomic radicals. Some examples follow to illustrate potential research directions and corresponding source requirements.

Although some photochemical studies have been carried out in the VUV region, using atomic resonance lines, the photochemistry of excited states of single bonds and of Rydberg states is almost completely unknown. Chemical analyses of photoproducts are often feasible with photon fluxes of 10^{12} per second. Thus, even at the high resolution required for

state-specific excitation in gases, such studies could be performed with the ALS. Furthermore, the fluence available from the ALS will permit product studies of VUV photoreactions of liquids and high-pressure gases to be carried out easily over time spans of minutes or hours.

ALS intensities are sufficient to produce detectable quantities of molecular hydrogen in single vibration-rotation levels of several excited electronic states. Rotational, vibrational, and electronic energy-transfer processes that occur in collisions may be studied. This is possible since, even at pressures of many torr, VUV fluorescence quantum yields are still near unity. With an excitation intensity as low as 1 photon per pulse within the 1 cm^{-1} bandwidth of a hydrogen absorption line, count rates of tens of photons per second of rotationally resolved fluorescence can be expected. With one to two orders of magnitude higher intensity, excitation of selected rotation, vibration, or electronic states of molecules, such as HCN, could be achieved. In this case, state-selective detection of the CN photofragments could be carried out with laser-induced fluorescence.

The high photon flux available with the ALS will make it possible to study the dynamics of many photoexcitation and photoionization processes in great detail. With a flux of 10^{13} photon/sec, it would become possible to investigate the primary photodissociation of polyatomic molecules in the VUV region using the method of molecular beam photofragmentation translational spectroscopy. Important questions related to the excitation of local electronic modes and specific bond dissociation could be answered. It would also be possible to investigate the dynamics of ionic processes by producing high-intensity, state-selected ion beams, and to develop many new schemes for obtaining energetic and spectroscopic information about important radicals and ions using VUV photons for either excitation or detection.

The middle ground between condensed-phase chemistry and the discrete quantum systems that typify gas-phase chemical physics is found in large molecules. The system or molecule to be studied can be chosen so that its number of atoms permits ultrafast dynamical processes to occur following pulsed-light excitation, even in the absence of collisions. The study of processes leading to adiabatic and nonadiabatic energy reorganization, changes in equilibrium geometry, atomic rearrangements, or photodissociation requires the combination of both picosecond and molecular beam techniques. If essentially isolated quantum states of molecules are excited, it should be possible to explore the time evolution of the nuclear positions. When bunches of levels are excited, as is the case at sufficiently high excitation energies in polyatomics and always for electronically excited states, picosecond methods can be used to explore the evolution of populations in the various quantum states involved. Both of these approaches probe fundamental questions of chemical dynamics and will help forge links between the *ab initio* methods of quantum chemistry and the chemistry of large molecules.

Materials Science

The broad tunable, wavelength range, high spectral brightness, and controllable polarization of synchrotron radiation (SR) provide new and improved techniques for exploring the bulk and surface states of matter. The relevant techniques are all based on measurements of x-ray absorption, diffraction, small angle scattering and fluorescent excitation to

produce detailed information about the geometrical arrangements of groups of atoms and their chemical bonding. Stimulated by the availability of high-brilliance radiation from insertion devices, refinements in current methods and the development of new approaches will occur soon.

Materials science at the ALS will fall into two broad catagories — studies of surfaces and studies of bulk materials. In as much as the ALS is primarily designed to maximize performance in the soft x-ray/VUV region, surface rather than bulk studies will form the major thrust of materials science at the ALS.

Understanding the reactions occurring at surfaces and the electronic properties of surfaces is crucial to understanding the behavior of surfaces, interfaces, catalysis, and even bulk materials formed atomic layer by atomic layer. Several tools utilizing soft x-rays for such studies have been developed in the past decade. Yet materials systems accessible for study by these surface techniques have been limited by the flux available at the sample. The increased brilliance of the ALS in the soft x-ray region will enable extended utilization and further development of these surface techniques, so that they can be applied routinely to numerous materials and to many types of problems. The high brilliance and the pulse structure of the ALS should also make feasible time-resolved experiments based on many of the new and developing techniques. Scientific opportunities available by using these techniques at the ALS are described in the following paragraphs.

Surface Extended X-Ray Absorption Fine Structure (SEXAFS) uses the surface-sensitive electron cascade from a photon absorption to measure the extended fine structure above a selected x-ray edge. Fourier analysis of the fine structure gives directly the distance from the photoemitter to nearby atoms. This method is particularly suited to studying disordered surfaces, where other surface methods cannot be applied. With the limited photon fluxes available at existing SR sources, long exposure times are required to make a SEXAFS measurement. A particularly important industrial application is studies of surface passivating films that are formed on metals by immersion in nitrate or chromate solutions. This method is a widely used, low cost—but little understood—means of protecting metals against corrosion.

Recent carbon K-edge absorption studies at SSRL have shown that the chemisorption geometry of a variety of carbon-bearing molecules can be determined from the angular variation of the absorption cross-section. For spherically symmetric initial states, the absorption probability is maximized when the electric field vector of the incident photon is in the direction of the empty (final) orbital density. Thus, photons at normal incidence probe for orbital density oriented along the plane of the surface and photons at near grazing incidence probe for orbital density oriented perpendicular to the surface. The high intensity of the ALS will allow this angle-resolved SEXAFS technique to be extended to a much wider class of materials.

Angle Resolved Photoemission Extended Fine Structure (ARPEFS) is another technique for studying surfaces. It measures the interference between direct and elastically scattered photoemission with an angle-resolved detector. The measurement can be quite sensitive, because the interference oscillations are large (50%), and scattering distances can be computed directly from Fourier analysis. But the intrinsically small angular acceptance required to c'tain adequate resolution slows the measurement. Increased brilliance would greatly shorten exposure times. Even greater benefit may be obtained, however, from the high energy resolution attainable with the ALS. When surface species undergo reactions.

their core levels show slightly different chemical shifts. A source with high spectral resolution can monitor these shifts during a reaction, giving structural information about reactants, products, and intermediates.

Photon Stimulated Ion Desorption (PSID) is a very new technique used to study adsorption site geometry at surfaces. Because PSID requires time-of-flight measurements, the time structure of the proposed ALS would allow for rapid development of this technique.

The finely divided metals used in heterogeneous catalysis can be as small as clusters of 20 atoms, and both surface and bulk SR methods are needed to determine their structure and chemical bonding. For example, in addition to determining surface structural and chemical characteristics with the methods described here, it is of interest to know how rapidly the cluster approaches bulk phase behavior as its size increases. Although the ionization potential characterizes this trend, conventional ionization techniques cannot yield the desired information. Electron impact lacks the needed energy resolution, conventional photoionization is much too weak, and excimer laser photoionization is not tunable. The ALS is an ideal tool, since it combines intensity with tunability over a broad range. Because of the low ionization potentials of metals, a low-energy limit of 5 eV is needed. The ALS high brilliance should allow ionization potentials to be measured for clusters in the appropriate size range.

The ALS beam lines equipped with standard wigglers will provide very intense x-rays in the important 3 keV to 10 keV range, and with the super-conducting wiggler very hard x-rays (up to 40 keV) will be available. Thus it will be possible to take full advantage of the new and advanced x-ray characterization techniques that are emerging from the remarkable renaissance in x-ray methodology. In addition to employing x-ray methods to probe the complex structures of specially synthesized advanced materials, the ALS capabilities will be used on a semi-routine basis for non-destructive characterization of samples whose catalytic, electronic, physical or mechanical properties are of interest. The results will provide data on the effects of unusual processing procedures.

Classical X-Ray Diffraction (XRD) using SR is still a very useful tool, especially for detailed analysis of atom positions in crystals. The high brilliance of the ALS will make it possible to use anomalous scattering near the absorption edge to decipher the crystal structure of very small crystals with volumes of only 50 μm^3 or less. This application is important in materials science to identify unknown phases obtained in very small crystallite size from the use of novel materials synthesis procedures or precipitated in alloys or ceramics. Real-time XRD to follow rapid phase changes, during synthesis and the occurrence of transient states, especially in high-pressure, high-temperature, or reactive-gas environments, could be applied to study reaction kinetics and mechanisms in many materials processing operations where this basic knowledge is still lacking. For example, pulsed SR should prove to be an extremely valuable monitoring tool for high-pressure experiments performed in a diamond anvil cell.

Time-resolved Small Angle X-Ray Scattering (SAXS) can be used to determine the arrangements of groups of the atoms and molecules in amorphous materials and polymers and to follow the evolution of ordered structures in these materials or complex alloys as a result of thermal or mechanical processing. For example, the extent of alignment of molecules by applied fields or during elastic straining or plastic forming of polymer films and fibers is of considerable interest.

X-Ray topography is a powerful tool for studying defects and strain fields in relatively perfect crystals. Recent experiments at SSRL have observed in real time the annealing behavior of dislocations in silicon wafers onto which devices have been made. A permanent topography set-up at the ALS would make this capability routinely available for the study of defects in electronic (and other) materials. Observations of the distribution and rapid movement of magnetic domains or elastic strain fields would contribute directly to the development of advanced materials and devices. Analysis of the strain distribution in heavily deformed or fractured metals is another important, albeit very challenging opportunity for SR research with the ALS.

The occurrence of low concentrations (down to parts per billion) of trace elements in bulk samples can be determined by high sensitivity x-ray fluorescence, and the clustering of such elements as well as their chemical bonding can be determined by K-shell Extended X-Ray Absorption Fine Structure (EXAFS) and X-Ray Absorption Near Edge Structure (XANES, also called NEXAFS). These methods, which take advantage of the high intensity of radiation in the 100 eV to 10 keV region have already been applied to a wide variety of materials, such as CaS in coals and TiN and VC in steels. Some examples of evidence for VC clusters in steels obtained by Huffman and Huggins of United States Steel are shown in Figure 3–8. Other techniques such as PSID and total electron yield (TEY) can also be used to obtain structure information and are particularly applicable to thin amorphous films such as those widely used in semiconducting devices.

The capability to do elemental imaging of the actual spatial distribution of trace elements with an x-ray microprobe will be particularly useful in learning about segregation of impurity elements near defects in electronic and structural materials. In addition to a very high signal to background ratio, i.e., excellent sensitivity, of an x-ray microprobe compared to an electron microprobe, a wide variety of samples can be studied without the preparation and vacuum environment required in the electron microprobe.

During the ALS/SSRL User's Workshop in May 1983, proposals were described by Bonse (Dortmund) and Barbee (Stanford) to utilize standing wave patterns in thin films and multilayer structures to study lattice deformation, solid-solid interface structure, location of impurity atoms, and so on (Figure 3–9). With the ALS this capability could be extended to the x-ray and VUV for detailed studies of anomalous dispersion. With the high spectral brilliance of the ALS it would also be possible to do standing-wave interference and fine-structure analysis of atomic positions at grain boundaries and interfaces between phases. The ultrashort time structure of radiation from the ALS might even be used to monitor interface migration and to identify active sites for atomic attachment. This nondestructive technique would nicely supplement atomic resolution studies being carried out at the National Center for Electron Microscopy at LBL.

Coherent Power and Mixed Beam Experiments

Spatially coherent soft x rays, with a longitudinal coherence of several microns and controllable polarization, will be available from ALS undulators at an average power level of about 10 milliwatts, (similar to a common He-Ne laser), fully tunable from about 100 eV to several keV. The early availability of this near-diffraction-limited, tunable XUV radiation at a facility accessible to all qualified users will provide new opportunities for exploring

atomic and solid-state systems. Interference techniques using coherent x rays (Figure 3–10) will become new tools for microholography, quantum interference studies, mixed spectral probing, and other types of experiments that are well known in the visible region of the spectrum. Moreover, tunable, coherent XUV radiation from the ALS should be available as much as a decade earlier than from other types of sources. As a consequence, the ALS will present U.S. scientists with forefront opportunities that are as yet not broadly anticipated in the field.

One potential application of coherent soft x rays, suggested by E.L. Hahn of the University of California Berkeley (Appendix B), is the use of picosecond-pulse radiation to prepare atomic states in a special way and thereby provide a measure of collision and other damping mechanisms in thin samples of solids and in gases. The technique is analogous to that described for pulsed coherent laser beams in the visible range by Kachru, Mossberg, and Hartmann [*Phys. Rev. Lett. 42*, 1665 (1979); *Opt. Commun. 30*, 57 (1979)]. The idea is to generate the equivalent of a "stimulated echo," as seen in transient NMR experiments, except that a photon echo in the visible region is generated. As shown in Figure 3–11, short x-ray pulses are applied with known frequency and wave vector to connect two quantum levels, 1 and 2. Using a laser, a third pulse is applied at a known time to connect level 1 to any other level 3, and a spontaneous coherent stimulated echo pulse signal will be radiated at a later time in a known direction. This echo pulse will give information about the degree of coherence of x-ray pulses, the spontaneous emission damping times in the sample, and the branching ratios and lifetimes of many states. It should be noted that increasing the coherent power and shortening the pulse width (preferably into the femtosecond range) will enhance the expected effect.

Many other classes of experiments will be possible with newly available coherent sources and improved x-ray optics. However, these opportunities have not yet been explored in a broad scientific forum—indeed are not yet widely recognized to be on the horizon. Further discussions in the scientific community will be required to identify the most suitable series of experiments to exploit these new capabilities.

National Defense Programs

Several scientific leaders at national defense laboratories such as Los Alamos, Livermore, Sandia, and the Naval Weapon's Center at China Lake have expressed the opinion that a high-brilliance, soft x-ray SR source with picosecond pulses is ideally suited to research and technological needs associated with their mission. Letters to this effect are included in Appendix B. Representatives of these laboratories recently made presentations to a Department of Energy review panel,* summarizing their jointly agreed needs. W. Trela of Los Alamos National Laboratory, spoke on behalf of the Department of Energy's defense-related laboratories (Los Alamos, Lawrence Livermore, and Sandia National Laboratories). Trela described mission and program related needs in weapons development, testing, and verification, fusion and isotope separation research, and a host of basic scientific and technological needs that would be served and enhanced by access to a modern soft x-ray SR facility of approximately 1 keV critical energy, high spectral brilliance and flux, with picosecond ($<$ 50 ps) pulse lengths. Charts from Trela's presentation

illustrate national defense needs for SR are shown here as Figure 3–12. These needs are echoed by many other scientific and industrial institutions. A similar presentation on behalf of Department of Defense research laboratories was made by V. Rehn of DOD's Naval Weapons Center at China Lake (Appendix B). Rehn gives added emphasis to dependable access to high-flux, high-brilliance facilities for planned technological and engineering developments.

Medical Applications

The application of x-rays for medical imaging is well known. Recently very interesting experiments have been done with a tunable 33-keV photon beam at SSRL to image the coronary arteries of a dog. These preliminary experiments indicate that it may be possible to image human coronary arteries noninvasively with SR. Cardiologist E. Rubenstein and physicist R. Hofstader, and their colleagues at Stanford and LBL, are currently developing equipment to test this concept at SSRL (Figure 3–13). Although a higher-energy electron storage ring would be preferred for this application, the team pointed out at the ALS workshop that the high-field superconducting wiggler at the ALS would have sufficient flux at 33 keV to perform angiography studies. The potential demand for this noninvasive diagnostic procedure and others that have yet to be developed suggest that medical use of SR is growing and that clinical/medical capabilities of all SR sources be examined.

Industrial Applications

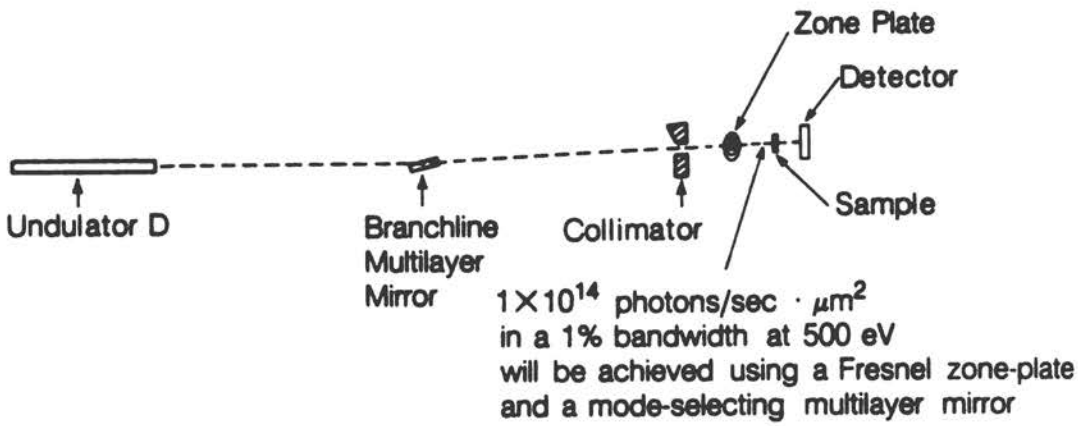
Access to spectrally brilliant XUV radiation promises to provide industrial scientists and engineers with valuable new manufacturing and research tools. The rich atomic and molecular structure can be used to optimize absorption processes for sub-1000 Å microfabrication, and to identify atomic species and their structural environment in chemical and solid-state materials (materials science). At present, utilization of XUV radiation is limited in industry by the very limited number of trained personnel and the underdeveloped nature of suitable radiation sources and transport techniques, e.g., x-ray optics.

According to industrial participants at the ALS/SSRL Users Workshop, LBL could contribute substantially to America's long-term industrial competitiveness by providing a focal point for industrial and academic collaborations. LBL's contribution would include the ALS with its spectral and brilliance characteristics, user-friendly beam lines, and newly developed x-ray optical techniques. These facilities would provide a natural meeting place for industrial and academic innovators, including those in the Bay Area's Silicon Valley. As examples, refer to correspondence (Appendix B) from J. Glaze of Physics International in San Leandro, and A. Neureuther of the UC Berkeley Department of Electrical Engineering and Computer Sciences. According to Glaze, the high cost of soft x-ray sources, prevents many companies from participating in the development of x-ray lithographic technology. To speed the development of this technology and others suitable for industry, Glaze urges that high-brilliance, soft x-ray SR sources be constructed as user facilities. Neureuther and his colleagues offer a specific proposal for using undulator radiation at the

*October 8–10, 1984, in Albuquerque, to DOE's Planning Study for Advanced National Synchrotron Radiation Facilities.

ALS to improve mask fabrication for the microelectronics industry; with this method finer feature sizes can be achieved at less demanding aspect ratios, while maintaining competitive writing speeds. Utilizing the ALS undulator power of several watts in 1% bandwidth, mask characteristics could be designed to be responsive to narrow-band radiation centered near near 15 Å where absorptive and diffractive trade-offs are optimized. Thus, the thickness of gold in the mask could be reduced by a factor of three, thereby allowing similar reductions in line widths. Linewidths approaching 1000 Å could be achieved in thinner mask materials, with less demanding aspect ratios (approaching 1:1 rather than 3:1). Additional research necessary to the development of x-ray lithography could be performed easily on the ALS (Figure 3–14). Continued research would provide further technical advances and valuable student and professional training while helping America's industry to compete in international markets.

X-ray Microprobes will Achieve Unprecedented Flux Levels on Small Samples, Using High Brilliance Insertion Devices, Low Emittance Storage Rings, and Modern X-ray Optics

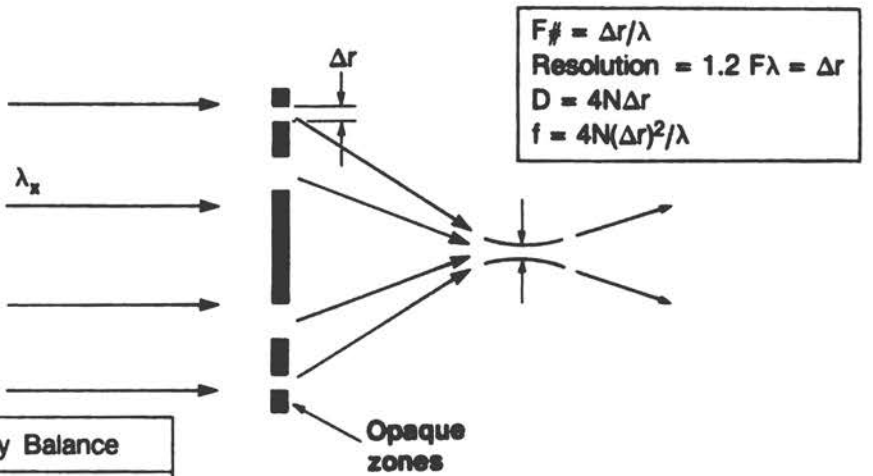


XBL 8311-781C

Figure 3–1.

Fresnel Zone Plate Lens for Diffractive Focusing of X-Rays:

(Feature sizes of order λ_x)



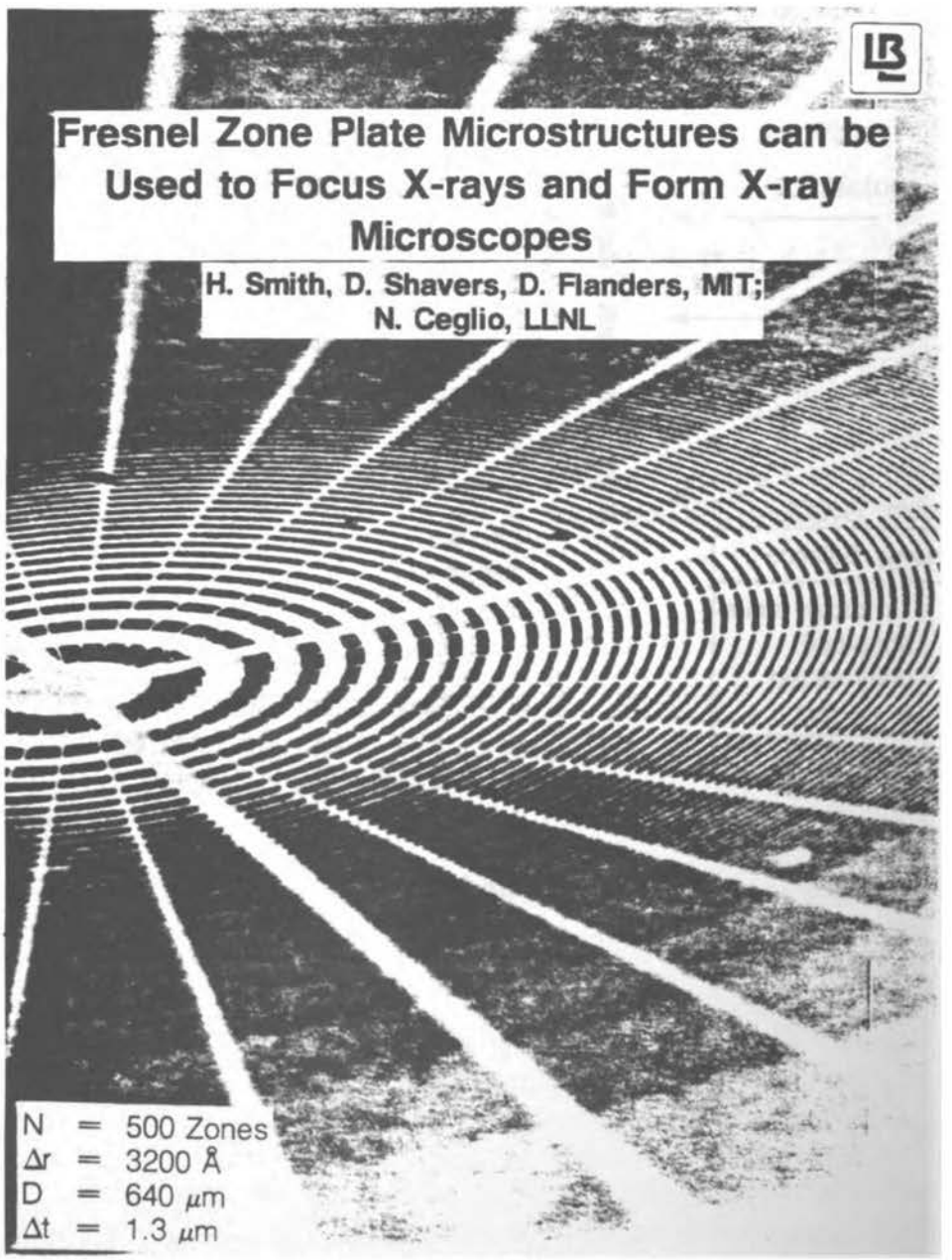
Energy Balance	
10%	1st order focus
50%	absorbed
25%	undiffracted
15%	other foci

References:

A. V. Baez, J. Opt. Soc. Am. 51, 405 (1961)
J. Kirz, J. Opt. Soc. Am. 64, 301 (1974)
N. M. Ceglio and H. I. Smith, LLNL, (1977)

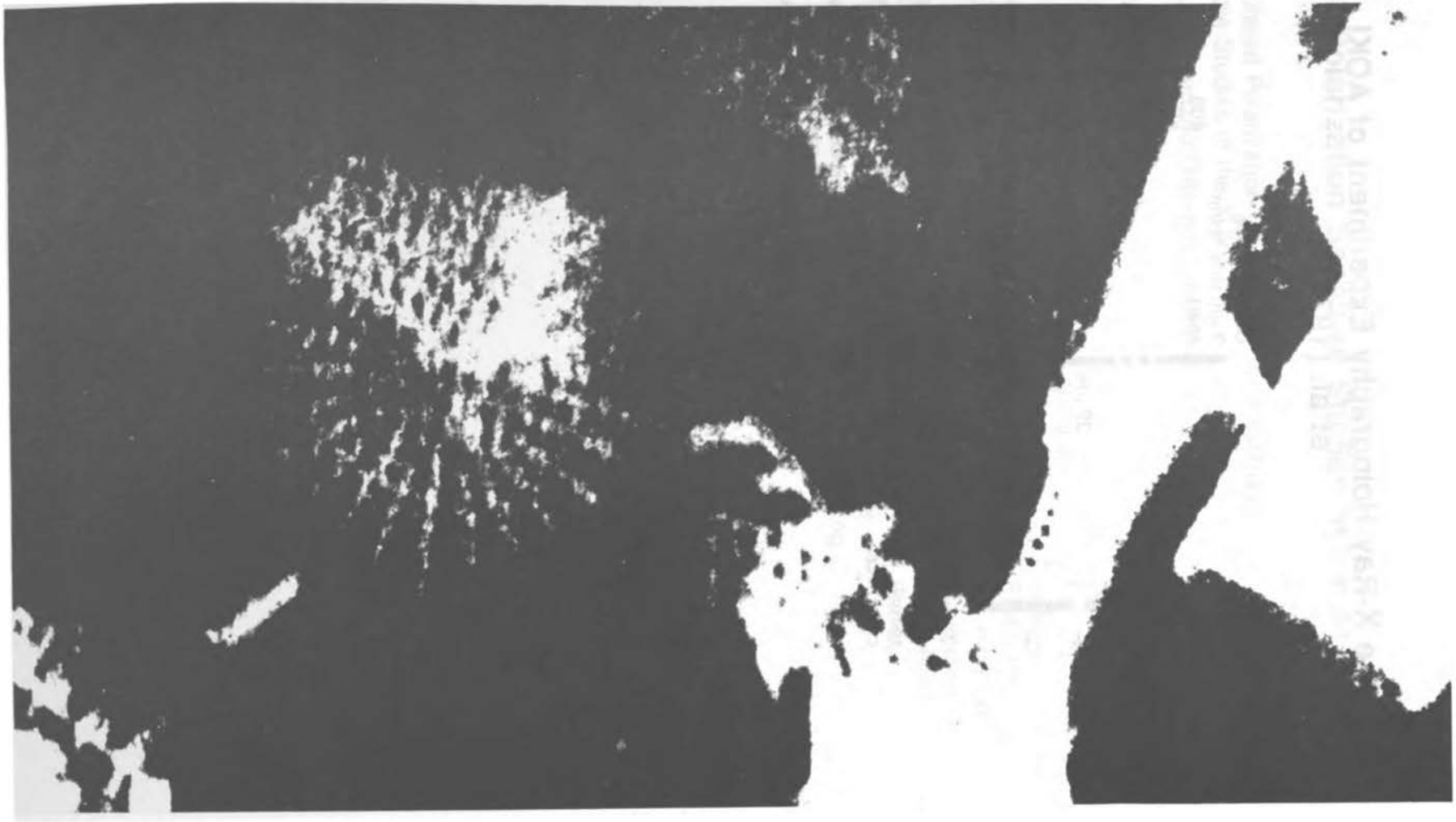
XBL 842-9405

Figure 3–2.


Fresnel Zone Plate Microstructures can be Used to Focus X-rays and Form X-ray Microscopes
H. Smith, D. Shavers, D. Flanders, MIT;
N. Ceglio, LLNL
N = 500 Zones
Δr = 3200 Å
D = 640 μm
Δt = 1.3 μm

1500 Å Biological Imaging with Soft X-Rays

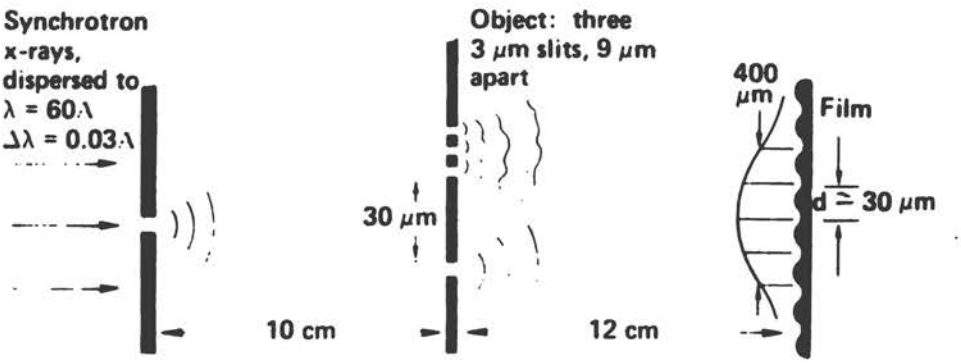
G . SCHMAHL, D. RUDOLPH AND B. NIEMANN, ANN. N.Y. ACAD. SCI. 342, 368 (1980)



$\lambda = 44$ Å, $\Delta r = 1200$ Å, $N = 625$

Diatoms ~1 μm tip to tip

The X-Ray Holography Experiment of AOKI et al. (1972)



7 μm slit for spatial coherence

2.5 μm slit, reference beam for "lensless" Fourier transform holography. Slit width sets spatial resolution.

Note. $\ell_{coh.} \simeq \frac{\lambda^2}{2\Delta\lambda} \simeq 6\ \mu m$ is excessive. This gives several cm coherence aperture at film plane. A factor of 30 less would reduce one hour exposure time to 2 minutes.

Reference: S. Aoki, Y. Ichihara and S. Kikuta, Japan J. Appl. Phys. 11, 1857 (1972).

Figure 3–5.

Polarization Sensitive Studies at the ALS

- Modulated Polarization Capabilities for Anisotropic Sample Studies in the XUV.
- Circular Polarized Differential Imaging

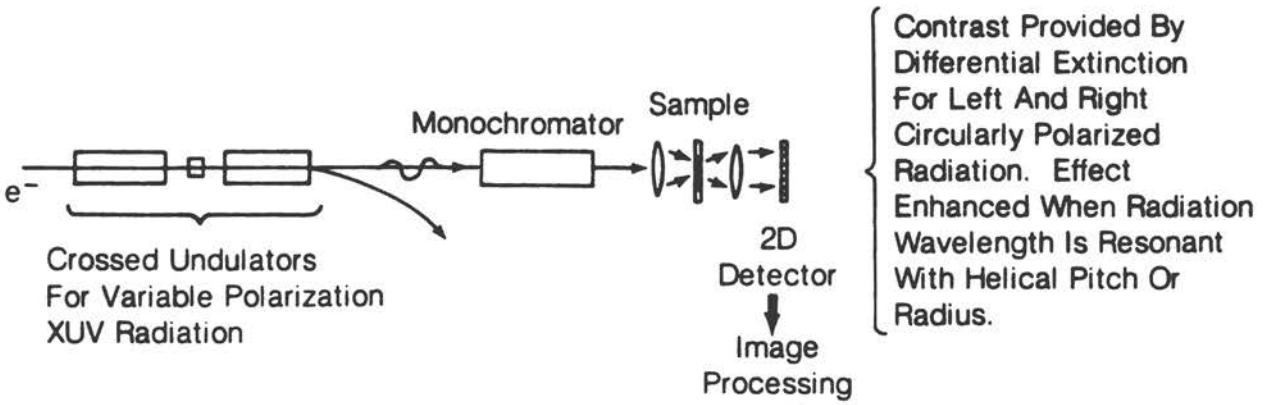
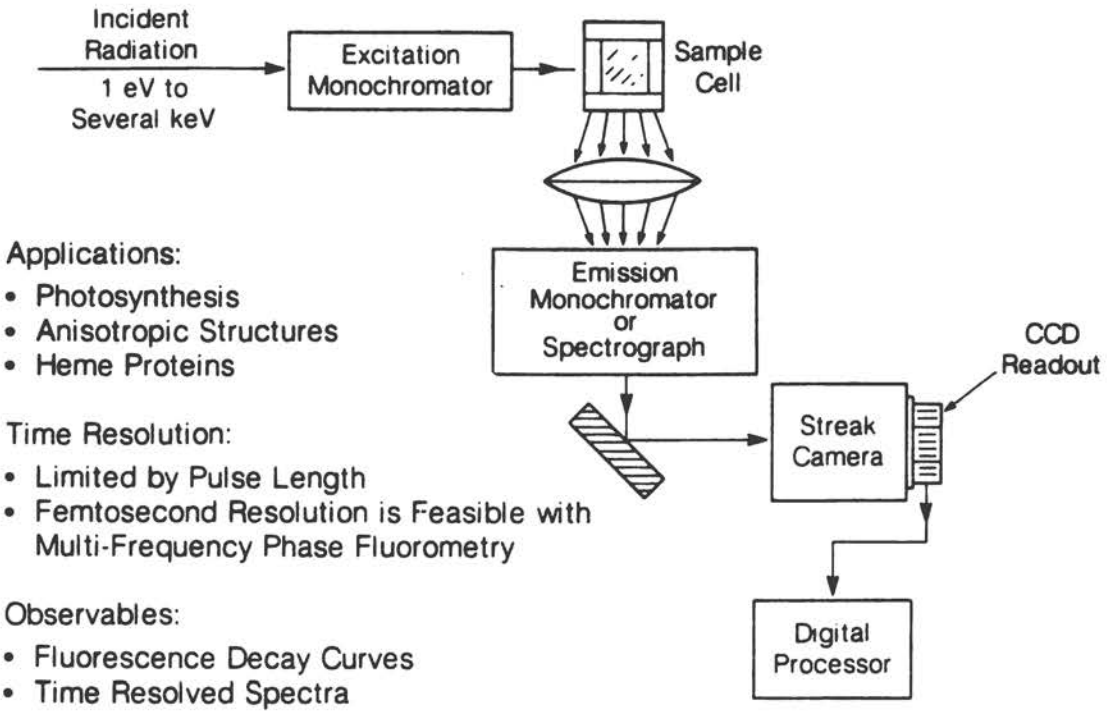


Figure 3–6.

Picosecond Chemistry with a Continuously Tuneable Source

Structural Chemistry via Time Resolved Fluorescence Spectroscopy



Applications:

- Photosynthesis
- Anisotropic Structures
- Heme Proteins

Time Resolution:

- Limited by Pulse Length
- Femtosecond Resolution is Feasible with Multi-Frequency Phase Fluorometry

Observables:

- Fluorescence Decay Curves
- Time Resolved Spectra

XBL 8311-653

Figure 3–7.

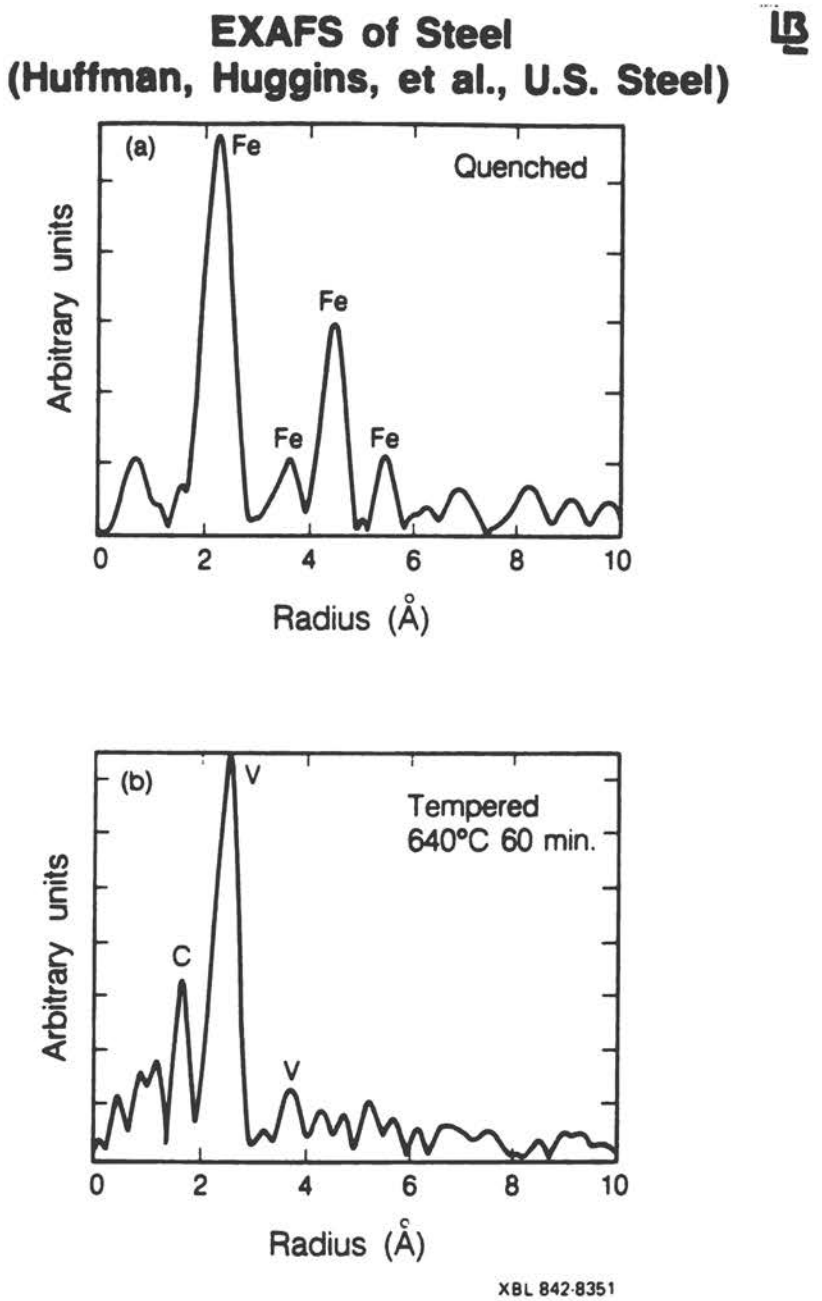
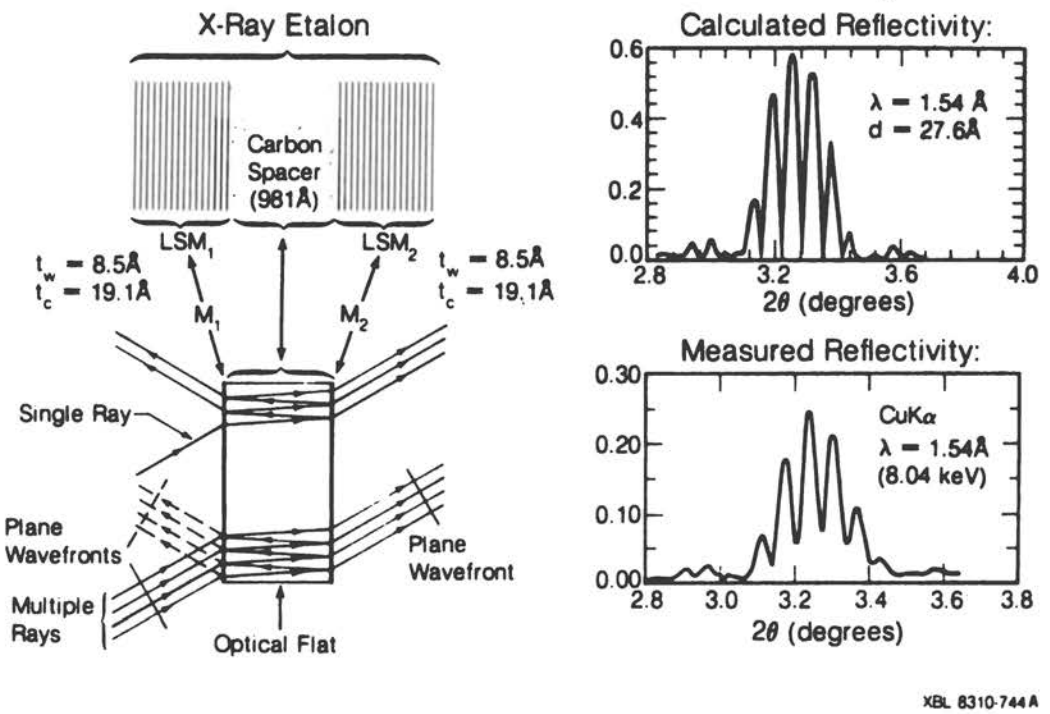


Figure 3–8. Fourier transform of EXAFS spectra of quenched (a) and tempered (b) steel containing 0.15 wt% V and 0.12 wt% C. In the quenched sample there is little indication of VC clusters, while in the tempered sample there is clear evidence of V-C cluster formation. Similiar real-time studies with steels, catalysts, ceramics, and other materials will be done at the ALS.

High Sensitivity Material Studies in the XUV Using Fabry-Perot Etalons

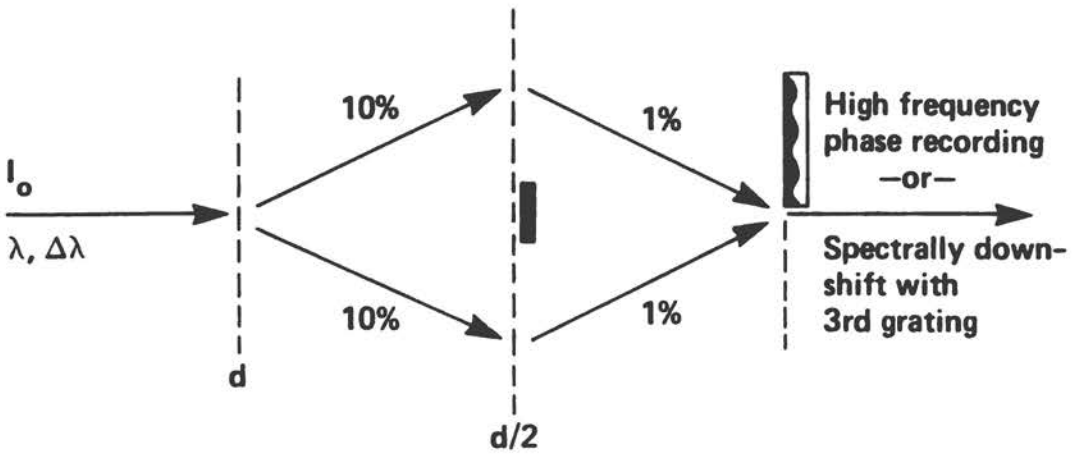
T. Barbee (Stanford) and J. Underwood (LBL)



XBL 8310-744A

Figure 3–9.

VUV and Soft X-Ray Interferometers can be Constructed



- Several hundred angstrom period gratings foreseeable
- Phase gratings possible with other materials
- Spatial coherence for grating interferometer minimal (Leith)
- Temporal coherence related to surface flatness and angular dispersion

XBL 842-9494

Figure 3–10.

Stimulated Photon Echos Produced By Coherent Soft X-Ray Pulse Sequences

(E. L. Hahn, UCB/Physics)

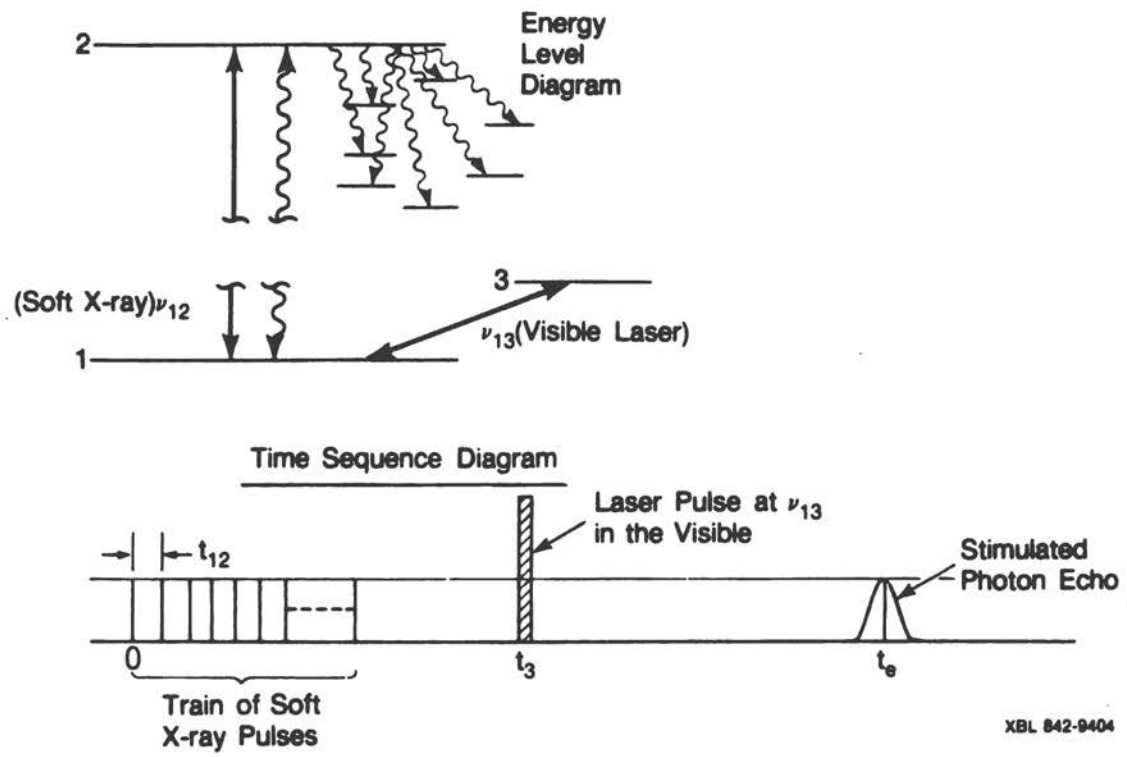


Figure 3–11.

Presentation by Dr. Walter Trela for Los Alamos, Lawrence Livermore, and Sandia National Laboratories:

Synchrotron Radiation Requirements for Mission- and Program-Related Needs

Research

Advanced Research Capabilities

- Materials Science
  - — Crystallography Exafs, Microprobe
- Solid State Physics
  - — Photoemission, Anomalous Dispersion, Optical Properties
- Surface Science
  - — Photon Stimulated Desorption, Sexafs
- Chemistry/Photochemistry
  - -- Photodissociation, Photoabsorption, Photoionization
- Atomic and Plasma Physics
  - — Photoionization, Photoemission, Inner Shell Threshold Measurements, Ionized State Absorption, Transmission Spectroscopy, Excited State Processes

Programmatic

State-of-the-Art X-Ray Measurement Facilities

- X-Ray Optics Development and Characterization
- X-Ray Detector Development and Calibration
- Low Energy X-Ray Data Base
  - — Attenuation Coefficients
  - — Coherent Scattering Factors
  - — Incoherent Scattering Factors
  - — Fluorescence Efficiencies
  - — Reflectivities
  - — Opacities of Stripped Ions
  - — Quantum Efficiencies
- Radiometry
- Materials Characterization

Summary

- Weapons Labs have a Large and Growing Need for Synchrotron Radiation
- Weapons Labs Believe that these Needs are Best Met by Participating in the Next Advanced (State-of-the-Art) Synchrotron Light Source with the National Scientific Community
- The Type of Advanced Light Source that Satisfies the Majority of the Weapons Lab's Needs has Low Energy (1 keV), High Intensity, High Brightness, Short Pulse Length Photon Characteristics

Figure 3–12.

XBL 842-9406

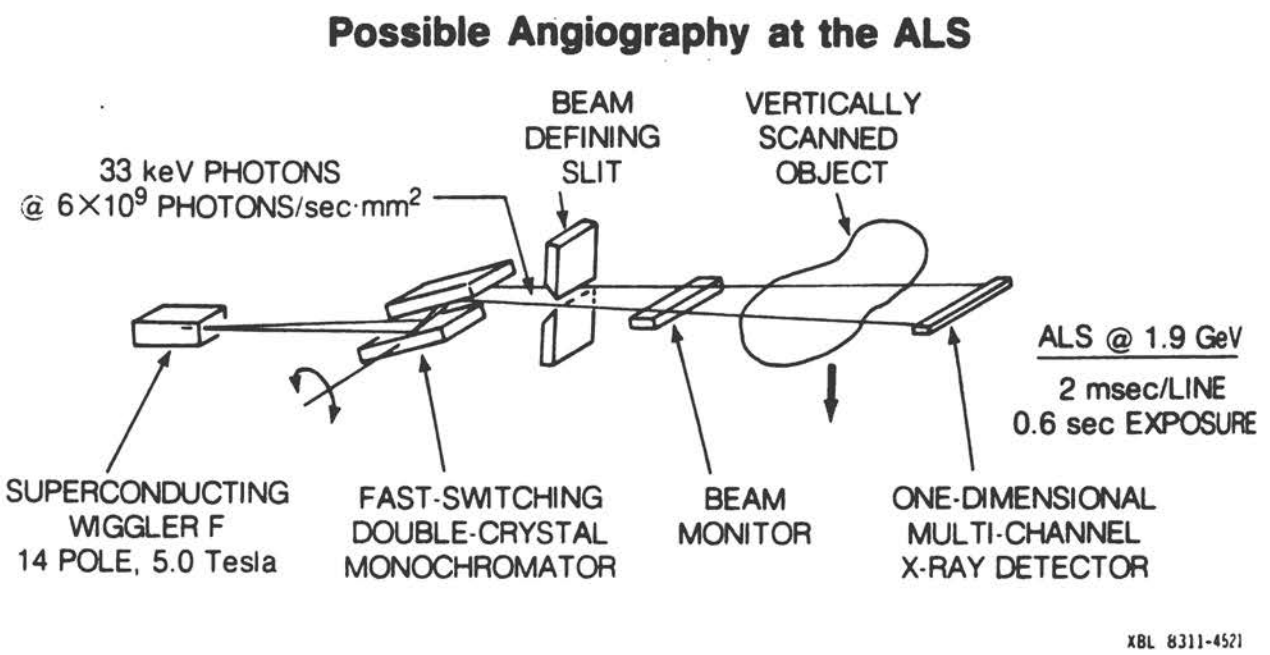
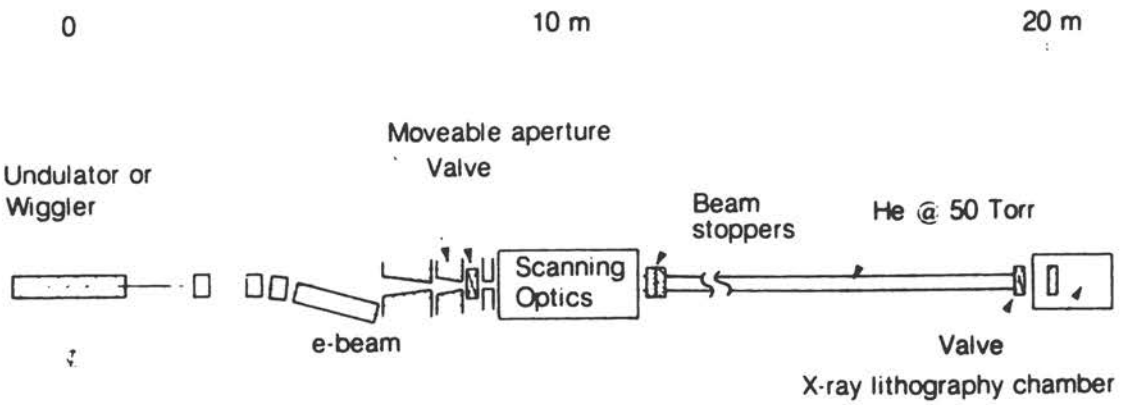

Possible Angiography at the ALS
BEAM
DEFINING
SLIT
VERTICALLY
SCANNED
OBJECT
33 keV PHOTONS
@ 6×10^9 PHOTONS/sec·mm^2
ALS @ 1.9 GeV
2 msec/LINE
0.6 sec EXPOSURE
SUPERCONDUCTING
WIGGLER F
14 POLE, 5.0 Tesla
FAST-SWITCHING
DOUBLE-CRYSTAL
MONOCHROMATOR
BEAM
MONITOR
ONE-DIMENSIONAL
MULTI-CHANNEL
X-RAY DETECTOR
XBL 8311-4521

Figure 3–13.

Lithography at the ALS



Type	Example	λ (A)	Mask (μm)	BW (%)	Power (w)	Efficiency (%)	Writing Speed (cm^2/s)
Bending Magnet	SPEAR 1.5 GeV 100 mA	8.4	0.6	50	0.24	17	0.05
Wiggler (Multilayer)	1.3 GeV 400 mA 1.6T, N - 25	15	0.2	1	1.7	9	0.8
Wiggler (Ne Filter)	1.3 GeV, 400 mA 1.6T.N 25	15	0.2	15	25.0	8	11.0
Undulator (Diff Pump)	1.3 GeV 400 mA N - 100	15	0.2	1	2.0	17	1.8

Figure 3–14.

4 Institutional Setting

The Advanced Light Source will be located at Lawrence Berkeley Laboratory, a multiprogram national research laboratory funded primarily by the Department of Energy and operated by the University of California. The ALS will be a national facility operated by LBL for all qualified investigators and will add to this country's heavily used SR capabilities. The location in Berkeley will enable the facility to draw on the Laboratory's noted strengths in accelerator physics, SR science, and instrument design; its experience in operating national user facilities; and its close associations with researchers and departments at the University of California's Berkeley campus.

The Lawrence Berkeley Laboratory was founded in 1931 by E.O. Lawrence for development of the cyclotron and pursuit of the unprecedented opportunities that invention opened in high-energy and nuclear physics. It is the birthplace of interdisciplinary big science. In the five decades since its founding, LBL has expanded its contributions into the fields of chemistry, earth science, biomedicine, computers, materials, and energy. Scientists in several LBL Divisions, including Materials and Molecular Research, the Center for Advanced Materials, and Applied Science expect to rely increasingly on SR for their research.

Lawrence Berkeley Laboratory is well qualified to design, build, and operate the first of the insertion-device-based SR facilities. LBL staff have played a pioneering role in the development of permanent-magnet insertion devices; the 54-pole wiggler installed at SSRL, the world's most powerful, was designed and built at LBL. The team that designed the ALS has participated in designing accelerators, accelerator devices, and particle detectors used at research centers around the world. Further, the laboratory is experienced in establishing and operating research facilities for the benefit of users throughout the United States and the world. On the average, more than 1100 guest investigators, visiting scientists, and regular users affiliated with other universities at LBL participate in research projects and use the national facilities. Notable among the national facilities at the laboratory are the Bevalac, the 88-Inch Cyclotron, the Neutral Beam Engineering Test Facility, and the National Center for Electron Microscopy, which houses five electron microscopes, including two state-of-the-art transmission electron microscopes—the Atomic Resolution Microscope and the High Voltage Electron Microscope. A new research center of great relevance to the ALS is the Center for X-Ray Optics. Described in Appendix D, this new center will play a major role in the design, fabrication, and testing of future synchrotron x-ray components and instrumentation. Finally, the site selected for the ALS includes buildings, utilities, machine

shops, accelerator-cooling facilities, and a high bay with crane, that will be used to good advantage by the new light source.

The Lawrence Berkeley Laboratory is unique among national laboratories in being a major research partner with an outstanding research and teaching university—the University of California at Berkeley. The combined human and material resources of LBL and UC Berkeley will assure that research programs at the ALS are world class in calibre. There are presently 174 joint faculty appointments at LBL and UC Berkeley. In addition, more than 500 graduate students pursue their research at LBL. Research opportunities at the ALS will attract additional students and professors from around the country, in many disciplines that are critical to the scientific and technological future of the United States. Training of future scientists at the ALS complex will be a major contribution to the national strength. Interaction and technology transfer will be accelerated through the use of this facility by scientists and engineers at major industrial R&D centers, universities, and government research laboratories, including these in the Bay Area. Silicon Valley, with its large industrial laboratories and high technology firms, is within an hour's drive of LBL. Also, nearby are Lawrence Livermore National Laboratory, Sandia National Laboratory at Livermore, and campuses of the University of California. Stanford University, as well as several other universities and colleges.

In addition, the location of the ALS in the western United States will provide a needed facility for regional VUV/soft x-ray users, complementing the x-ray capabilities at SSRL, where it has already become difficult for prospective users to gain access, with only about 15 weeks per year of dedicated time to be divided among them.

To summarize, LBL's strong programs and expertise in accelerators, SR science, and instrument design; its experience in running national facilities; and its unique association with an outstanding research and teaching university make it an excellent site for the Advanced Light Source. Research at the ALS will benefit from established relations and strong expressed interest from UC Berkeley faculty. LBL's already major role in graduate education will be enhanced by providing more opportunities for student research and training in an emerging field of pure and applied science where a lack of qualified personnel is limiting national potential. As a national user facility, the ALS will fill a critical need for the SR user community. The opportunities it presents in both basic and applied research will stimulate the kinds of interactions between national research laboratories and academic and industrial scientists that must flourish if the United States is to maintain its position of leadership in high technology.

SSRL'S Planning for a New Synchrotron Radiation Facility including a 6 GeV Storage Ring

March 1984

SSRL's PLANNING FOR A NEW SYNCHROTRON RADIATION FACILITY INCLUDING A 6 GeV STORAGE RING

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INTRODUCTION

In this paper, we describe a synchrotron radiation facility based on a 6 GeV storage ring optimized for the production of high flux and high brilliance x-ray and soft x-ray synchrotron radiation from many wiggler and undulator insertion magnets. This facility will provide 10 beam lines with about 15 experimental stations and, thus, extend markedly the nation's capabilities to perform the most demanding and important research in this spectral region. It could be enlarged at some later date to include as many as 30 beam lines. In addition, a 1-2 GeV storage ring could be added to it for the production of soft x-ray and vacuum ultraviolet radiation. Alternatively, the existing SPEAR storage ring could be modified to provide high flux and high brilliance in this lower energy spectral region.

We begin with a brief discussion of the facility itself, and then present the scientific and technical reasons for constructing a 6 GeV ring. There then appears a discussion of why such a facility should be constructed at Stanford University by the Stanford Synchrotron Radiation Laboratory. Finally, our estimates of the costs of such a facility are provided.

THE SSRL 6 GeV DESIGN CONCEPT

Facility Description

The main component of the proposed facility, as it is presently planned, is a storage ring in which a beam of electrons or positrons circulates in a vacuum chamber embedded in a magnetic guide field. The circumference of the ring is about 537m and is composed of 10 equal units called superperiods. Each superperiod provides for one 4m long and two 2m long straight sections which can be used for the installation of wiggler and undulator magnets. These magnets are the sources for high intensity beams of synchrotron light. The beam guide magnets are constructed such that the photon beams can leave the ring vacuum chamber tangentially through exit pipes without interference. The photon beam lines lead to an experimental hall around the storage ring. The storage ring is located in a tunnel of heavy concrete walls to provide radiation safety.

The electrons or positrons to be stored are produced in a

small linear accelerator, then injected into a booster synchrotron where they are accelerated to the operating energy, and finally transferred into the storage ring. In order to save cost, the booster synchrotron is placed in the same tunnel as the storage ring. An inexpensive option allowing injection of electrons or positrons from the existing SLAC LINAC also exists.

The energy lost from the beams by synchrotron radiation is restored by a high power radio frequency system which employs klystrons to drive the accelerating structure at a frequency of about 350 MHz. The system is capable of delivering about one megawatt of rf-power. Since much of this power appears as synchrotron radiation which strikes the outer wall of the vacuum chamber, that wall has to be water-cooled. Moreover, the radiation causes the desorption of gases from the vacuum chamber surface. These gases must be pumped away very rapidly, since a low pressure (about 5×10^{-9} Torr) must be maintained in the vacuum chamber both to achieve adequate beam lifetimes and to minimize the background radiation to the experimenters. These low pressures will be sustained by means of sputter ion pumps distributed around the ring.

Wiggler and undulator magnets are both periodic arrays of alternating magnetic poles. Wiggler magnets provide photon beams covering a wide spectrum of photon energies similar to the radiation from a bending magnet. In a wiggler magnet, however, the beam is alternately deflected into opposite directions by each pole of the magnet. This way as many radiation sources as there are magnet poles line up to form one source of radiation with much enhanced intensity.

An undulator magnet operates at lower magnetic fields than a wiggler and is designed to enhance interference effects in the radiation from the many individual poles. Through coherent radiation of x-rays from the entire undulator structure, the spectral quality of the radiation is greatly improved over wiggler radiation for many experiments. The entire beam of radiation is emitted into a cone of angular radius of about 100 microradians, and the spectrum is peaked at odd multiples of a fundamental energy which is determined by the electron energy, the magnetic field and the undulator period. At these peaks, the radiation is emitted into a cone which is yet an order of magnitude smaller in angular dimensions. As a result of the spectral concentration and small angular divergence, a photon beam with a brilliance which is several orders of magnitude greater than that obtained from existing wiggler sources can be obtained. Such an undulator, producing 1 KeV radiation, was developed in an SSRL/LBL collaboration and has been used for soft x-ray experimentation at SSRL. A beam line, resulting from a Xerox/Stanford collaboration, and devoted to such experimentation with undulators is to be installed at SSRL this summer.

Unfortunately, the highest useful photon energy which can be reached with the fundamental mode radiation from an undulator on SPEAR is only about 5 KeV. Much of the motivation for

building a 6 GeV storage ring comes from the need to obtain fundamental mode undulator radiation in the 8-20 keV photon energy range which is so important in the determination of atomic arrangements in condensed matter.

Considerable effort has been employed to develop the magnetic focusing structure, called the lattice, of the storage ring. It is important to achieve a very small beam size, which in turn will result in a photon beam of very high brightness. Most existing synchrotron radiation facilities use the radiation from storage rings optimized and constructed for colliding beams for high energy physics experiments. The lattices were designed to produce the maximum feasible beam size to maximize the luminosity for high energy physics experiments. It is for this reason that storage rings, specifically optimized for small beam sizes, can provide photon beams with a brightness which is several orders of magnitude greater than those of existing sources.

The fundamental limits on the performance of such a storage ring are instabilities created by the electromagnetic interaction of the beam with the surrounding chamber walls. The total particle beam is composed of between one and up to several hundred bunches, each about 100 psec long and separated in time by 1800 nsec in the one bunch mode, and by $1800/N_b$ nsec for N_b equally distributed bunches. Each bunch can interact with itself and other bunches via the interaction with the surrounding chamber, thus creating possible instabilities. Each of the known instabilities in existing storage rings has been studied. This storage ring has been designed to minimize the known causes of instability. Hence, the maximum desired current of 100 ma should be obtainable. It should be noted, however, that single bunch instabilities limit the current per bunch to about 10 ma.

It should be realized, however, that technological improvements by several orders of magnitude are not easy to achieve. Some of the improvement can be realized rather easily with present day knowledge by designing the storage ring for synchrotron radiation production rather than for collding beams, where large beam cross sections are utilized. The ultimate design performance, however, will require significant machine development. It is, therefore, imperative that the storage ring be designed such that it can be operated initially with less difficulty, but at reduced performance. Then, as the understanding of the storage ring is improved, the design should allow a gradual transition to higher and higher performance. This development can go in parallel with the usage of the ring for synchrotron radiation experiments. The proposed SSRL 6 GeV ring has this feature and can be operated initially with a brilliance which is about an order of magnitude below the ultimate design value, but with considerably reduced difficulty in operating the storage ring.

Around the ring tunnel is the experimental hall which radially extends about 30m. Such a hall allows photon beam lines as long as 75m. The siting of the facility will be such

as to allow for the construction of some much longer beam lines in order to make use of the highest possible photon flux at acceptable power densities. A crane provides support for the installation of beam lines and experiments as well as the initial installation of the storage ring, booster ring and the shielding wall. A service gallery is located radially inside the ring tunnel to provide necessary space for controls, power supplies, etc. Above this service gallery there are two stories of office space, light shops etc. Figure 1 shows an artist's view of the facility. Some of the main parameters of this storage ring are compiled in Table 1.

WHY BUILD A 6 GeV STORAGE RING?

In this section, the logic which led to the decision to plan a 6 GeV storage ring for insertion-device synchrotron radiation production is discussed.

Insertion Devices Make Possible Important X-Ray Science

Two types of scientific endeavors illustrate the major advances in synchrotron radiation science which occurred with the development of the wiggler. The first of these is the evolution of EXAFS analysis. EXAFS makes possible the determination of the average surroundings of individual atomic species in complex, polyatomic materials. It is now employed to obtain atomic level understanding of the fundamental properties of materials as diverse as metalloproteins and glasses. The initial bending magnet line of SSRL provided sufficient flux for the development of EXAFS analysis of high concentration constituents in amorphous and crystalline alloys, as well as concentrated metalloproteins and enzymes.

Soon after its introduction, however, the approach was broadened considerably through the development of fluorescence EXAFS. The fluorescence detection technique markedly increased the signal-to-noise ratio obtained when studying the surroundings of a dilute constituent such as a metal atom in a protein present at biological concentrations or atoms introduced to modify the physical properties of materials like semiconductors or glasses. As a result, we have been able to determine the surroundings of atoms present in concentrations as low as one part in 10^5. This, in turn has led to considerable new understanding of biological, physical and technological properties. At these low concentrations, however, the absolute signal becomes very small because of the small number of atoms participating in the absorption and subsequent fluorescence processes. As a result, inserton devices are needed to provide enough flux to yield a sufficiently strong signal.

With the introduction of the various forms of electron-yield EXAFS, it also became possible to determine the average surroundings of atoms on the surfaces of both crystalline and amorphous materials. Again, a tool of immense scientific and technological importance was provided to the community, but the effective cross section in the process studied is extremely

small because of the small number of atoms involved. As a result, wiggler sources have been essential to making the approach effective.

The latest development in this field is photon-induced desorption EXAFS. This approach makes it possible to study the average surroundings of specific types of atoms which, in turn, are surrounded by other specific species. Thus, for example, one can study the early stages of the oxidation of a metal by examining the surroundings of those metal atoms which are adjacent to oxygen atoms on a partially oxidized surface. Similarly, one can study the poisoning of a catalyst by studying the surroundings of those metal atoms which are adjacent to sulfur atoms on the surface of the metal. The signal associated with this process is extremely small, since it involves the desorption of an atom through the absorption of a photon. That process is one with a very small cross section and, in addition, there are very few atoms of interest in such a system. Again, such an approach is made extremely effective through the availability of high intensity radiation.

Thus, while bending magnet radiation made possible the anticipated development of EXAFS, it very soon brought with it the development of approaches that had not been anticipated. Whereas, the first EXAFS experiments were "photon-rich" with bending magnet radiation, the newer experiments were "photon-poor" and were helped dramatically by the introduction of the wiggler beam lines at SSRL.

The field of x-ray scattering has followed a very similar path, but with a need for greater brilliance as well as greater intensity becoming increasingly apparent. Bending magnet radiation made possible major advances in structure determination in both crystalline and amorphous materials. Indeed, the bending magnet radiation also made it possible to study the time evolution of material systems as they underwent natural processes, albeit on a relatively slow time scale.

With the introduction of wigglers, we have seen the true development of structural studies of two-dimensional systems. It has become possible to study atomic arrangements on biological membranes and to monitor the details of phase transitions in two dimensions. More recently, it has even been possible to perform structural studies of thin amorphous layers. Such studies could very effectively use considerably greater brilliance than is provided by SSRL's wigglers on SPEAR. In the studies of two-dimensional phase transitions, for example, it is frequently desired to study long range structural correlations as the liquid is cooled towards the solidifaction temperature. Such studies require extremely high Q-space resolution, or low beam divergence. On the other hand, the samples are often quite small, so that small beam size is required. The obtaining of both small divergence and small beam size can only be achieved by increasing the brilliance of the synchrotron radiation, since optical elements which decrease one of these increase the other.

Significantly higher brilliance is also required for the

study of the structures of very thin amorphous films on substrates. Such studies are performed using the phenomenon of x-ray total reflection, in which the x-rays are incident at an extremely small glancing angle and only penetrate 20 to 1000 angstroms. During this penetration, they are diffracted as well as reflected. It is analysis of the diffracted beam which leads to the structural information.

In such studies, the beam divergence must be extremely small to control the x-ray penetration depth. In addition, the beam size must be small because the beam is incident at a very small angle, so that even a small beam has a very large cross-section on the sample. The high brilliance needed in most such experiments can only be obtained through the use of undulators on a high energy storage ring.

With the evolution of appropriate detectors, we may also anticipate the determination of the changes of atomic arrangements in both natural and techological processes on increasingly rapid time scales. Again, we have gone from experiments which were "photon-rich" to experiments which are "photon-poor".

There Is a Widespread Need For Insertion Device Radiation

In the short time since SSRL introduced wigglers and undulators for synchrotron radiation experiments, it has become apparent that the need for the experimental techniques made possible by them pervades a vast portion of the scientific and technological world. There are, for example, many biological, polymeric and inorganic materials whose physical properties are strongly influenced by dilute constituents. The desire to determine the surroundings of such constituents in order to understand these properties at an atomic level is found over the range from biophysical laboratories to those of paint and glass companies. The present insertion device facilities and those which can be constructed on existing storage rings cannot possibly meet a significant part of that need. As a result, it is extremely important to build a new generation of facilities.

Choice of Machine Energy

If one were to construct a storage ring exclusively for the production of x-ray synchrotron radiation by wigglers a lower energy ring, say a 3.5 to 4 GeV machine, would probably be quite adequate. As one examines such machines in more detail, however, it becomes obvious that it would be much wiser to build a machine which is capable of functioning at 5 to 6 GeV. The reasoning which leads to this is the following.

First of all, unlike bending magnet machines, the circumferences of these insertion-device machines are largely determined by the number and length of the straight sections. The number of straight sections is, in turn, determined by two considerations. The first of these is the need to keep the bend angles small to achieve a low emittance. This requirement dictates a minimum number of straight sections for any given emittance and ring energy. The second is the number of

straight sections desired for the facility.

In the 6 GeV machine discussed here, the emittance considerations led to the design of a ring with 30 straight sections. A lower energy machine with the same emittance could have as few as 20 straight sections.

Further, the total cirumference-related costs of the ring are small compared to the total cost of the facility. For example, we find that the minimum circumference for a ring containing 30 straight sections is about 537 meters. A lower energy ring could have about two-thirds that circumference, leading to a cost reduction (including other considerations) of a little less than $10M out of a total project cost of about $126M. Thus, the difference in cost is small relative to the total investment in the storage ring and beam lines.

Given this small difference, it is prudent to build the 6 GeV machine to avoid the construction of a machine which will not meet important needs. This high energy is required in order to achieve fundamental mode x-ray undulator radiation with photon energies as high as 20 kilovolts. Such undulators offer the possibility of considerably higher brilliance than can be achieved with x-ray wigglers, given the thermal limits imposed by the first optical elements in the system. The brilliance will make possible the performance of a number of experiments which require high flux, small beam size and small angular divergence of the beam. Given the pervasive need for high flux, the advances which are already within reach with the large increases in brilliance to be obtained from undulators, the small difference in cost between a lower energy and a 6 GeV storage ring, as well as the technical factors discussed immediately below, it seems unwise to build an x-ray synchrotron radiation storage ring with energy less than 6 GeV.

The final considerations that led to the choice of 6 GeV machine rather than a lower energy machine are related to technical performance. It is our assumption that any next generation x-ray synchrotron radiation storage ring will be designed for extremely low emittance. At constant emittance, however, the Touschek lifetime of the electron or positron beam tends to increase as the square of the storage ring energy. Thus, the Touschek lifetime of the lower energy ring would be less than one-half that of the 6 GeV machine. For many experiments to be performed on such a ring, this would be a major disadvantage.

This difficulty could be overcome, in some case, by utilizing a higher voltage rf system. The increase in cost of the rf system would, however, partially offset any cost advantage the lower energy machine might have.

Similarly, all beam instabilities are worse at lower energies. If the beam current is limited by such instabilities, then the problems will be enhanced considerably by reducing the energy.

Finally, there is the effect of Coulomb scattering. Due to it, the aperture at, say, 4 GeV has to be larger by 50% in

both the vertical and horizontal planes. This means that undulators cannot have as small a period and become even less effective than would be anticipated by the decrease in stored electron energy alone. This effect can also be overcome, partially, by decreasing the storage ring ambient pressure. This solution will be very expensive, however, and the additional cost will tend to offset the cost advantages of the lower energy ring.

Thus, a lower energy ring appears to offer no real cost savings relative to a 6 GeV machine. The 6 GeV machine offers the possibility of obtaining extremely bright, fundamental mode, undulator x-ray radiation at photon energies as high as 20 KeV, with harmonics providing still higher energies. At the same time, it is a conservative machine which is more likely to function effectively than a lower energy machine. Such considerations have led us to plan for the higher energy machine.

All our experience with wiggler radiation indicates that the high flux has made possible experiments which were not even anticipated a decade ago when bending magnets were first being utilized for x-ray synchrotron radiation research. The same historical path was followed in laser utilization. Thus, it seems extremely likely that the availability of extremely high brilliance undulator radiation at photon energies as high as 20 keV will yield even more important experimental techniques than are presently foreseen. Such radiation will only become available when a very low emittance, 6 GeV, storage ring is available on a dedicated basis for synchrotron radiation production.

WHY THE 6 GeV MACHINE SHOULD BE BUILT AT STANFORD

Stanford Can Design and Construct the Machine So That It Functions Effectively.

Stanford has many years of experience in the successful design and construction of electron-positron storage rings. Three such storage rings are presently functioning at Stanford: SPEAR (4 GeV), PEP (16 GeV) and the SLC Damping Ring (1.2 GeV). The latter has achieved an emittance which is comparable to that which we plan to achieve in the 6 GeV machine. In addition, Stanford is presently undertaking the design and construction of a 1 GeV storage ring with extremely low emittance to be utilized for free electron laser research and for the production of extremely bright VUV radiation through wigglers and undulators. The construction of this last ring, which is being designed by H. Wiedemann of the SSRL machine physics group, will yield experience which is directly applicable to the development of the 6 GeV. (Professor Wiedemann was responsible, as well, for the design of the SLC Damping Ring and also played a major role in the designs of PEP and the DESY machines, DORIS and PETRA.)

In this 6 GeV storage ring endeavor, Dr. Wiedemann will be joined by J. Cerino, A. Hofmann and H. Winick of the SSRL Machine Physics group, as well as visiting scientists and additional staff to be added during the next four years.

The capabilities of this group will have been enhanced considerably by the development of the 1 GeV free electron laser ring on the Stanford campus. This ring is designed specifically for free electron laser development. Part of any such effort must be experimentation in the achievement of low emittance, high current configurations of the sort to be employed in the 6 GeV ring. Thus, the United States will have an electron storage ring for which one main purpose is experimentation in ring design itself. All of the storage rings constructed in the United States have been utilized almost immediately after commissioning for either high energy physics or synchrotron radiation production. This new ring will undoubtedly lead to increased understanding of the machine physics required to produce high brightness synchrotron radiation through wigglers and undulators.

The machine is also an ideal one for the training of graduate students in accelerator physics. The type of experimentation discussed in the previous paragraph is likely to yield exciting Ph.D. theses and to reduce American dependence on accelerator physicists from Europe. Some of these graduate students will, in turn, be well prepared for participation in the development of the 6 GeV ring. Indeed, Professor Wiedemann already has four graduate students working with him on problems which are related to both the 1 and the 6 GeV rings.

Supporting this group is, of course, the Stanford Linear Accelerator Center. Here, the complete ability to design,

fabricate, assemble and effectively commission electron-positron storage rings has been demonstrated. SSRL will also have acquired more experience in the utilization of insertion devices and the utilization of many insertion devices on a single ring than any other facility. There are presently three wigglers functioning on SPEAR. In the summer of 1984, SSRL's first beam line dedicated to undulators will be installed. In the summer of 1985, a multi-undulator system is expected to be added to that line. This development is extremely important because it partially overcomes one disadvantage of undulators, their relatively narrow tuning ranges. During the same summer, SSRL will install the world's first hard x-ray undulator on the 16 GeV storage ring, PEP, and an additional x-ray wiggler line on SPEAR. In the summer of 1986, still another wiggler line, devoted to x-ray scattering, will be installed on SPEAR. These developments will provide much needed opportunities for the development of techniques for dealing with the existence of many insertion devices on a single ring, as well as with hard x-ray undulator radiation. The former are very much needed because extremely precise electron beam control is required for the multiple, long, small aperture paths associated with the insertion devices to be employed on a 6 GeV ring.

In September, 1983, Stanford University established a committee to examine whether it is appropriate for the University to submit a proposal to construct a 6 GeV synchrotron radiation facility. That committee is expected to report out soon, and we anticipate a favorable response.

The establishment of this committee followed a statement concerning SLAC participation in the design and construction of the 6 GeV ring in June, 1983 by W. H. K. Panofsky, Director of SLAC, that "SLAC policy remains that SLAC is perfectly willing to cooperate in this respect, provided arrangements can be made so that such cooperation does not interfere significantly with SLAC's designated mission, which is research and instrumentation in high energy physics. This requires (a) adequate talent at SSRL to plan, design, and coordinate the construction of new facilities, and (b) sufficient advance notice to SLAC to augment its staff and readjust its workload should SLAC collaboration be required." Thus, SSRL has good reason to anticipate SLAC cooperation and collaboration should the University decide to submit the proposal and the Federal Government to fund it. Nevertheless, the role of SLAC in this endeavor, and the relationship between SSRL and SLAC should it be undertaken, are still to be determined.

The Beam Lines Will Be Effectively Developed and Utilized.

SSRL and those closely associated with it have demonstrated their ability to develop and utilize the high power beam lines associated with wiggler and undulator synchrotron radiation. Much of the now commonplace x-ray and soft x-ray instrumentation was developed at SSRL. The first three wigglers for synchrotron radiation research were developed and implemented by SSRL. Similarly the first x-ray undulator was developed in collaboration with the Lawrence Berkeley Laboratory. Interestingly enough, the first permanent magnet

undulator was developed over 30 years ago at Stanford. At the present time, SSRL is building up its internal capabilities to construct permanent magnet undulators for Beam Line V on SPEAR and the new beam line on PEP. Similarly, much of the now-commonplace x-ray optics for synchrotron radiation were first utilized at SSRL.

The local groups involved are the SSRL scientific and engineering staffs, 19 Stanford University faculty from 8 departments participating heavily now in SSRL synchrotron radiation research, a number of scientists from "Silicon Valley" corporations whose research programs are heavily centered around SSRL as well as scientists and engineers from the University of California at Berkeley, the Lawrence Berkeley Laboratory, the Lawrence Livermore National Laboratory, Sandia National Laboratory in Livermore and the University of California, Santa Cruz. This extremely high concentration of relevant scientific and technical talent within easy driving distance of SSRL has helped the Laboratory to flourish over the past decade and will help make possible the effective development of beam lines for the 6 GeV ring.

At the same time, the Laboratory has benefited from the active participation of scientists from quite distant laboratories. Scientists from the Bell Telephone Laboratories, EXXON, the University of Washington and Boeing Corporation, for example, have contributed heavily to the development of SSRL and continue to do so. We have every reason to believe that this support will continue if SSRL develops the 6 GeV ring.

It is presently anticipated that approximately 15 experimental stations will be developed on the 10 beam lines to be constructed initially. Each of these stations will be devoted to a specific type of experiment (e.g., small-angle x-ray scattering or large-angle x-ray scattering), in accordance with a plan to be developed in concert with SSRL's Proposal Review Panel and the SSRL Users' Organization Executive Committee. In our present planning, some of the beam lines will be designed and constructed by SSRL's scientific and technical staff. Others will be developed by outside scientists, in consultation with SSRL's staff, using federal funds allocated for this purpose. By following this mechanism, we anticipate making the most modern and sophisticated experimental equipment available to all of SSRL's users. Individual scientists participating in the development of experimental stations or beam lines will be entitled to some priority time as a result of their intellectual contributions.

Experience in Synchrotron Radiation User Support

SSRL has shown its ability to support many scientists in an effective manner. Over the past decade, at least a 1,000 scientists have utilized SSRL, approximately 650 proposals have received beam time and well over 150 graduate students have received Ph.D.s as a result of research at SSRL. At the present time, there are 196 active proposals from 146 different principal investigators representing approximately 600 scientists.

The development of systematic procedures for meeting the needs of such a large number of scientists has not been straightforward and simple. It has required many attributes, including careful attention to the concerns expressed by many users. That expertise will make utilization of the 6 GeV ring by outside users considerably more effective.

Effective Graduate Student Training

Stanford University and the University of California, Berkeley, are renowned for the high quality of their graduate students. Locating the 6 GeV ring at Stanford will assure the continued education of outstanding students in the various scientific fields utilizing synchrotron radiation. This process is further assured by the large number of Stanford faculty whose students perform research at SSRL. That number will necessarily increase, by design, if Stanford is selected as the site of the 6 GeV machine. Presently, 56 Stanford University students and approximately 20 University of California, Berkeley students are actively working on their Ph.D.'s using SSRL's facilities. SSRL, together with the Applied Physics Department at Stanford, has also started a graduate student training program in Accelerator Physics. This program is very much needed to ease the demand in this country for accelerator physicists.

COST ESTIMATE AND SCHEDULE

The estimated cost of the whole facility including positron injector and 10 photon beam lines stated in FY 1985 dollars is $125.9 million. In this estimate, a stand-alone facility was assumed. (See Table 2)

This estimate includes ED&I as well as contingencies.

A more detailed breakdown of the cost is shown in Table 3.

The completion date is expected to be 1990 assuming significant R&D funds in FY 1986 and full authorization in FY 1987.

The schedule and the total cost estimate are of course related. If the schedule is delayed or stretched out for any reason, the total cost will rise because of inflation and also because of some loss of efficiency in ED&I work.

Table 4 shows the estimated power consumption for the facility.

The power costs, using power rates projected by SLAC, for the year 1990 are also shown on Table 4. The actual cost of power from PG&E for 1984 is $0.045/kWh.

In Table 5, the estimated operating costs are shown. It is assumed that 10 beam lines with 15 experimental stations are operational. The staff projections are scaled from the present SSRL staff. The operating costs are derived from actual costs for the storage ring SPEAR and from actual costs for photon beam lines at SSRL.

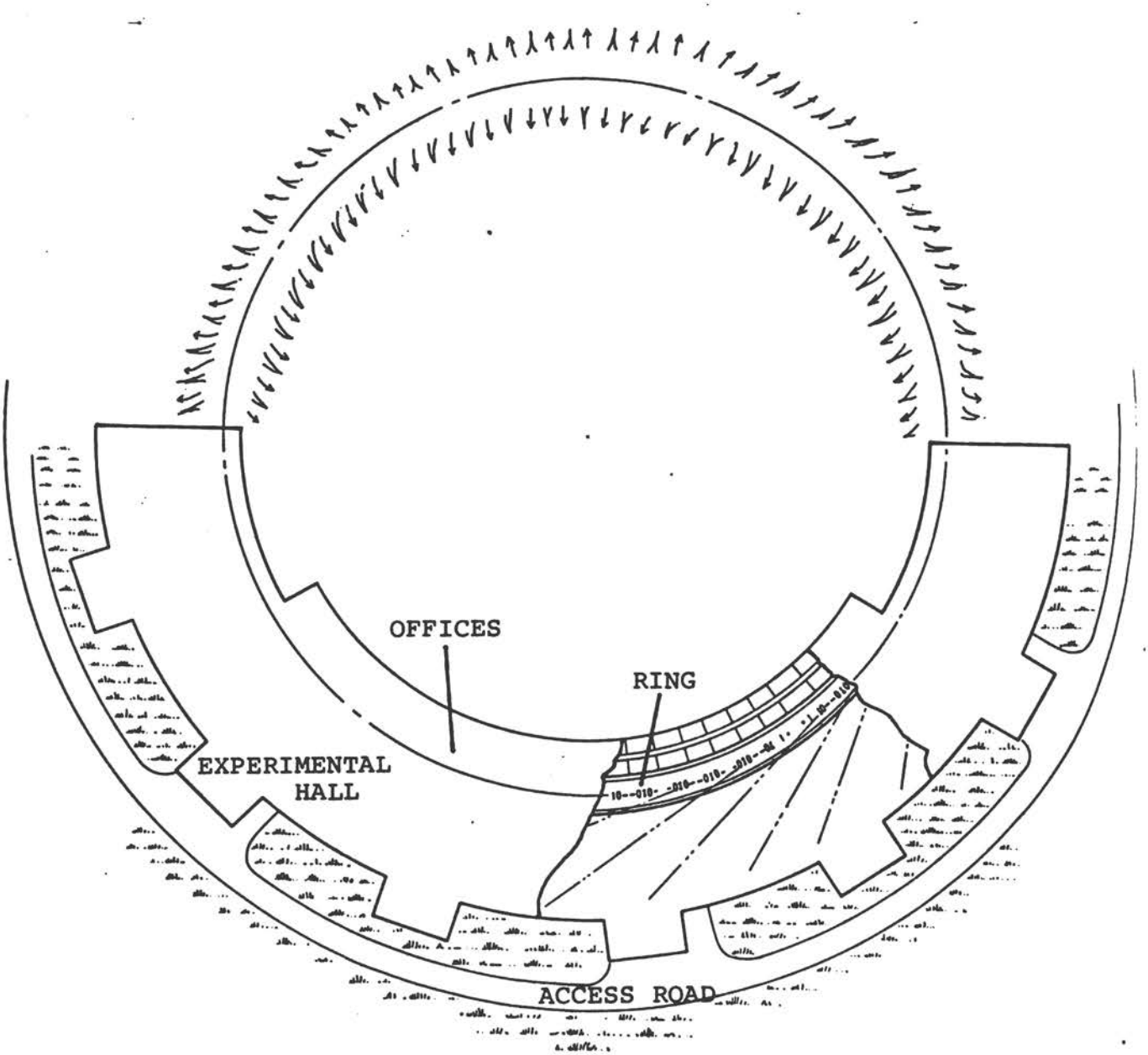


FIGURE 1

SCHEMATIC LAYOUT OF THE FACILITY

Ring Parameters

Particle Beam Energy	6	GeV
Circumference	537	m
Beam Current (max)	100	mAmp
Beam Emittance	0.007	mrad mm
Insertions		
4m long	10	
source width σ	0.400	mm
source height σ	0.120	mm
2m long	20	
source width σ	0.100	mm
source height σ	0.030	mm
Photon Flux (1.2 tesla, 54-pole wiggler)	10^{14} to 10^{15}	ph/sec/mrad/.1% BW
Brilliance (for photon energies of up to 20 keV)	1 to 3 10^{19}	ph/sec/mm /mrad /.1% BW
Brightness	1 to 5 10^{17}	ph/sec/mrad /.1% BW

TABLE 1

New Ring Cost Summary

FY 1985 M$

Storage Ring and Buildings	**74.6**
Dedicated 6 GeV Injector	**14.1**
Positron Source	**1.9**
Cost for 10 Photon Beam Lines	**35.3**
Grand Total Facility	**125.9**
Operating Cost Estimate	**18.1**
Total Electrical Power Consumption MW	**3.6**

TABLE 2

New Ring Cost Estimate

FY 1985 k$

Conventional Facilities	
tunnel,50% circle experimental hall	
lab/shop/office building,utilities	**25445**
Technical Components	
w/o photon beam lines	
w/o injector	**26942**
Standard Equipment	**226**
ED+I and Administration	
10%conv.fac.,25%techn.comp.	**933**
Contingency	
15%conv.fac.,25%techn.comp.	**12688**
Total	**74637**

Options :

Dedicated 6 GeV Injector	**14100**
Positron Source	**1900**
Beam Transport Line from SLAC	
conv.fac.2287k$, techn.comp.1630k$	**3917**
Unit Cost for Photon Beam Lines	
incl. ED+I and contingency	**3531**

TABLE 3

New Ring Power Consumption

Magnets		
Bending Magnets	444 kW	
Quadrupoles	270 kW	
Sextupoles	100 kW	
Steering etc.	50 kW	
Total	864 kW	
(PS-efficiency 85%)		1016 kW
RF-System		
Synchrotron Radiation	600 kW	
Cavity Losses	340 kW	
misc. Losses	50 kW	
Total	990 kW	
(overall AC/RF-efficiency 50%)		1980 kW
Photon Beam Lines		
(3kW/beam line avg.;10kW rating)		100 kW
House Power		500 kW
Total Power Consumption		3596 kW
est.power cost in 1990 (5000hr/yr):		
WAPA : 4.9¢/kWhr 245k$/yr/MW		880 k$/yr
PG&E : 9.4¢/kWhr 470k$/yr/MW		1690 k$/yr

TABLE 4

Estimated Operating Cost

(10 beam lines,15 exp. stations)

FY 1985 k$

Staff :		
Laboratory Management	**10**	
Administration	**17**	
User Support	**23**	
Scientific Staff		
(1 sen.physicist/beam line)	**10**	
(1 jun.physicist/station)	**15**	
Accelerator Operations	**36**	
Beam Line Operations	**17**	
Accelerator Physics	**10**	
Engineering	**25**	
Total Staff	**163**	
Total Staff Salaries		**9943**
Operations (Materials and Services):		
Accelerators	**2025**	
Beam Lines	**800**	
Electrical Power	**875**	
Scientific Program	**4462**	
Total		**8162**
Total Estimated Operating Cost/yr		**18105**

TABLE 5

The Argonne Neutron Plan

February 1984

THE ARGONNE NEUTRON PLAN

I. Objectives and Overview

II. Neutron Scattering - Accomplishments and Oportunities

- A. Most Significant Recent Scientific and Technological Accomplishments
- B. Argonne's Role in Pulsed Neutron Research
- C. The Future

III. The IPNS User Program

IV. The Argonne Plan

- A. IPNS Upgrade
  1. Enriched Target System and Cold Moderators
  2. Accelerator
  3. Instrumentation and Computer System
- B. ASPUN
  1. Sketch of Plan
  2. Critical Features - Why Build a Prototype?
- C. Mini-ASPUN
  1. Plan
  2. Address of ASPUN Critical Features
- D. Synopsis of Plan and a Timetable

V. Resources Required to Implement the Plan

- A. The Current Situation
- B. The Upgrade and Mini-ASPUN
- C. The Steady State with Mini-ASPUN Operating

VI. Why at Argonne?

- A. Scientific Climate and the Role of Neutron Scattering
- B. Scientific Support Systems

THE ARGONNE NEUTRON PLAN

I. Objectives and Overview

The goal of the neutron program at Argonne is to provide the United States with a peerless pulsed neutron facility that meets the specialized research requirements of a wide range of scientific disciplines, and is available to all qualified users from universities, industry, and government laboratories. Argonne embarked on this path a decade ago with the construction and operation of ZING-P, a modest prototype, which was the first proton spallation source in the world instrumented for neutron scattering. The current system, the Intense Pulsed Neutron Source (IPNS), is the most intense spallation source in the world; it has been and continues to be the test bed for technology, instrumentation, and techniques in the developing world of spallation neutron science.

IPNS is run as a national user facility. The excitement of the new science from this source, and the resulting demand for beam time are well documented. In the last round of proposals (December 1983), scientists from over 50 institutions made 104 requests for beam time; the demand was so great that only 40% of the proposals could be accepted.

While IPNS is indeed a success story, we still see it as a prototype. Its peak flux of approximately 4×10^{14} n $cm^{-2}s^{-1}$ is less than the steady state flux of the world's most intense reactors (approximately 10^{15} n $cm^{-2}s^{-1}$). Moreover, in late 1984 the Spallation Neutron Source (SNS) in England will come on line and have an anticipated flux some 15 times that of IPNS. The Germans have even more ambitious plans.

Argonne developed IPNS and its spallation predecessors to test the merit of spallation sources. With this merit now strikingly established, the Argonne goal has become a U.S. commitment to construct a dedicated 10^{17} n cm^{-2} s^{-1} source (250 times more powerful than IPNS) in the 1990s. An innovative design for this remarkable source, which we call ASPUN, is described briefly below. The proposal being made herein charts a clearly delineated development path such that this unprecedented source can be constructed with confidence; this represents a continuation of the "development center" role that Argonne has played so well in the spallation neutron realm. In addition, the proposal has been designed to maximize opportunities for pulsed neutron science, consistent with our recognition of the importance of exploring the scientific scope and extending research opportunities to an ever-expanding and multi-disciplinary user community.

The Argonne proposal involves four major parts, three which address an upgrade of IPNS and the fourth and most important of which deals with a prototype of ASPUN. More specifically:

1) Installation of an enriched uranium target system, and construction of a new cold moderator assembly.

2) Installation of a third RF cavity to improve beam handling and decrease losses in the Rapid Cycling Synchrotron (RCS) and

replacement or modifications of some accelerator subsystems in order to improve reliability and performance.

3) An upgrade of the IPNS instruments, the building of two new instruments, and major improvements in the data acquisition and handling procedures.

4) A test of the key ASPUN accelerator features, using IPNS as a base. Our design for ASPUN is centered about a 1500 MeV, 3.8 mA fixed-field alternating gradient (FFAG) accelerator, a system promising superb performance at a cost far lower than that of comparably performing linear systems. The FFAG prototype (Mini-ASPUN) would deliver in FY89 a proton beam of 100 μA time-averaged current at 500 MeV into the existing IPNS target facility. This would increase the peak IPNS flux to 7 x 10^{15} n $cm^{-2}s^{-1}$ and maintain IPNS as a world-class facility into the early 1990's, while at the same time, this prototype would allow crucial features of the ASPUN design to be tested.

II. Neutron Scattering - Accomplishments and Opportunites

A. Most Significant Recent Scientific and Technological Accomplishments

Over the past 25 years, the unique characteristics of the neutron as a probe of condensed matter have transformed much of our fundamental understanding of the physics and chemistry of materials. In the last decade a new generation of cold and thermal neutron instruments has been developed (particularly in Europe), which have extended the wavevector range and energy resolution for neutron experiments by orders of magnitude. These in turn have opened up new research and have greatly expanded the application of neutron scattering.

The impact of these emerging neutron research opportunities on U.S. science has been addressed by three reports over the past six years: the NAS sponsored study "Neutron Research on Condensed Matter" in 1977; the "Report of the Review Panel on Neutron Scattering," sponsored by DOE in 1980, and the "Current Status of Neutron Scattering Research and Facilities in the United States" sponsored by the NAS in 1984.

As documented in these reports, the most significant recent scientific and technological accomplishments have been the development and utilization of cold neutron sources. For example, highly sensitive cold-neutron time-of-flight spectrometry and ultra-high resolution back reflection and spin-echo spectrometers have expanded the spectral range of neutron scattering by five orders of magnitude, down to 10^{-9} eV. This capability, combined with the unique wavevector regime available with neutrons, has opened up entirely new and exciting applications of neutron scattering in chemical spectroscopy, condensed matter physics, polymer science, and biology. In chemical applications, low-energy neutron spectroscopy is an extremely sensitive tool for probing the intermolecular potentials and the details of rotation and diffusion of molecular species in condensed systems; for example, rotational ground-state splittings (tunneling) can be measured by spin-flip scattering.

The principal biological areas in which neutrons have been applied during the past decade have been in high- and low-resolution macromolecular crystallography, in studies of molecular assemblies and molecules in solution, and in the study of some partially ordered systems. In all cases the difference between the scattering of hydrogen and the scattering of deuterium

has been used as an important tool. For example, cold sources have been used for small angle scattering to extend measurements to much lower wavevector and thus permit the study of larger structures. Recent work on locating the positions of proteins in complex structures such as ribosomes will be extremely useful in understanding functional relationships of different parts of the structure.

Probably the most dramatic, recent application of cold sources has been in the area of polymer science. Polymer molecules are long chain structures which are largely coiled, with molecular weights varying roughly between 10^4 and 5×10^6, and having a characteristic linear dimension, the centroidal radius of gyration, lying between 25 Å and 800 Å. The study of these large molecules requires the very small momentum transfer (down to 4×10^{-4} Å^{-1}) that is only available from cold neutron sources. For example, recent measurements have confirmed that the overall chain conformation of a polymer molecule in the bulk is a random coil with no measurable excluded volume repulsive effects and not an ordered structure with neighboring chains strongly influencing mutual conformational arrangements.

The exciting extension of the useful neutron spectrum downward in energy is now paralleled by the promise of a similar extension upward in energy using the new spallation systems. It has been only since the full-time operation of the Japanese, English, and more intense IPNS sources (1981) that the potential of these facilities has become evident. In recognition of the dominant role that Argonne has played in the development of pulsed sources, we address this new frontier for neutron scattering in the next section.

B. Argonne's Role in Pulsed Neutron Research

Argonne has been, and continues to be, the world's leader in the development and innovative use of pulsed neutron facilities. Among the considerable technical achievements, the following should be noted:

- First uranium target fabrication. ANL is now building a target for the KEK Laboratory facility in Japan. We will also be the first to install an enriched uranium target.
- First choppers phased to a pulsed neutron source. Three such choppers now run at ANL.
- First position-sensitive scintillation detector operated at a diffractometer. ANL is now fabricating a next generation detector for the Institut Laue Langevin, Grenoble, France.

Scientifically, pulsed neutrons are beginning to make a considerable impact. The current favorable position of U.S. pulsed neutron research provides an ideal opportunity to develop the spectral and pulse characteristics of such sources over the next few years. We already know that pulsed sources are superbly matched to highly effective research in both high resolution and low resolution diffraction from powders, glasses and liquids. They exceed reactor sources for applications requiring high momentum or extreme environments. In addition, it is clear that time-of-flight spectroscopy above the thermal neutron range will rapidly become the province of these sources, as improved instruments and higher peak intensities are achieved. The competitive application of pulsed sources to subthermal neutron scattering research, and to studies of the dynamics of ordered or single crystal specimens requires new generation sources and instrumentation. It

should be remembered that intense pulsed sources have operated for only a few years - as compared to the 40 year development of reactor beam technology. Sources now exist at Argonne, Los Alamos, KEK (Japan), and Harwell (England).

The most important single challenge and opportunity for pulsed neutrons is how to make the best use of the rich epithermal neutron spectrum available from these sources. Argonne here has been the pace setter, for example, in the deep inelastic scattering experiments to measure the momentum distributions of elementary solids (collaboration with University of Illinois); in the high-energy, low-wavevector studies of magnetic excitations (collaborations with University of Maryland, University of Missouri, University of Colorado, ORNL, and KFA/Julich); and in the measurements of the dynamics of amorphous solids and liquids over a range of wavevector (collaborations with Pennsylvania State University and MIT). All these experiments utilize epithermal neutrons, of unique intensity at a spallation source, and are therefore either impossible or extremely difficult to conduct at reactors. They have all been performed on the two chopper instruments designed and built at Argonne. Only one other machine of this type exists at Harwell.

Other important contributions from Argonne include the exploitation of the high resolution obtained from a pulsed source in diffraction experiments. The powder diffractometers routinely solve complex crystal structures, often at high pressure or extreme temperatures. The time-of-flight method is particularly well matched to special environments as all the information can be obtained through a single small window. We see this area as one of rapid growth for pulsed neutrons and one that will extend into the area of time resolved studies that will exploit the time structure of the source.

Argonne has also started to explore the possible uses of cold neutrons from a pulsed source. In this field the Japanese have led the world but IPNS now has a cold moderator with three instruments using cold beams (i.e., $\lambda > 4\text{Å}$). In this area as well, we foresee a considerable expansion of our activities and plan to build a quasielastic spectrometer (resolution approximately 20 μeV) and make major modifications to our small-angle diffractometer.

The industrial involvement at IPNS has also been appreciable. Exxon, SOHIO, and Amoco all have strong interest in using the high resolution of the powder diffractometers for studies of catalysts and have purchased (or will soon) proprietary beam time. Schlumberger-Doll has launched a major program at IPNS (and has purchased beam time) to measure the neutron scattering from many hydrocarbons and is now discussing with us the possibility of assisting financially in a major upgrade of one of the instruments as well as stationing a staff member at IPNS. IBM has shown interest in the surface magnetism studies at IPNS using cold neutron beams. Further industrial involvement can be expected as our small-angle diffractometer is upgraded and our capabilities in residual stress determinations enhanced.

C. The Future

Neutron science has always been intensity limited. The advent of pulsed sources at the 10^{16} and ultimately 10^{17} n $cm^{-2}s^{-1}$ level opens up totally new horizons, which are difficult even to predict at this stage. In diffraction experiments we can expect routine experiments on polycrystalline or amorphous samples of a few milligrams with a variety of special environments, e.g., high and low temperature, pulsed magnetic or electric fields, and pressures up to

approximately 100 kbar. Single crystal samples of much less than a milligram will be examined with the Laue technique and with position-sensitive detector arrangements to open new possibilities in molecular biology and play a crucial role in a variety of materials synthesis programs. The copious supply of cold neutrons from cold sources will allow spin-echo machines, quasielastic scattering, and small-angle diffractometers of unprecedented resolution to be built.

But it is in inelastic scattering using the rich epithermal spectrum from spallation sources that the most dramatically new science will emerge. In addition to sophisticated high resolution chopper spectrometers working between 50 and 1000 meV, we can expect to see constant-Q machines challenging conventional 3-axis spectrometers in the study of elementary excitations, new eV spectrometers based on nuclear resonances working in the energy transfer range of 1 to 20 eV and thus complementing inelastic x-ray and electron spectroscopy, and the analog of the spin-echo machine used in the range 0.5 to 5 eV.

Promising and exciting new experimental opportunities have already emerged after relatively little pulsed neutron source operation. During the month of February, 1984, two IPNS sponsored workshops will examine these opportunities and further define future directions:

- o High Energy Excitations in Condensed Matter - Joint with Los Alamos National Laboratory.
- o IPNS Workshop on Scientific Possibilities and Instrumentation for 10^{16} and 10^{17} n/cm^2-sec Pulsed Neutron Sources - Argonne neutron scientists, IPNS users, and Los Alamos scientists.

A more detailed discussion of the future of pulsed neutron science will be found in the proceedings of these workshops.

In summary, the utilization of cold neutrons pioneered in Europe during the last decade has opened up new fields of science. We now stand on a similar frontier with the epithermal spectrum from pulsed sources and there is every reason to believe that new and important science will emerge. This has been the lesson of neutron scattering for the last 30 years whenever new capabilities have become available.

III. The IPNS User Program

From its inception IPNS has been operated as a user facility. The beam time is apportioned 25% to the in-house Argonne programs and 75% to the user program. We do not intend to change this ratio for the foreseeable future.

The role of IPNS as a national user facility is now well established. In the first two years of operation approximately 200 experiments were performed at IPNS, 75% of which have had outside scientists as the principal investigators. Some 140 scientists from 77 different institutions all over the world have visited IPNS to perform experiments. The University of Chicago has supplied funds for travel and housing for IPNS users from North American universities. If scientists do not have sufficient funds, the total cost of coming to IPNS to perform an experiment can be covered. In addition, a car is available for use by scientists during their stay.

At the most recent round of proposals (December 1983), 758 instrument days were requested on the seven user instruments whereas 300 were available, representing a 60% rejection rate. Of these 758 days, 620 were requested by non-Argonne scientists. The growth of the involvement of U.S. universities has been particularly gratifying, increasing from a demand of 120 instrument days in March 1982 to over 300 in the latest round.

The success of this user program has not simply come from having a "proposal and peer review system" for beam-time allocation. Argonne embarked on a program of workshops and continuing education for the U.S. scientific community that represents a totally new, and long overdue, initiative from the U.S. neutron community. Starting in July 1981 with a Faculty Institute, Argonne has sponsored seven workshops on a wide variety of topics, including Resonance Radiography with Neutrons, Chemistry with Neutrons, Powder Diffraction, Neutrons as Applied to Engineering Materials, and eV Spectroscopy with Neutrons. Two of these workshops have been sponsored jointly with Los Alamos National Laboratory. These workshops have each attracted between 50 and 100 participants, a great number of whom have never used neutrons before. Many of the workshops included hands-on experience at IPNS, an aspect greatly appreciated by the many new users who attended. In addition, Argonne has hosted three major international conferences in this period and our first User Meeting (November 1983), attended by 120 scientists. An IPNS Progress Report was prepared for the User Meeting giving all details of the IPNS program, together with many reports of work in progress. Twelve hundred copies were circulated throughout the world.

In summary, the IPNS User program continues to set new standards for the neutron community in the United States. The rewards of this policy accrue not only to IPNS but also to the total neutron community in the United States.

IV. The Argonne Plan

A. IPNS Upgrade

1) Enriched Target System and Neutron Cold Moderators

The IPNS target facility has performed impeccably since installation. We are already embarked on a program to install an enriched uranium target; safety analyses and neutronics calculations are in progress, and the preliminary estimates are that we can have the target installed and operating by June 1985. Calculations show that this will give a factor of from three to five in intensity with no appreciable loss of resolution due to pulse width broadening and no meaningful increase in the delayed neutron background. The completion of the enriched target assembly, which will be built by Argonne, is our highest immediate priority. No enriched target assembly operating at the projected current level now exists in the world; thus, this effort represents an important technological experiment as well as a "flux enhancer."

Argonne experience with cold moderators at IPNS has been extensive. At the present time, we have installed two separate cold (approximately 90 K) moderators, one for the ultracold neutron experiment and one for the three instruments (small-angle diffractometer, polarized neutron beam and ^{3}He project) that require the long wavelength neutrons from the cold moderator and are not affected by pulse width degradation. These moderators will be modified to operate at 20 K in 1984. The larger

heat load from the enriched target will require a new moderator system. In 1986, we plan to install a new cold (20 K) moderator assembly. Heterogeneously poisoned moderators will be used for some of the instruments. Experience is continually being gained on moderator design at IPNS as well as at KENS in Japan and the SNS in the UK.

2) Accelerator

The IPNS accelerator is the world's highest-average-intensity proton synchrotron at 7.5×10^{13} particles per second, and operates with remarkable reliability. We have scheduled over 9000 hours of neutron science these past two years and have run more than 90% of the scheduled time. The neutron yield increase during that period from proton current and energy increases has been 120%, and the 12-μA average beam current now available exceeds the goal stated to the Brinkman Review Panel in 1980 by 50%. The highlight of accelerator improvement has been the development of a higher current H^- ion source. Improvements in the control flexibility and stability of various power supplies have allowed for efficient utilization of the increased H^- beam.

While the Rapid-Cycling Synchrotron (RCS) has performed very well, a modest investment can make it perform even better. Our upgrade plan provides for a 50% increase in the beam current and an improvement in long-term reliability by better control of beam losses. Operation of the IPNS accelerator for up to eight months per year is consistent with the implementation of this plan. These modifications will be handled in a fashion consistent with the fact that the RCS is scheduled to run only until the completion of the prototype FFAG.

Our plan, based upon two years of operating experience, derives from the following observations: a) the accelerator runs beam-loss-limited; b) the RCS is operating near its space-charge density limit, but significant improvements in beam capture and early acceleration efficiency can be made by improving injection stability, by better aperture utilization, and by space-charge density reduction through beam-bunch dilution; and c) beam losses above 250 MeV can be reduced by significantly higher first-harmonic rf voltage.

To address these limitations, we propose:

Addition of a 150-kW RF System. The current two rf systems operate near their 11-kV voltage limits. Measurements and calculations indicate that high-energy beam losses can be reduced up to 50% by 5 to 8 kV more first-harmonic rf voltage during the last 10 ms of the acceleration cycle. Accelerator research has demonstrated that one of three rf systems could be run on the second harmonic of the beam-rotation frequency for the first 4 ms of the cycle. This dilutes the beam bunch and reduces low-energy space-charge density by 30%. It has been demonstrated that it is possible to make the harmonic transition with little beam loss.

Better Low-Energy Orbit Control. This plan calls for the addition of 3 sets of trim dipole magnets to allow "tuning" to maximize the radial and vertical low-energy accelerating apertures of the RCS and changes in the linac transmitter modulator to make the 50-MeV beam energy and energy spread less subject to line voltage variation. This improvement will effectively enlarge the aperture through which the beam

circulates. This allows more beam in the synchrotron and reduces sensitivity to beam steering errors.

Replacement of Ring-Magnet Tuning Choke. The RCS ring-magnet power supply includes a high-Q tuned circuit to supply most of the 5 kV to drive the ring magnet guide field. The 3000-A, 16-mH inductance in this circuit is now formed by accelerator magnets surplused by Cornell in 1967. The higher inductance replacement will improve the stability of the ring-magnet guide field.

3) Instrumentation and Computer System

Currently there are ten instruments working at IPNS. Seven are in the user mode, including two high-resolution powder diffractometers; a single-crystal diffractometer operating on the time-of-flight Laue principle with a position-sensitive detector of the scintillation type; a small-angle diffractometer, also with a position sensitive detector; a crystal-analyzer spectrometer primarily for observing H-modes in chemical systems; and two chopper spectrometers with incident energies ranging from 50 to 1000 meV, which allow scattering measurements over a broad range of energy and momentum transfer. Three additional instruments are also operating but not yet in the user mode: a polarized-neutron instrument for studying refraction from surfaces; a diffractometer built to search for ordered nuclear-moment arrangements in He^3 below 1 mK; and a spectrometer for experiments in the eV range. The upgrade proposals are:

- Complete installation of the high-angle flight path of the High-Resolution Medium-Energy Chopper Spectrometer (HRMECS); equip the spectrometer with a full complement of detectors at small angles, and an adequate number of detectors at large angles. The larger momentum range made possible by the extra large-angle detectors is essential for studies of atomic dynamics in condensed matter at higher resolution than is possible at the Low-Resolution Medium-Energy Chopper Spectrometer (LRMECS). The additional detectors at small angle will double the counting rates in measurements of magnetic scattering, which are so far unique and at present very difficult.

- Upgrade the small-angle diffractometer, which has already proved valuable in metallurgical, biological, and polymer science, by increasing the flight path, acquiring a new detector, and installing a section of guide tube.

- Upgrade the single-crystal diffractometer by increasing the flight path, adding another detector, improving the electronics on both detectors, and increasing the dedicated computer capability at the front end.

- Increase significantly the capability of the data acquisition system including new front-end computers (some instruments currently share front-end computers, a decision forced by budget constraints in 1979 and 1980), new PDP computers for the eV spectrometer and quasielastic machine, and a new VAX system for data analysis. It should be realized that time-of-flight instruments with multiple-counter (especially two-dimensional)

assemblies produce large quantities of data that must be processed by sophisticated computer systems. This is particularly important when we are dealing with a large throughput of outside users, and essential for rapid data analysis.

- Build two new instruments.

  Correlation Chopper Spectrometer. In the past year, structural measurements on glasses have been made at the two powder diffractometers at IPNS. Pulsed sources are very powerful for such measurements since the short-wavelength neutrons provide excellent spatial resolution. On the basis of these initial measurements, it is proposed to build and design a new spectrometer that will have several features (high intensity, low-angle detector, low background) optimized for measurements on glasses. The spectrometer will also be able to separate the elastic and inelastic components of the scattering - a separation that is often crucial in comparing experimental data with modeling calculations.

  A quasielastic spectrometer designed to study polymers, and chemical and biological systems. This instrument, largely modeled on the instrument that works successfully at the KENS facility in Japan, will be installed on a neutron guide tube looking at the cold moderator.

B. ASPUN

As noted above, the goal of the Argonne Super-Pulsed Spallation Neutron Source (ASPUN) project is to provide a facility that can deliver pulsed neutron fluxes exceeding 1×10^{17} neutrons/cm^2-sec in few-hundred nanosecond bursts at a repetition rate around 50 Hz. The core of the ASPUN design is an FFAG proton accelerator (1500-MeV, 3.8-mA average current) that has the potential to deliver the beam power needed to achieve the desired neutron yield and has many other features that make it attractive for generating the proton bursts for an intense neutron source. These include dc excitation of the main ring magnets so that the capture and rf acceleration process can be optimized. Metal vacuum chambers can be used, which allows an extremely low impedance to reduce beam instabilities by permitting higher-beam thresholds before disruptive beam instabilities set in. This phenomenon is further helped by the fact that injection and extraction elements are located only on the very inside and outside edges of the vacuum chamber reducing the perturbation of the smooth wall to a small fraction of the acceleration cycle. The acceleration cycle is so rapid that the beam moves through instability regions before damaging beam growth can occur.

Another important feature of an FFAG accelerator is the ability to stack beam internally, i.e., accelerate several bunches from injection energy to some intermediate energy, merge these bunches into one bunch, and finish the acceleration cycle with the stacked bunch. Because the magnet is dc excited, it is possible to recapture essentially all of the particles that are left behind from the injection and stacking processes and extract them into a beam dump at the injection energy.

1) Sketch of ASPUN Plan

Design parameters for the ASPUN accelerator are given in Table I. The FFAG accelerator will fit into an existing ring building previously used for a high-energy physics accelerator (the Argonne ZGS). The extracted beam lines and target stations can be accommodated in existing buildings that are also part of the high energy physics complex. The injection radius of the FFAG accelerator is 25.888 m and the extraction radius is 28.139 m.

Table I
Parameters for the ASPUN and Mini-ASPUN Accelerators

	ASPUN	Mini-ASPUN
Injection Energy, MeV	200	50
Extraction Energy, MeV	1500	500
Stacking Energy, MeV	1250	350
Injection Closed Orbit Length/2π, m	25.888	8.407
Extraction Closed Orbit Length/2π, m	28.139	9.666
Number of Sectors	20	16
Angular Width of Magnet, degrees	3.6	5.625
Field Index, k	14	8
Spiral Angle, ε, degrees	61	57
Magnetic Field at Injection, T	0.413	0.489
Magnetic Field at Extraction, T	1.327	1.5
Radial Betatron Frequency, ν_x	4.25	3.25
Vertical Betatron Frequency, ν_y	3.3	2.3
Radial Beam Emittance @ Injection, mm-mrad	650 π	200 π
Vertical Beam Emittance @ Injection, mm-mrad	500 π	150 π
Maximum RF Voltage per Turn, kV	400	60
Space Charge Limit	10^{14}	5.25×10^{12}
Extracted Beam Repetition Rate, Hz	≥50	29.9
Number of Beam Stacks	6	4
Average Beam Current, μA	3800	100

The FFAG accelerator consists of 20 identical sector magnets that are designed to intersect perfect circles at a 61° spiral edge angle. The magnet field increases with radius according to

$$B = 0.413 \left(\frac{R}{25.957}\right)^k \qquad (1)$$

where B is the magnetic field in Tesla at a radius R measured from the machine center in meters. The factor k is known as the field index, which for the ASPUN machine has the value 14.

The combination of the entrance and exit edge angles and the field gradient in the sector magnets provide the transverse focusing of the beam resulting in a betatron tune of 4.25 in the horizontal plane and 3.30 in the vertical plane.

An H^- beam is accelerated in an Alvarez linac to 200 MeV. The H^- ions are injected at the inside radius of the accelerator through a carbon stripper foil to produce H^+ ions. The stripper foil is displaced slightly away from the normal equilibrium orbit for the injected beam. Four bumper magnets, two before and two after the stripper foil, produce a local bump in the orbit to bring the beam through the foil. The magnetic fields in the bumper magnets decrease during injection so that beam injected earlier in the cycle is drawn away from the stripper foil. This technique is used to distribute the injected beam more uniformly in space to minimize space charge effects. A beam of 32 mA

for 500 μsec is injected into the accelerator in order to reach the design value of 10^{14} protons per pulse.

Beam is adiabatically captured and accelerated on the second harmonic from 200 to 1250 MeV. The process is repeated six times with the individual bunches stacked into a single beam. The six stacked beams are recaptured into a single bunch at 1250 MeV and accelerated to the full energy of 1500 MeV and extracted in one turn. Calculations indicate that the process of stacking and recapture should be very efficient; however, for protection against unwanted radiation, the fraction of the beam not recaptured in the stacking process is rebunched and decelerated back to 200 MeV for one turn extraction into a 200-MeV beam dump. Likewise, calculations for initial capture after the 200 MeV injection indicate low losses; in the same interest of maintaining low-residual radiation, the uncaptured injected beam will be rebunched and extracted into a beam dump in one turn.

The maximum rf voltage required for the total cycle is 400 kV generated by 10 cavities located around the ring. The frequency range during the second-harmonic acceleration period from 200 to 1250 MeV is 2.087 to 3.09 MHz and during the first harmonic acceleration period phase from 1250 to 1500 MeV is 1.545 to 1.565 MHz.

2) Critical Features - Why Build a Prototype?

The FFAG is a new and exciting entrant in the field of high-current drivers for spallation neutron sources. Yet, past experience does exist with FFAG accelerators and generically similar machines such as ring cyclotrons and sector focusing cyclotrons. The FFAG concept was extensively studied in the early 1960's at the MURA laboratory in Stoughton, Wisconsin. Small electron machines were successfully built and operated and much of the theory developed at that time. Beam stacking was demonstrated. Two large high-current ring cyclotrons, similar in many respects to FFAG's, are currently in operation, one in Canada (TRIUMF) and another in Switzerland at the Schweizerisches Institut für Nuklearforschung (SIN). The latter routinely operates with 100 μA at 590 MeV with a loss rate that is so low that hands-on maintenance of the machine is possible. An upgrade in current to 1 mA is now underway and will be completed in 1984, thereby providing additional information as to the low-loss capabilities of such machines.

Although this previous experience does exist and is suggestive of the capability of the ASPUN accelerator, the fact remains that ASPUN does represent innovation in the area of high current accelerators. After looking critically at this reality, Argonne has concluded that a small-scale prototype would provide the data necessary to produce with confidence a definitive design for ASPUN. A design has been developed in which the existing rapid-cycling synchrotron (RCS) of IPNS is replaced by a 50 to 500-MeV FFAG. This design is called Mini-ASPUN. The intent of the Mini-ASPUN plan is to provide a configuration affording critical tests of the principal ASPUN ideas, for instance, efficient capture and acceleration, the design of the magnets, removal of uncaptured beam, and the success or limitations of beam stacking. Further, Mini-ASPUN has been planned to serve as an important scientific entity in its own right.

C. Mini-ASPUN

1) The Mini-ASPUN plan

Location of the 500-MeV FFAG on the IPNS site is shown in Figure 1. The parameters for the 500-MeV FFAG are given in Table I. Most of the IPNS 500-MeV beam transport line and the IPNS target and experimental configuration will be utilized in their current form. The existing 50-MeV linac is also used, but the modulator, rf driver, tank cooling, and ion souce need upgrading. The existing 50-MeV transport line from the linac to the RCS is used.

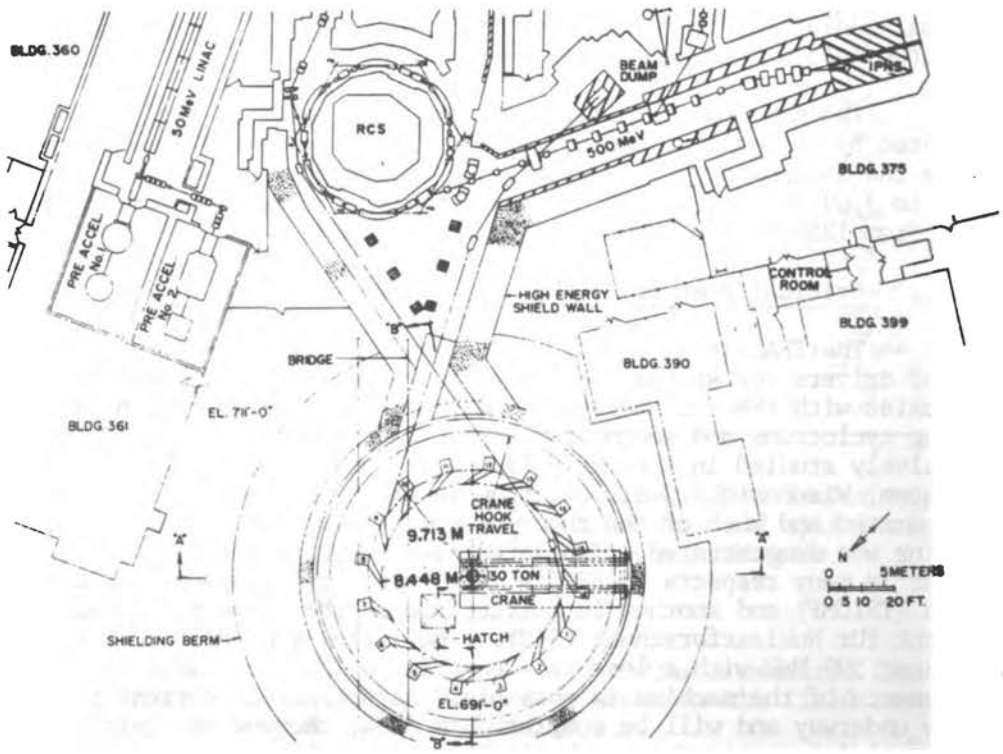


Figure 1: Mini-ASPUN Layout on IPNS Site Plan

An analysis of the linac, designed for operation at 10 Hz, has led to the conclusion that it is capable of operating without damage at much higher repetition rates. The linac tank will require added cooling but this can be provided by connecting existing water channels in parallel rather than series, thus increasing the ΔP across the drift tube cooling circuits. Increased cryo-pumping, a better buncher, and a new pulsed bouncer would also be required for high frequency opration. Existing rf drivers for the linac will also be replaced.

The existing ion source operates near the limit set by power dissipation, which makes it marginal for Mini-ASPUN. We propose switching to a new ion source.

The operating character of Mini-ASPUN is similar to that of ASPUN. Beam is injected through a stripper foil using a magnet bumper system similar to that described for ASPUN; such a system is currently in operation on the IPNS RCS. After injection, the beam is captured and accelerated to a stacking energy of 350 MeV on the second harmonic. Four cycles are merged and accelerated from 350 to 500 MeV on the first harmonic, and, finally, the stacked bunch is extracted in one turn. The nominal repetition rate for the extracted beam is 29.9 Hz and the linac operates at 119.6 Hz. The average injection radius is 8.407 m and the average extraction radius is 9.666 m. The magnetic field increases with average radius according to

$$B = 0.489 \left(\frac{R}{8.438}\right)^k, \qquad (2)$$

where k = 8. The design current is 100 μA. A more detailed view of the ring layout for the 500-MeV FFAG is shown in Figure 2.

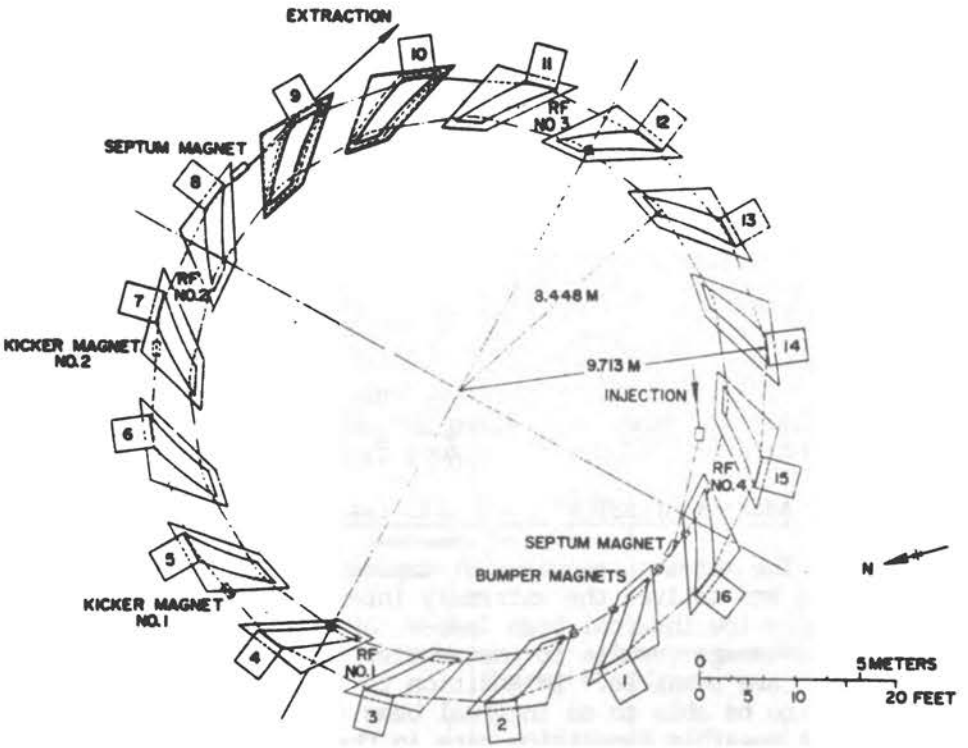


Figure 2: Details of 500-MeV FFAG Ring for Mini-ASPUN

The spiral angle for a main-ring sector manget is 57°, and the nominal angular width of a magnet is 5.625°. The magnet gap starts at 18 cm on the inner radius, is constant to an average radius of 9.0 m, and then reduces to 9.0 cm at the outside edge. Two sets of excitation coils are used to energize the magnet and generate the correct field profile. The main excitation coils circle the full pole face. Pole-face windings start between the inner radius and an average radius of 9.0 m and return beyond the outer radius of the pole face.

The injection bumper magnets are located in two straight sections shown in Figure 2. The stripper foil is located at the edge of the vacuum chamber on the upstream end of magnet 1. The pulsed bumper magnets are designed to have a useful aperture of 6 × 6 cm and a length of 20 cm. Rise time of the field is designed to be 150 μsec and decay times are independently programmed around 100 μsec. The injection septum magnet operates with a 0.57 T field, has a length of 60 cm, and a useful aperture of 3 × 4 cm. The septum magnet is dc operated.

The maximum rf voltage required for acceleration is 60 kV. The rf frequency range for the first part of the acceleration from 50 to 350 MeV on the second harmonic is 3.565 to 6.926 MHz, and for the second part of the acceleration from 350 to 500 MeV on the first harmonic is 3.463 to 3.741 MHz. Four rf cavities are located in straight sections between magnets 3 and 4, 7 and 8, 11 and 12, and 15 and 16. Each cavity has a cross-sectional area of ferrite equal to 0.0625 m^2 and a total volume of 0.279 m^3. The peak rf power per cavity is 115.4 kW including beam power and the average power per cavity is 25.3 kW. Each cavity has one accelerating gap of approximately 10 cm and the ferrite is divided into two sections, one on each side of the accelerating gap.

Extraction is accomplished in one turn with the use of two fast ferrite kicker magnets and a septum. The location of the elements is shown in Figure 2. The first kicker deflects the bunch inward by 7.384 mr. The second kicker is located 180° in betatron phase from the first kicker so that its deflection of 7.384 mr adds to the first deflection. This places the beam 4.7 cm outside of the unperturbed equilibrium orbit at the septum magnet, sufficient to clear the magnet septum and get a final deflection of 77.99 mr. Each ferrite kicker magnet is 0.4-m long, operates at 0.07 T, and has a good field region of 5 × 6 cm. The field rise time is 90 nanoseconds and the flattop is 170 nanoseconds. The final extraction septum magnet is 0.6-m long, has a field strength of 0.473 T, and a good field of 3 × 6 cm.

2) Address of ASPUN's Critical Issues

The foremost requirement imposed on ASPUN is to be able to accelerate and deliver the extremely intense beams needed with sufficiently low internal beam losses, or with the removal of lost beam, so that no damage results to the accelerator and ordinary maintenance techniques are possible. In addition to this requirement, it is desirable to be able to do internal beam stacking in ASPUN to achieve the lowest possible repetition rate in the extracted beam so that long wavelength neutrons can be provided without the necessity of adding an external stacking ring.

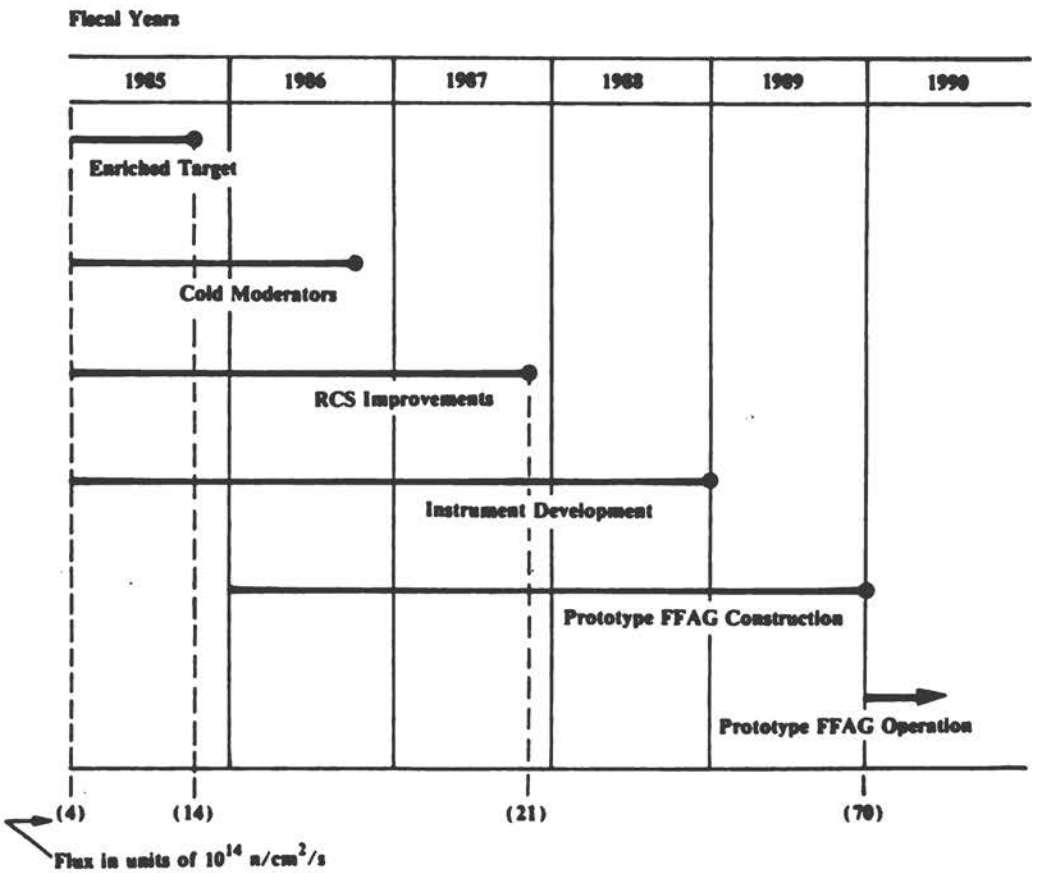
Calculations indicate that the intensity goals at the overall beam efficiencies can be achieved. The ability to achieve internal beam stacking, although encouraging, is not as theoretically certain. Mini-ASPUN provides the opportunity to demonstrate the former and test the latter. In particular, the injection, capture, and acceleration process of Mini-ASPUN will be identical to ASPUN so these processes can be studied in detail, and theory and practice compared. The development of optimal techniques for removing the uncaptured injected beam into external beam dumps will be pursued. The design and performance of

actual accelerator hardware items such as the magnets and their correction coils, rf system, and diagnostics will be tested under actual beam conditions. Such elements as the optimal control of beam tune by edge windings on the magnets will be studied.

Beam stacking on Mini-ASPUN will be a principal area of study. Key questions such as whether unforeseen instabilities occur and whether they can be damped will be tested. The size of beam losses in the stacking and recapturing processes can be measured and the ability to remove this beam by rf deceleration to the injection energy and kicking it out into the beam dump will also be tested.

The use of Mini-ASPUN as a prototype for ASPUN will provide a solid demonstration of the technology and will also provide important technical information relevant to the design and cost of ASPUN.

D. Synopsis of Plan and Timetable *



* An alternative accelerated schedule for ASPUN construction is outlined on the final page of this document.

V. Resources Required to Implement the Plan

A. The Current Situation

IPNS is now being run for six months per year for users and Argonne staff members. The effort and costs in FY 84 for facility operation, the user program, and Argonne neutron research are:

	FTEs	Cost (FY84 M$)
Facility Operation	38	4.10
User Interface	21	2.01
Argonne Neutron Research	16	1.72

Incremental costs for an additional week of operation are approximately $35K. It should also be noted that Laboratory discretionary funds totalling $240K have been provided in FY84 toward the construction of the enriched target.

B. The IPNS Upgrade and Mini-ASPUN

Our current estimate for the cost of the IPNS upgrade, including the renovation of the linac and ion source, is (FY 84 M$):

FY	84	85	86	87	88	Total
Gen. IPNS Upgrade*	0.30	0.93	1.29	0.78	-	3.30
Linac & ion source renovation**	-	-	0.15	0.45	0.30	0.90

* Includes:

Enriched target	0.49
Cryogenic Moderator(20K)	0.28
RCS Modifications	0.92
Instrument Upgrade	0.56
Correlation Chopper Spectrometer	0.25
Quasielastic Scattering Instrument	0.30
Computer System	0.50

**Contingent upon Mini-ASPUN.

The cost estimate for Mini-ASPUN is (FY 84 M$):

	Oper., Eqpt. and R&D	Construction	Total
FY 1985	0.65	-	0.65
FY 1986	1.41	2.35	3.76
FY 1987	1.07	6.40	7.47
FY 1988	0.25	6.43	6.68
FY 1989	0.53	5.50	6.03
FY 1990	1.06	-	1.06
Total	4.97	20.68[+]	25.65

[+]Includes contingency of $2.40M

In our judgement, the ASPUN design effort should be reemphasized

beginning in FY 1987 to a level of 6 FTEs with annual costs of $500K. This design effort, which would continue into the early 1990s, has not been included in any of our budgets.

C. The Steady State with Mini-ASPUN Operating

When Mini-ASPUN is operating, together with the new and renovated instrument complement, research opportunities will be strongly enhanced over those available at IPNS as currently configured. For running eight months per year, our operations, user interface, and research plans involve:

	FTEs	Costs (FY84 M$)
Facility Operation	52	6.46
User Interface	28	2.53
Argonne Neutron Research	18	1.93

VI. Why at Argonne?

A. Scientific Climate and the Role of Neutron Scattering

Neutron science has been a central feature of Argonne programs since the inception of the Laboratory, with the early emphases being radiation effects and cross section measurements. Neutron scattering, in particular, was initiated at the Laboratory in 1948, continued as a key Argonne activity at the CP-5 reactor (1954 - 1979), and then, through a series of intermediate steps, moved into the "time-of-flight" realm utilizing the pulsed spallation source IPNS in 1981.

Argonne work in neutron scattering is embedded to a large extent within the Materials Science and Technology (MST) Division, a materials organization of extraordinary size ($28M in FY 1984) and scope. The large and talented neutron scattering group incorporates a diversity of interests and is involved in programs dealing with, inter alia, catalysts, fast ionic conductors, superconductors, molten salt chemistry, amorphous systems, glasses, crystallography and magnetic materials; scientists from MST have borne and bear much of the responsibility for instrumentation design and implementation. In addition, the wealth of materials perspective at Argonne leads to novel applications of neutron scattering as well as constant pressure on the state of the art. Recent examples include the work on residual stress determinations in complex solids and investigations of surface magnetism via polarized neutron scattering. Further, Argonne has a tradition of pioneering studies directed toward the most fundamental questions in condensed matter physics, such as the measurement of the fundamental excitations in liquid ^{3}He, a seminal experiment in the physics of quantum fluids. This tradition continues with the collaborative program (Northwestern University, Studsvik Research Laboratory in Sweden, Argonne) directed toward the determination of the ultra-low temperature spin ordering in ^{3}He, an experiment of enormous complexity and of great interest.

It should be noted that the extensive chemistry-based Argonne effort in crystallography is situated programmatically within the MST Division. This effort has both "user" and "Argonne program" character.

Another important component of the IPNS program is that conducted by biologists from the Biological and Medical Research Division, utilizing small angle scattering for investigations of biological systems. The small angle

scattering diffractometer is also of particular interest to the chemists looking at the structure of, for example, crystals comprised of large molecules (molecular weights in the range of 100,000 units), and to the metallurgists working on alloy development and properties.

The critical role that neutron scattering plays in the extensive Argonne materials programs is thus clear. Equally important is the fact that these programs impart perspective to the neutron scattering effort, in kinds of experiments attempted as well as instrumentation. Indeed, the success of the IPNS User program can be attributed in substantial measure to the extensive interest at Argonne in neutron scattering, which provides a fertile ground for conceptualizing and initiating new ventures and opportunities for continuing collaborative activities.

B. Scientific Support Systems

A wealth of support services are available to expedite scientific accomplishment and to assist users, which make siting major facilities at Argonne attractive. Some of the services available and siting advantages are:

Convenience and Accessibility

Argonne is located 25 miles southwest of Chicago. It is centrally located in the nation and is only about one-half hour driving time from O'Hare Airport, the world's busiest airport with daily service to every major airport and most minor airports in the country. The Laboratory has a lodging facility with 112 rooms and apartments on site for visitors, a travel office and a cafeteria.

Multidisciplinary Research Staff

Argonne has approximately 20 technical and scientific research divisions which employ more than 4200 people, of whom about 1,550 are scientific and professional staff. Argonne scientists can provide a valuable resource of consultation and collaboration over a wide range of interests to neutron users. Argonne technical groups have designed and built the two uranium targets that are used at pulsed neutron sources.

Machine Shop Services

Central Shops has a staff of 105 people including approximately 85 journeymen machinists, manufacturing engineers, instrument makers, model fabricators, welders, grinders, precision opticians, and other specialists. The shops contain basic machines such as lathes, milling machines, planers, and grinders, but also specialized equipment such as numerical controlled machines, electron beam welders, electro-discharge machines, and x-radiography and ultrasonic testing equipment.

Plastics Shop

The plastics shop is a 6400 sq. ft. area dedicated to building custom apparatus needed for the operation and experimental exploitation of a large particle accelerator facility. Some 60 major items of equipment are installed there. Of special interest are the ovens, pumps, etc. to vacuum impregnate and cure the insulation systems of large magnets coils and high-power rf structures; facilities for vacuum deposition of thin metal films, ceramic flame spraying, and scintillator manufacture are of particular importance.

Electronic Services

Electronics Division personnel collaborate with scientists to define and solve instrumentation and detector problems. Areas where assistance is provided include application techniques, systems specification, circuit design, circuit construction, maintenance, circuit modification, and documentation. The division has staff in six groups: Data-Acquisition and Processing Systems, Digital Instruments and Systems, Fabrication and Maintenance, Measurement and Control Systems, Radiation Instrument, and Reactor and Low-Frequency Electronics.

Engineering Services and Graphic Arts

The Engineering Division staff of 152 provides facility engineering, design and drafting services. This Division designed and built IPNS and has extensive experience in design and safety analyses of "nuclear" systems. The Graphic Arts Department has 60 staff members to prepare copy, print and bind technical reports and other printed matter, provide industrial photography facilities for black-and-white and color material, and prepare visual material such as displays, exhibits, slides, and illustrations.

Occupational Health and Safety

The Occupational Health and Safety Division has extensive experience and expertise, built on thirty years of close collaboration with the Laboratory's experimental program and seven years direct experience with the pulsed sources at Argonne. They perform hazard evaluation and safety reviews of experimental arrangements and equipment, monitor and measure generated radiation fields, perform necessary personnel radiation dosimetry both internal and external, and evaluate personnel exposures to non-ionizing radiation, noxious gases, mists, vapors, smokes, dusts, and excessive noise.

Computing Services

Argonne's computing facilities include three large IBM computers, two 3033's and one 370/195 using the MVS and VM, and OS/MVT operating systems, respectively. These computers and their associated peripheral equipment provide 19 billion bytes of on-line storage in disks and drums, 24 magnetic tape drives, 55 remote job entry stations distributed throughout the laboratory complex, a multiplicity of input and output devices, and extensive libraries of mathematical, statistical, and graphical programs and subroutines. The central computing facilities are linked to the IPNS complex by a communications network with local terminals.

Library Services

The Technical Information Services Division of Argonne operates eight library locations on the site. The media collection includes 75,000 books, 3000 journal titles, 1500 journal subscriptions, and 750,000 technical reports. Thirty-three experienced professionals assist in on-line data base searches, reference service, interlibrary loans, and journal translations.

Other Services

These include a fire department with firemen and paramedics on duty at all times, a medical office, site security protection and rigging services.

ARGONNE NEUTRON PLAN

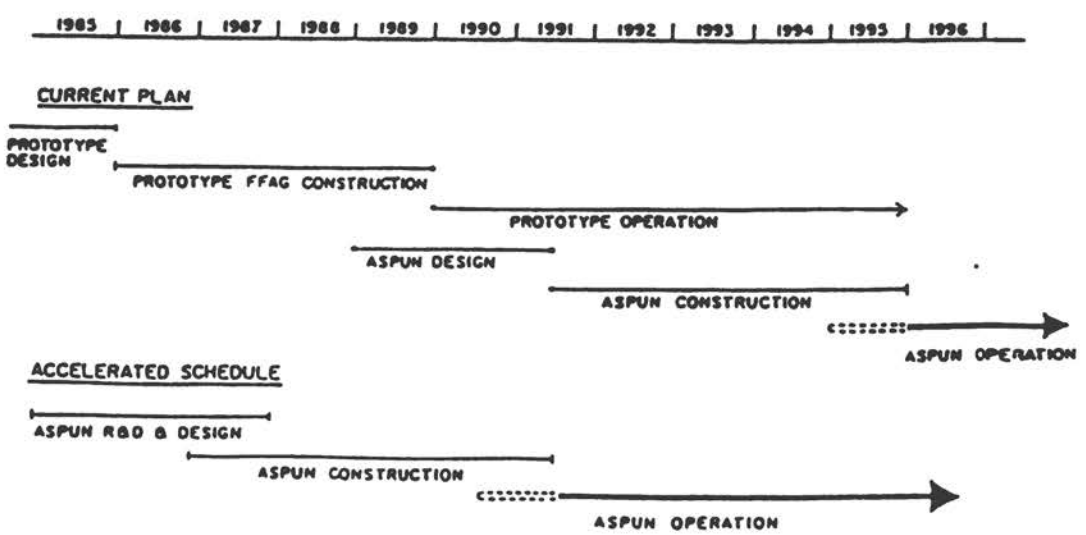
Optional Schedule for ASPUN

The Argonne Neutron Plan proposes building a prototype machine that will result in a neutron source of approximately 10^{16} n/cm^2-sec and that will provide information for the design of the extraordinarily powerful ASPUN accelerator. Argonne has adopted this step-wise approach for arriving at a 10^{17} n/cm^2-sec source. However, an optional schedule for ASPUN without the prototype could be adopted which would advance operation of ASPUN by five years, from 1996 to 1991. Figure 1 shows the schedule for the current plan leading to ASPUN in 1996 and the accelerated schedule leading to ASPUN in 1991.

The current plan allows testing of all of the ASPUN hardware on a lower-intensity accelerator. Furthermore, a critical examination of injection and capture techniques, effective removal of uncaptured injected beam, the use of pole-face and pole-edge windings to adjust horizontal and vertical tunes, and beam stacking will be performed at Mini-ASPUN.

Although the current path offers these advantages, it is possible to bypass the prototype with a substantial analytical study program and with additional contingency in the technical design. This possibility is suggested by the fact that FFAG-type accelerators constructed to date have achieved design performance with relative ease. Essentially, the experimental studies on Mini-ASPUN would be replaced by detailed computer studies of the injection, capture, and stacking processes. An aggressive program of building and testing model magnets and rf cavities, and of developing beam diagnostic equipment would be needed. This R&D program would require $13.75 M for fiscal years 1985, 1986, and 1987.

The ASPUN design has a factor of about 2.8 safety margin in achieving the design goal of 10^{17} n/cm^2-sec. This factor is built in to allow for the possibility that linear scaling from IPNS experience may not be valid due to the high-power density in the target. We believe that, with experience in operation, greater than 10^{17} n/cm^2-sec will be achieved. With or without the prototype, the initial schedule for commissioning ASPUN would be basically the same, 20% of full current at turn-on and 65 to 70% of full current within one year of turn-on. However, the percentage of the initial year's operating time spent on achieving the schedule rather than in operation for condensed matter research will undoubtedly be greater for the optional plan without the prototype.



Guide Hall at the High Flux Beam Reactor

Brookhaven National Laboratory

Presentation to the Neutron Scattering Subpanel

of the Major Materials Facilities Committee

National Research Council

National Academy of Sciences

February, 1984

1. Introduction

The National Synchrotron Light Source (NSLS) and the High Flux Beam Reactor (HFBR) at Brookhaven National Laboratory constitute a unique environment for research in physics, chemistry and biology. The two facilities are complementary: scattering experiments with electromagnetic radiation and neutrons combine to provide microscopic information of importance for many diverse fields of science.

The HFBR has been in operation since 1965. At its present power of 60 megawatts, it provides a thermal neutron flux of 1×10^{15} neutrons/cm^2-sec, and is one of the best thermal neutron sources in the world. It runs 24 hours per day during operating cycles of 24 days, separated by 3 to 6 day shutdowns for refueling and maintenance. At present, there are 9 beam ports supporting 15 experimental stations.

The scope of the scientific activities at the HFBR is exceptionally wide, spanning:

Biology: - structural biology
Chemistry: - chemical crystallography; cooperative phenomena
Physics: - neutron scattering studies and slow positron research in all areas of condensed matter physics and materials sciences
- nuclear structure

In the past few years, conceptual advances and developments in instrumentation have led to the clear recognition that it is essential to expand the facilities for neutron scattering in the United States, particularly at the steady state sources. It is extremely appropriate to undertake such an expansion at Brookhaven in view of the diverse scientific program based upon a first rate neutron source in close proximity to a forefront facility for research with synchrotron radiation.

In order to provide the increased experimental space necessary to accommodate the proposed new facilities, it is intended to take advantage of advances in neutron beam optics in order to extend beam lines into a guide hall, external to the present reactor. In this way it will be possible to house eight new experimental stations and, by making constructive use of the

features of the new building, to establish a unique center for research with low energy positrons.

The HFBR is operated as a national users facility: workers from other laboratories are able to carry out experiments there, after peer review of their research program. In order to have a unified policy for use of the two major facilities, Brookhaven has adopted for the HFBR the Participating Research Team (PRT) system, already established at the NSLS. Existing and future spectrometers will be constructed and/or operated by PRT's, organized by discipline, and consisting of members from the Laboratory, universities, industry and government laboratories.

The proposed expansion of the HFBR has been developed in consultation with an External Advisory Committee consisting of R. J. Birgeneau (Massachusetts Institute of Technology), B. Craven (University of Pittsburgh), D. M. Engelman (Yale University), R. W. Hoff (Lawrence Livermore Laboratory) and J. J. Rush (National Bureau of Standards). The views of the users community at large were solicited at an open workshop held on November 3, 1983 and attended by about 150 people. The guide hall concept was well-received, and a lively discussion produced a number of suggestions which have been incorporated into the present form of the proposal.

2. Developments in Research with Neutrons

Over the past thirty years, it has clearly been established that neutron scattering is of fundamental importance for physics, chemistry and biology. In particular, the microscopic information obtained by magnetic and inelastic scattering of neutrons, and by the elastic scattering of neutrons from low-Z materials has not so far been matched by any other technique. The scope of these contributions and the parallel developments in low-energy positron scattering and in reactor-based nuclear structure physics are illustrated by a brief listing of recent research accomplishments in the various fields.

A. Condensed Matter Physics

1. Coexistence of magnetism and superconductivity
2. Effects of magnetic fields on dilute magnets
3. Charge-density waves, Peierls' and spin-Peierls' instabilities
4. Incommensurate systems

5. Low-dimensional magnetism
6. Structures of surface phases
7. Large-amplitude anharmonic excitations
8. Paramagnetic scattering in itinerant magnets
9. Conformational studies of polymers
10. Critical phenomena at magnetic and structural phase transitions
11. Transitions in intercalated systems
12. Spin glasses
13. Mixed valence materials
14. Momentum distribution in quantum fluids
15. Local modes in hydrides

Major contributions to all of these topics except 9 and 14 have been made at Brookhaven and, in several cases neutron scattering studies were initiated there. Without exception the microscopic information obtained from these experiments has led to new theoretical developments and to a deeper understanding of the underlying physics.

B. Chemistry

1. Structural analysis of organometallic compounds
2. Studies of framework structures (zeolites etc.)
3. Ionic conductors
4. Hydrogen in metals
5. Electron charge-density and spin-density distributions
6. High resolution studies of small molecules
7. Spontaneous polarization in pyroelectrics and ferroelectrics

Contributions have been made at Brookhaven to all areas. Some of the first work on framework structures, organometallic compounds, electron charge-density distributions and spontaneous polarization in pyroelectrics was carried out at the HFBR.

C. Biology

1. Determination of molecular weights and shapes
2. Nucleic acid-protein-lipid distribution in large complexes

3. Structural studies of membranes
4. Determination of hydrogen positions in proteins
5. Hydrogen-deuterium exchange studies in proteins
6. Determination of bound water in biomolecules
7. Determination of polymer structures
8. Micelle studies
9. Virus structures

The use of neutron techniques for the analysis of biological structures was pioneered at Brookhaven and major contributions have been made, particularly to topics 1-6. Neutrons have played an important role in many of the most fundamental areas of modern biology.

D. Nuclear Structure

A main thrust of the nuclear structure program at the HFBR has been to map out the structure and symmetries of excited states of nuclei with excitation energies up to 2 MeV. Complementary experimental work has been carried out at the Institut Laue-Langevin in Grenoble. At Brookhaven, the experimental data have been used to establish and refine the Interacting Boson Approximation (IBA) - a model which incorporates the essential symmetry of Cooper pairs in the nucleus and allows the detailed calculation of collective modes. The IBA is regarded as one of the most significant advances in nuclear structure physics in the past twenty years. Recent work at the HFBR has provided the first evidence for multi-j supersymmetry in nuclei.

Another major aspect of the program has been the study of heretofore inaccessible nuclei far off stability with the isotope separator TRISTAN. These programs are the only ones of their kind in the United States.

E. Low Energy Positron and Positronium Research

In the past decade, great advances have been made in the development and exploitation of mono-energetic low-energy positron beams: technical progress has led to a thousandfold increase in the positron current, using conventional positron emitting sources. Some notable achievements during this period are:

1. Positron-atom scattering
2. Low energy positron diffraction (LEPD)
3. Study of imperfections at metal-metal, metal-semiconductor and metal-metal oxide interfaces
4. Measurement of vibrational levels of adsorbed molecules
5. Study of surface magnetism of ferromagnetic metals
6. Studies of defects in metals
7. Discovery of negatively charged positronium
8. 1S-2S transition in positronium

Brookhaven has been a leading center for research in this field and carried out the projects 3, 4, 6 listed above.

A collaboration involving Brookhaven, Bell Laboratories, City College New York and Brandeis University is now engaged in establishing a new pilot facility at the HFBR. Various members of the collaboration were responsible for initiating all of the advances listed above. The new facility is based upon short-lived high-intensity ^{64}Cu sources produced by neutron irradiation and, with the aid of brightness enhancement techniques, it is designed to increase the positron current by an additional factor of ten thousand.

F. Technical Developments

1. High energy resolution instruments
2. Extensive use of neutron guides
3. Cold neutron moderators
4. Use of neutron spin polarization analysis
5. Development of focussing monochromators, multilayers and supermirrors
6. Powder profile analysis
7. High resolution area detectors
8. Neutron interferometry
9. Use of phase contrast methods for large biological molecules

Brookhaven has made significant contributions to 3, 4, 5, 7 and 9 of the above. It is felt that the United States has not fully utilized 1, 2 and 6 and they constitute a major component of the proposed guide hall expansion at the HFBR.

3. Proposed Guide Hall Construction at the High Flux Beam Reactor

The major element of the HFBR expansion plan is the addition of a guide hall of 15,300 square feet to house new scientific instruments with 4,300 square feet of adjacent laboratory space. In addition, the guide hall building will also provide office and support space for external users and the Reactor Division staff, as well as space to house mechanical equipment.

The location of the guide hall, as determined by its relationship to the beam from the cold neutron moderator and a suitable thermal port, is restricted to the western area, near the lobby of the HFBR. The same considerations determine the width of the guide hall and, since the beam lines are 21 feet above grade, suggest a two story building (see Figures 1 and 2). The ground level can then accommodate laboratory and office space, and provides a natural site for a slow position facility, which must be located close to the reactor. The overall depth of 100 feet is required by the optical properties and location of the planned neutron instruments.

A number of approaches were investigated in order to develop solutions which would meet the scientific requirements.

Brief Description of Scientific Programs

Recent advances in material science, nuclear physics, chemistry and structural biology opened up new fields of investigations, particulary in the dynamics of atoms and molecules in solids. Such studies demand an expansion of existing neutron facilities, with new neutron instruments for the use of the scientific community. In order to place such new devices and improve the utilization of the High Flux Beam Reactor (HFBR), the construction of a guide hall that will house up to ten additional spectrometers is planned. The development of new neutron optical devices (multilayer monochromators and super mirror guides) has made it possible to place neutron spectrometers at a greater distance from the reactor without losing flux, thus allowing the placement of many more instruments and enhancing the use of reactor neutrons.

Apart from innovations in ongoing research projects, instruments are needed to allow novel research activities in material science, metallurgy, polymer chemistry, medical investigative techniques and structural biology. The presently planned general layout of the facility is given in Figures 1

and 2. The final location of instruments will be reviewed close to the date of installation to assure the best utilization of the cold and thermal neutron beams. In consultation with external users, the following new instruments have been identified as most urgently needed:

1. Powder diffractometer
2. Backscattering spectrometer
3. Nuclear structure facility
4. Medical prompt γ station
5. Spin echo spectrometer
6. Time-of-flight instrument
7. Small angle station
8. Crystal spectrometer
9. Positron facility
10. Triple Axis instrument

High Resolution Neutron Powder Diffractometer

In the past few years the application of neutron powder diffraction techniques to the analysis and determination of crystal structures has been very successful in a variety of materials research problems where single crystals are unavailable. The main advance has been the use of profile methods of data fitting first introduced by Rietveld, in which the raw intensity data obtained in an angular step scan are fitted point by point directly to some structural model. In this way, it has been possible to determine in some detail the structures of many quite complex inorganic materials of current interest, including hydrides, fast ion conductors, superconductors and more recently zeolites.

The most important consideration in the appliction of the profile technique is the overall resolution of the neutron pattern, which depends mainly upon the collimation and the mosaic width of the monochromating crystal, typically 20-30' in most existing diffractometers. The proposed instrument is designed to have collimation and mosaic widths in the region of 5-10', together with a high take-off angle for the monochromator which will

optimize the resolution over the angular range of interest. The resulting loss of intensity will be compensated for principally by a multi-detector system, and also by the use of wide vertical apertures, more efficient Soller slits and a vertically focussing germanium monochromator. With such an instrument, it is anticipated that complete data sets can be collected within a 24 hour period with a factor of at least three improvements in resolution. This will enable considerably more complex structures to be tackled, and also a wider variety of problems involving phase transitions and determination of the unit cell symmetry in pseudo-symmetric structures. Further, the possibility exists of combining such data with similar data taken on the high resolution x-ray diffractometer being constructed at the National Synchrotron Light Source, which should be particularly useful for hydrogenous materials.

This kind of instrument is comparatively simple to operate and should present no problems for outside users. It should find wide application in a variety of structural problems of interest to chemists, crystallographers and metallurgists in the materials community.

Back Scattering Spectrometer

Although conventional 3-axis spectrometers have been and will continue to be the instruments of choice for most applications in condensed matter physics, there are special circumstances in which higher energy resolution combined with relatively large momentum transfer and/or relaxed momentum resolution are required. A backscattering spectrometer using ~2Å neutrons can fulfill these requirements, by making use of the very high energy resolution associated with Bragg scattering at nearly normal incidence. However, such an instrument has limitations for low-symmetry powder samples and it may prove desirable to have the option of placing it on a cold beam. Three back scattering instruments are in routine use in Western Europe but no comparable instruments are available in the United States.

This spectrometer will prove very useful in the following kinds of measurements:

1. Elastic Incoherent Scattering. Accurate determination of elastic incoherent structure factors for rotating or tunnelling molecules in solids, which requires high energy resolution to clearly separate elastic and quasielastic scattering components.

2. Inelastic Incoherent Scattering. Rotational and tunnelling states of molecules in solids, as well as hyperfine splitting can be directly investigated. Single particle diffusion, for example of H in metals, is also an area for possible application.

3. Inelastic Coherent Scattering. Soft phonon modes, central peaks and collective diffusive modes in solids, glasses or viscous liquids can in principle also be studied.

Nuclear Physics in the HFBR Guide Hall:
The (n,γ) Reaction and 2) Neutron Rich Nuclei From TRISTAN.

1. One of the most powerful techniques for studying the structure of atomic nuclei is that of radiative neutron capture, in which a beam of low energy neutrons from a reactor is allowed to impinge on a target sample containing nuclei of some element. These nuclei capture the neutron to form a new isotope of the same element. This resulting nucleus is formed in an excited state and it must divest itself of this extra energy. It does this by emitting a sequence of γ rays each leaving the nucleus in successively lower states of excitation. By studying these γ rays the nuclear structure (shapes, modes of motion and excitation, interactions of the protons and neutrons within the nucleus) can be unravelled. This technique, usually called (n,γ), is particularly powerful because it populates essentially all low-lying excited states of the resulting nucleus and thus offers a unique test of modern comprehensive nuclear models that attempt to account, not just for the properties of a few excited modes, but for all of them.

In all such experiments a perennial problem is unwanted background γ radiation from the reactor itself. If a neutron beam can be guided to an isolated distant environment, this problem can be greatly reduced. The guide hall beams will do just this and will provide a "quiet" environment in which very sensitive experiments can be carried out.

2. TRISTAN uses the fission of uranium to produce exotic atomic nuclei that have many more neutrons than protons. Such nuclei are not usually found in nature and so are difficult to study. Due to their unique combinations of protons and neutrons they often evidence new phenomena or additional examples of familiar ones that allow us to understand them

better. These "neutron rich nuclei" are studied by means of their emitted γ radiation and thus also benefit from a low background environment. They are produced in the form of ionized beams and thus can be focussed and directed by the use of electrostatic and magnetic "lenses". It is proposed to lead these ions to a set of instruments in the Guide Hall, thus benefitting from the shielded, low background enclosure, substantially improving the sensitivity of the measurements and expanding the producitivity of the TRISTAN facility nearly two-fold.

Medical Physics, Prompt γ Spectrometer

Neutron capture therapy.

Current improvements in radiation therapy have been achieved by using target agents in conjunction with neutron capture therapy. The aim is to target a stable boron isotope (^{10}B) to a tumor for later activation with an external neutron beam. The γ emission of the irradiated boron target agent provides a localized radiation dose to the tumor. The success of this approach will depend on the selective uptake of target molecules by the tumor in sufficient concentrations. To study target affinity, conventional wet chemical microanalytical techniques for boron analysis were not satisfactory, particularly for the polyhedral boranes. The development of a prompt-γ-boron analysis facility in the HFBR guide hall will be of prime importance in these studies. This technique has a sensitivity of ~ 0.2 μg $^{10}B/ml$, and allows non-destructive testing of biomolecules such as monoclonal antibodies. The prompt-γ facility is unique within the United States.

It is anticipated that these studies will provide a borated (third generation) compound showing physiological binding to tumor, and clearance from normal tissues.

High Energy Resolution Neutron Spin Echo Spectrometer

Neutron Spin Echo (NSE) spectrometers are capable of measuring exceedingly small energy transfers, down to 1 neV. With this resolution, the internal modes of vibration of polymers and the energy widths of critical scattering at phase transitions in organic substances can, for example, be studied. Precision measurements of phonon linewidths or lifetimes can also, in principle, be performed.

The remarkable energy sensitivity of the NSE spectrometer is achieved by using the Larmor precession of the neutron magnetic moment in an applied magnetic field as a clock. The phase of the precessing polarization can be substantially shifted after an inelastic scattering process involving only a minute transfer of energy. Furthermore, because the spin precessional frequency is independent of neutron velocity, a spin echo technique can be employed which allows a wide band of incident neutron energies with correspondingly high intensity but without signficant loss of energy resolution.

NSE instruments have already become established research tools at the ILL, Grenoble, France, although no such machine yet exists in the United States.

Low Energy Time-Of-Flight Spectrometer

The proposed time-of-flight spectrometer would chop a polarized monochromatic incident beam, either in a single pulse mode or according to a more complicated modulation code, electronically with a "π" spin-flipping device. The incident beam would be polarized and monochromated by a combination of polarizing multilayer mirrors and an energy-dependent spin-flipper. Neutrons scattered from the sample would then be time-of-flight analyzed in a conventional manner.

This instrument would be a simple yet versatile tool for inelastic scattering studies of interest to both physicists and biologists. For example, low energy excitations in magnetic systems, the diffusive motion of H in metal hydrides and inelastic scattering from molecules on surfaces are subjects physicists could investigate given an energy resolution of the order of 10 μeV. Problems of special interest to biologists which could be studied with this spectrometer include C-C bending and stretching modes in systems such as viruses, proteins, muscle membrane and protein complexes.

High Resolution Small Angle Neutron Scattering

Small angle neutron scattering provides unique information about polymer structures like the complexes found in biological systems, plastics and lubricants.

The construction of a guide hall and the presence of a cold moderator provides an opportunity to install a versatile, highly efficient small angle spectrometer. The existing small angle instrument was designed to fit into the available space, thereby reducing the resolution and usable flux. With the planned new guide hall, an instrument with a total length of 60 feet can easily be placed, increasing the available resolution and, for the average experiment, increasing the usable flux five fold. The planned instrument with variable collimation, using focusing multilayer monochromators will permit the measurement of very large complexes up to 10,000 Å. For fast and accurate data collection, the spectrometer will be equipped with a large two-dimensional detector and on-line electronics for direct data reduction and analysis. This instrument will also be equipped with a time-slicing device and a chopper that will allow inelastic scattering measurements of moderate resolution, complementing the high-energy resolution of the spin echo spectrometer. The new instrument will allow more sophistication in determining the structure of nucleic acid-protein complexes. It will be used for the structural analysis of polymers and will allow us to engage in the structural analysis of viruses (so far only possible at the Institut Laue-Langevin in Grenoble).

The application of inelastic scattering in Biology is in its infancy. Only a few papers have been published, but it is clear that significant insights into the dynamics of biological systems can be obtained by dynamic neutron experiments. Of particular interest is the possibility to examine the motion of a macromolecule as a function of biological activity.

Crystal Spectrometer

The proposed crystal spectrometer for chemical crystallography would employ three advanced position-sensitive neutron detectors. These two-dimensional multi-wire counters would be filled with a gas containing ^{3}He, and would dramatically increase the rate of data collection. Runs presently requiring up to one month on a conventional instrument with a single counter thus could be completed within a few days. It would be possible to carry out many additional experiments on complicated systems, such as transition metal hydrides, metal cluster compounds and zeolites, among others. Work currently being pursued in these areas is leading to highly precise structural data, with interatomic distances often being determined to within one part per

thousand. The additional data that would be made available by the multi-detector instrument would be of great value in understanding chemical bonding in zeolites, metal clusters and other organometallic systems which are of direct relevance to both homogeneous and heterogeneous catalysis. With the addition of position-sensitive detectors, there should be exciting new opportunities for studying the kinetics of solid state reactions and the response of crystals to stimuli such as electric fields. The new neutron crystal spectrometer, together with the chemical crystallography instrumentation at the NSLS X-ray source, would constitute an unparalleled national resource for structural chemistry research.

Positron Facility

The high thermal flux available in the reactor will be used to produce sources of ^{64}Cu in the 0.1 - 10 kCi range. These sources will permit the production of variable energy positron beams having 10^2 - 10^4 times the current of any of the beams presently operating (on the order of 10^8 - 10^{10} positrons per sec). Because of the very high levels of radiation involved, these sources cannot be readily transported beyond the immediate vicinity of the HFBR. Representative experiments that would be undertaken using a high flux variable energy positron beam of the type described herein include several exciting prospects. We have already proposed the first studies of the interactions of neutral positronium atoms with clean surfaces, with plans to measure positronium diffraction. Momentum distribution of electrons residing at the surface will be measured using the angular correlation technique on the annihilation radiation resulting from electrons annihilating with positrons bound to surfaces in an image potential. Other experiments include measurements of surface magnetism, positron stimulated desorption of surface impurities, positron stimulated Auger electron spectroscopy, high-precision spectroscopy of the positronium atom as a means of testing two-body formulations of QED, and studies of eleastic and inelastic scattering of positrons and positronium reflected from or emitted through various well-characterized surfaces. Moreover, a number of promising future studies should become feasible using the new machine. Construction of a high spatial resolution positron microscope should be within our reach in the next few years. Such an apparatus would greatly enhance the existing capabilities of imaging defects on surfaces and in thin films.

The test beam is already under construction on the operations level of the reactor. Several disadvantages exist; in the present location, for example, every experimenter and technician needs either to have an "L" clearance or be escorted while working on the beam, which has turned out to be a critical problem both in time and expense. In the new area proposed in the guide hall, no restrictions concerning clearance would be necessary and more space would be available, permitting larger experimental systems, as well as opening the way to splitting the beam to feed a numnber of experiments simultaneously. Several useful support facilities which are critical, none of which can be developed on the operations level, could be made available, among them a more flexible overhead crane, exhaust hood, water, sample cleaning and preparation facilities, overhead baking facilities for the UHV chambers in the beamlines, and larger on-line computing and data collection systems. These enhancements would greatly expand the scope and number of experiments feasible using the new location.

Triple Axis Spectrometer

The original plans for the HFBR expansion did not include the relocation of the present triple axis spectrometer situated at the cold moderator beam, H9A. Since those plans were formulated, it was realized that a considerable increase in intensity can be achieved by redesigning the instrument and moving it into the proposed guide hall. This move has been urged by several current users of the existing triple axis instruments including those who have had experience with the H9A instrument. The new spectrometer will be based upon the H4M instrument which is currently being built under the auspices of the US-Japan collaboration.

The main advantage of the new H9A spectrometer will include a lower incident neutron energy and a high flux at the sample due to a larger beam size and better focusing capabilities with a single monochromator. A new flexibility will be provided due to the tanzboden design. The range in energy and momentum transfer of the new H9A spectrometer will be similar to that of the Grenoble IN12 spectrometer.

Neutron Guide Tubes

A. Nickel Coated Guide Tubes. The effectiveness of neutron guides in transporting thermal and cold neutrons over distances of the order of 10-100 m is now universally recognized. The main advantages of neutron guides are: 1) they give large intensity gains over non-reflecting collimators since they can transport neutrons without loss in solid angle, 2) curved guides can be used to filter out fast neutrons and gamma radiation, 3) neutrons can be transported to spacious experimental regions where the background is expected to be lower.

The solid angle of the beam transported by a guide tube is determined by the critical angle of neutrons for the material of the coating. Conventional guide tubes are made from plates of glass thinly coated with nickel. The critical angle per unit wavelength for such a surface is $\theta_c/\lambda = 0.097$ rad Å^{-1}, this being the largest value of readily available mirror materials. The thickness of the nickel film should be about 1,000 Å to keep the reflection losses below 2%.

B. Multilayer Supermirror Guide Tubes. Thin film multilayer monochromators, made by depositing thin films of two materials in an alternating sequence on a glass substrate, have been developed at Brookhaven and are presently in use at two stations. It is proposed that "supermirrors" be made by introducing a continuous gradation in thicknesses of the films, such that the greater d-spacing gives rise to a reflection coincident with the critical-angle reflection from the substrate. The supermirror will then act as a total reflection surface with an effective critical angle $\theta_c/\lambda = 0.465/d_{min}$ rad Å^{-1}, where d_{min} is the smallest d-spacing in the supermirror. For $d_{min} = 50$ Å, this gives $\theta_c/\lambda = 0.533$ deg Å^{-1}. The effective critical angle for such a supermirror will be five times that of nickel, resulting in a very large increase in intensity. The gain factor in neutron flux transported by a guide tube over that observed at the end of a non-reflecting collimator is proportional to the solid angle of the beam transmitted by the guide which, in turn, is proportional to the square of the critical angle. The actual gain in intensity will depend on all the geometrical parameters.

A good supermirror should have its bilayers deposited in a way so that the reflectivity is greater than 0.90 for all angles up to the critical angle. Fabrication of such supermirrors will require substantial effort in research and development. O. Scharpf and T. Ebisawa et al. have shown the feasibility of making supermirrors. However the reflectivity of their supermirrors was not uniformly high over the range of interest. Our setup uses RF sputtering for making thin films and can give uniform and stable deposition rates over a long period. Unlike in a multilayer monochromator, the number of layers in a supermirror has to be kept to a minmimum to avoid absorption losses. This will involve searching out proper deposition materials and parameters for making uniform, non-globular films with small interdiffusion between layers. Complete automation of the system will be required for a) sensing and controlling the parameters which affect the deposition rate or the quality of films, and b) changing the thickness of the layers in a predetermined manner. Each supermirror will then be tested with a neutron beam, and its characteristics compared with the expected values.

Substrates of the mirrors for waveguide sections should have minimum microscopic surface defects and macroscopic roughness or waviness. Specially polished borated plate glass will be used for depositing multilayers.

C. Waveguide Assembly. Neutron guides will be assembled in small (about 30 cm long) segments, and these segments will be aligned to form the guide tube. A polygonal approximation will be made for the curved guide, and each section will be offset by a fixed angle from the one preceding it. The supporting tables for the guide tubes will be made of a material with small thermal expansion such as granite. The assembled waveguides will be covered with shielding layers of boron epoxy, steel and lead.

4. Cost Estimate Guide Hall Facility
(In Thousand Dollars)

1.	Conventional Construction (Ammann and Whitney)		$13,640
	a. Site work	$ 244	
	b. HFBR building modifications	329	
	c. New addition (58,000 sq. ft. at $163/sq ft.	9,456	
	d. Site utilities	337	
	e. Special equipment (cranes, etc.)	1,634	
	f. Design and engineering	1,500	
	g. Standard equipment	140	
2.	Scientific Stations		10,704
	a. Powder diffractometer (Cox)	852	
	b. Backscattering spectrometer (Axe)	1,183	
	c. Nuclear physics station (Casten)	912	
	d. Medical physics prompt γ station (Fairchild)	70	
	e. Spin echo (Shapiro)	1,356	
	f. Time-of-flight instrument (Majkrzak)	1,292	
	g. Small angle scattering (Schneider)	1,316	
	h. Crystallography (Koetzle)	1,267	
	i. Positron facility (Lynn)	1,715	
	j. Triple axis spectrometer (Shirane)	741	
3.	Reactor Plugs (Rorer)		813
	a. H3 plug (thermal)	313	
	b. H9 cold moderator	500	
4.	Neutron Guides (Schoenborn/Axe)		1,423
	a. Thermal guides (supermirrors)	723	
	b. Cold guides (Ni)	700	
Guide Hall Facility in $ FY 1984			26,580
Contingency and escalation (Completion - end of FY 1989)			8,320
Total Cost Guide Hall Project			$34,900

5. Users Policy

A. Participating Research Teams

The policy for utilization of the HFBR is designed to enable scientists at Brookhaven, other national laboratories, universities and industrial laboratories to cooperate in the utilization of existing spectrometers and in the design, fabrication and utilization of new instruments. Research should be conducted with a minimum of formal administrative interaction and with maximum room for spontaneous development. In order to achieve these objectives, present and future experimental instruments at the HFBR will be divided into two categories--general user facilities, and a number of spectrometers managed, designed and/or instrumented by Participating Research Teams (PRT's). Such a policy has been in effect at the NSLS since its inception, and works well. Its adoption for the HFBR produces a unified approach for the two large facilities.

A PRT will consist of a group of qualified scientists with common research interests. In return for their management and development of spectrometers, the PRT will be given priority usage of those spectrometers for a maximum of three quarters of the scheduled beam time.

Non PRT members have access to the general users facilities and to the unawarded fraction of time on the spectrometers assigned to the PRT's. Non-PRT members will not be required to enter into a collaboration as a condition for using a PRT spectrometer.

A Program Advisory Committee with broadly based membership from outside the Laboratory and within gives advice to the Director on the general utilization of the HFBR, the formation of PRT's and the approval of specific proposals for experiments.

B. Users Profile

The following tables illustrate the distribution of users of the HFBR for 1982.

Table 1

Discipline	Number of Users
Physics	115
Chemistry	58
Biology	56
	229

Table 2

Origin	Number of Users
Brookhaven	42
Other DOE Laboratories	11
Other Government Laboratories	5
Universities	102
Industry	13
Foreign	55
Other	1
	229

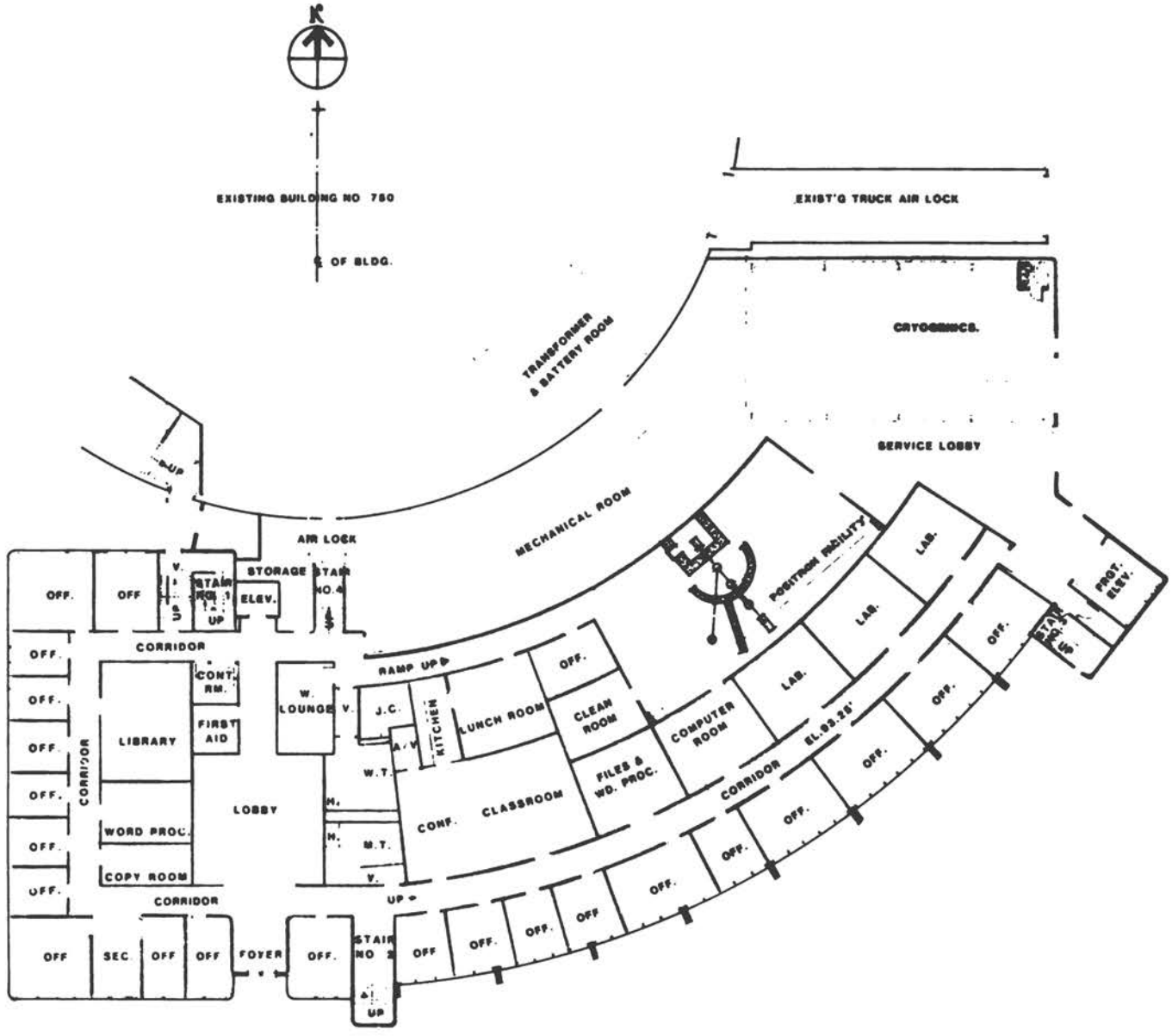
6. Laboratory Environment

Brookhaven National Laboratory was established in 1947 as a multidisciplinary research institution with emphasis on the utilization of large-scale facilities by scientists at the Laboratory and from the outside. There is a long-established program for users and short-term visitors, who are accommodated at apartments and dormitories at the Laboratory.

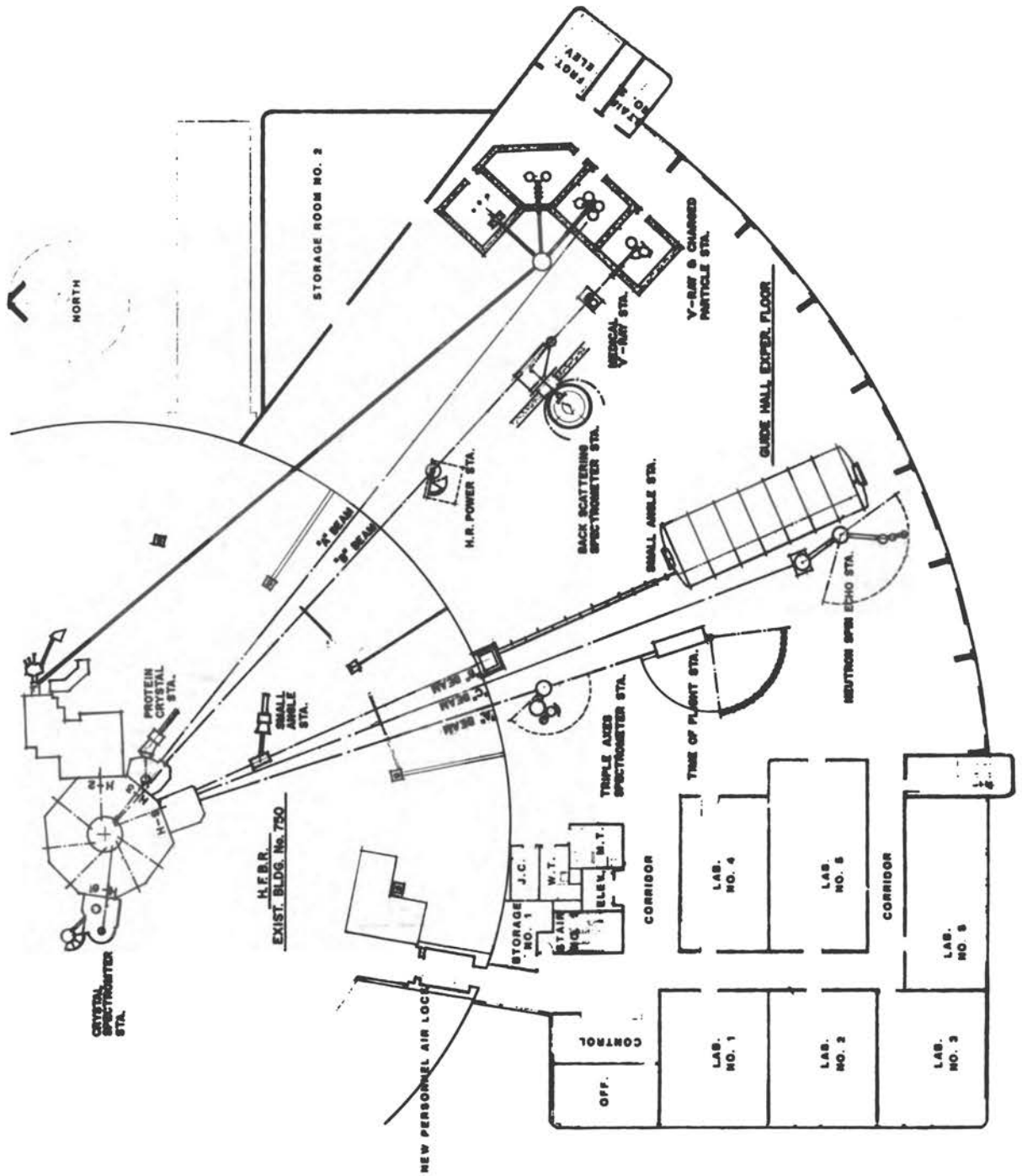
The Instrumentation Department and the Central Machine Shops have resources and extensive experience in the design and fabrication of instruments for research at large facilities. The Central Scientific Computing Facility operates two Control Data 6600, one Cyber 76 and one DEC VAX 11/780 computers which are extensively used for data analysis. The scientific departments have engineering, design and technical support staff with current experience in building spectrometers for neutron scattering research.

Brookhaven's scientific staff carry out research at all of the major facilities. It has been the general experience that a strong in-house program is an essential ingredient for the smooth and effective performance of experiments by all users.

Brookhaven is the only laboratory in the world with a neutron source and a synchrotron light source at the same site. The advantages of this have been recognized in discussions of a site for the European Synchrotron. There is already an interaction between research programs related to the HFBR and the NSLS, and this will increase as the NSLS comes into full operation. It would be greatly enhanced by the expansion of the neutron scattering program envisaged in the HFBR Guide Hall proposal.



GROUND FLOOR PLAN
HIGH FLUX BEAM REACTOR BUILDING ADDITION



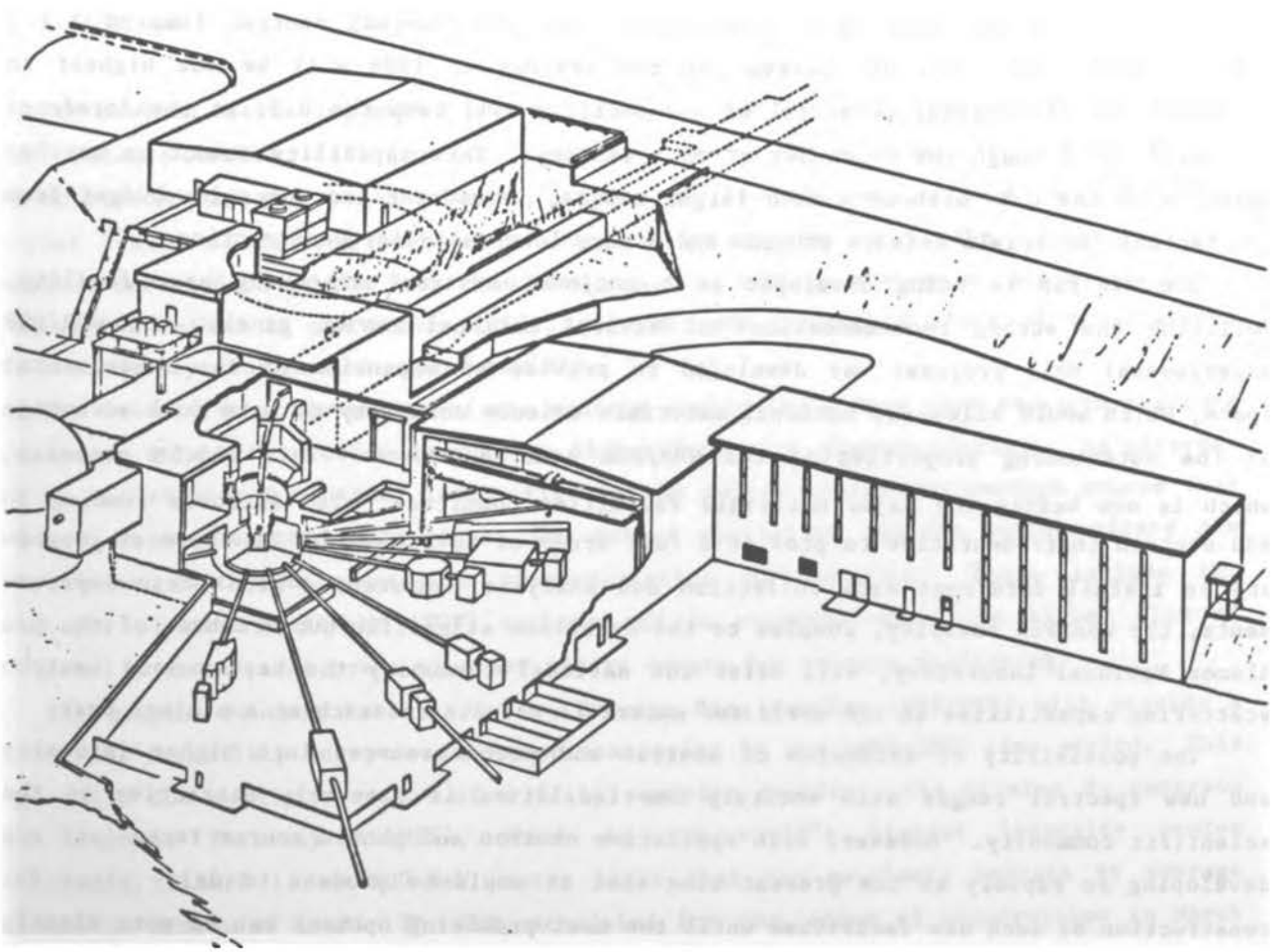
2ND. (EXPERIMENTAL) FLOOR PLAN
HIGH FLUX BEAM REACTOR BUILDING ADDITION

WNR/PSR EXPERIMENTAL HALL EXPANSION

Presentation to Major Materials Facilities Committee
Subpanel on Neutron Scattering

February 26, 1984

Los Alamos National Laboratory



EXECUTIVE SUMMARY

The power of neutron scattering methods for condensed matter research continues to grow as new techniques, particularly those associated with pulsed spallation sources, are developed and applied. Higher pulsed neutron source intensity will make possible a much broader range of techniques, allow major improvements in resolution, and increase productivity for the developed time-of-flight methods. The pulsed neutron intensity that can be achieved in the immediate future at the WNR/PSR facility of the Los Alamos National Laboratory will make possible a research program fully as diverse and productive as that of the best steady-state reactors. The WNR/PSR pulsed neutron scattering program will complement the reactor programs by investigating the new energy and momentum transfer range offered by the high epithermal flux, by utilizing the time-of-flight method with the high peak thermal flux, and by exploring the potential of the pulsed source for cold neutron research. The peak thermal neutron flux of 1.7×10^{16} $n/cm^2 \cdot sec$ that will be achieved at the WNR/PSR in 1986 will be the highest in the world and the upgrade potential of the facility will keep the U.S. at the forefront of this field through the remainder of this century. This capability cannot be matched anywhere in the U.S. without a much larger capital investment and operation budget from the national materials science program and a very long delay for construction.

The WNR/PSR is being developed as a national neutron scattering user facility. Following the strong recommendations of several national review panels, the WNR/PSR Experimental Hall proposal was developed to provide an expansion of the experimental space, which would allow the national materials science community to take full advantage of the outstanding properties of the WNR/PSR neutron source. This $15.5M proposal, which is now before the Major Materials Facilities Committee, also includes funding to add neutron instrumentation to provide a full array of spectrometers to the user program and to install forefront data collection and analysis computers. With these improvements, the WNR/PSR facility, coupled to the excellent scientific support base of the Los Alamos National Laboratory, will offer the national community the best pulsed neutron scattering capabilities in the world for materials science research at a minimal cost.

The possibility of extension of neutron and photon sources into higher intensity and new spectral ranges with entirely new facilities is extremely attractive to the scientific community. However, both spallation neutron and photon source technology are developing so rapidly at the present time that it would be prudent to delay plans for construction of such new facilities until the most promising options can be more clearly established. We recommend full development and exploitation by the materials science community of the best of the existing and developing neutron and photon sources. We urge support for the WNR/PSR Experimental Hall project as the key element in providing the national community with the world's best pulsed neutron scattering facility for materials science research.

I. INTRODUCTION

The WNR/PSR facility nearing completion at the Los Alamos National Laboratory is a pulsed spallation neutron source for neutron scattering research in condensed matter science. When compared with other US and foreign neutron sources currently under construction or proposed, it is the only existing facility that can keep the United States competitive in pulsed neutron scattering research through the remainder of this century. The peak thermal neutron flux of the WNR/PSR in 1986 will be 1.7×10^{16} n/cm^2•sec, which is almost two orders of magnitude over present pulsed source capabilities in the U.S. The proposal before the Major Materials Facilities Committee would provide for the expansion of an experimental hall, and the provision of instrumentation and computers, which are essential to exploit this opportunity for U.S. materials science research.

II. BACKGROUND

The neutron scattering method has a record of outstanding contributions to condensed matter science (solid state physics, chemistry, materials science, biology). This is well-documented in the recent (draft) report of the National Academy of Sciences, "Current Status of Neutron Scattering Research and Facilities in the United States," hereafter referred to as the Rush Committee report. Neutron scattering has developed as an essential method in the above fields, and the user demand and range of applications will undoubtedly continue to expand rapidly.

The scientific achievements of the neutron scattering method with research reactors have led to a rapidly growing demand for higher intensity neutron sources. An alternative to the reactor for higher intensities is the pulsed spallation neutron source that is based on accelerator technology. The pulsed spallation neutron source offers new capabilities that complement the characteristics of reactors. These include the advantages of time-of-flight (TOF) methods and an orders-of-magnitude higher flux of epithermal neutrons that opens up a new energy domain for neutron scattering.

The Weapons Neutron Research/Proton Storage Ring complex (WNR/PSR) will provide a world-class capability for pulsed neutron scattering in the 1985-2000 time period. This is possible due to the presence of a truly superior facility, the Clinton P. Anderson Meson Physics Facility (LAMPF), which is the world's highest intensity proton accelerator. LAMPF is an 800-MeV proton linac that can routinely operate at average currents in excess of 1 mA. The PSR, scheduled for completion of construction in March 1985, will accumulate LAMPF proton beam into pulses appropriate for neutron scattering. The present PSR schedule is to inject its first protons in early 1985 and to achieve 12-Hz, 270-nsec proton pulses with an average current of 100 μA to the neutron scattering program by September 1986. Although the capability in 1986 will already be

world-class, the LAMPF/WNR/PSR complex has the potential for significant upgrades, which would maintain this status until the end of this century.

The pulsed neutron scattering research program at Los Alamos National Laboratory was started in 1978 with the goal of developing the WNR/PSR facility into a world-class center for pulsed neutron scattering research in materials science. This effort received a strong impetus in 1980 from the report of the Neutron Scattering Review Panel chaired by W. Brinkman of Bell Laboratories. The WNR/PSR effort was reviewed again by the Pulsed Neutron Sources Review Panel appointed by the Division of Materials Sciences of BES/DOE in 1982. The origin of the construction proposal before the Seitz committee lies in the recommendations of this report, from which we quote:

> "One of our principal conclusions is that optimal use should be made of DOE resources to ensure a natural, gradual shift to and buildup of the Los Alamos facility by the 1986-87 timeframe. At that time, the WNR/PSR facility is scheduled to achieve an order-of-magnitude increase over current US pulsed source capabilities. It is important to recognize that an increasing financial commitment by the Materials Research Division is necessary for the success of the WNR/PSR. We emphasize that the experimental area is small and accessibility is limited, and we consider it essential that an expansion of the experimental area making it suitable for a national facility of this magnitude be undertaken." (The underline is our emphasis.)

Subsequent to this report, we developed a construction proposal that provided for a major expansion of the experimental floor space, for additional neutron scattering instrumentation, and for a new computer and data acquisition system. This proposal was reviewed in January 1983 by a user committee chaired by M. Rowe of the NBS, and their recommendations were incorporated into a Schedule 44 proposal that was submitted to the DOE in March 1983. This panel concluded:

> "...The current experimental area is totally inadequate for a facility that will undoubtedly be the premier pulsed neutron facility in the USA and one of the best in the world in the 1985-95 timeframe."

> "The Los Alamos staff has produced a very good overall design. In particular, the expanded facility should greatly facilitate the execution of experiments. Further, it has the promise of providing a comfortable, aesthetically pleasing environment that will attract users from both the national and international communities. We would emphasize, however, that we consider the proposed expansion to be the minimum necessary to make the WNR/PSR acceptable as the US national pulsed neutron facility and we would not like to see any regression in the plans."

The Los Alamos proposal before the Seitz panel is a low-cost construction project that would provide an excellent experimental area, dedicated to neutron scattering, and would be capable of handling future increases in neutron source intensity that are possible with the WNR/PSR. This plan allows the neutron scattering program to go forward without interference with other programs, such as national defense and nuclear science, thereby retaining the multiple sources of support for the WNR/PSR. This provides the neutron scattering capability to the national materials science community at minimal cost.

III. CONDENSED MATTER SCIENCE RESEARCH AT THE WNR/PSR

A. SCIENTIFIC POTENTIAL OF THE WNR/PSR

The WNR/PSR facility will provide the condensed matter science community with the world's best capabilities in the new domain of energy and momentum transfer provided by the very high epithermal neutron flux. The high peak thermal flux (1.7×10^{16} $n/cm^2 \cdot sec$), combined with the TOF method, offers experimental capabilities in the thermal range that can compete favorably with the best steady-state reactor facilities in the world. In addition, the use of the TOF technique at the WNR/PSR pulsed source offers many characteristics that are complementary to steady state sources.

There are many areas of condensed matter science where an advanced pulsed source, such as the WNR/PSR, is advantageous compared to other methods.

PHASE TRANSITION PHENOMENA - These can be studied by using TOF methods to cover a large range in momentum and energy transfer simultaneously. For example, diffuse scattering can see domain formation, superlattices, amorphous structures, and critical scattering in planes or rods. Inelastic scattering with TOF mathods can be used to conduct surveys of unknown dispersion curves of elementary excitations. TOF methods are particularly useful in the study of phase transitions induced by high pressures, electric fields, or magnetic fields.

HIGH ENERGY EXCITATIONS - The momentum distributions n(p) of quantum solids and fluids (e.g., the Bose condensate in HeII) can be studied by recoil scattering with epithermal neutrons in the impulse approximation limit. The WNR/PSR may play an essential role in unraveling the mysteries of itinerant magnetism through the measurement of high-energy ($50 < \omega < 500$ meV) magnetic excitations such as spin waves and Stoner excitations. It should also be possible to measure presently inaccessible high-energy phonons in materials such as metal hydrides, graphite intercalates, etc. Pulsed sources are already established as the method of choice of high-energy chemical spectroscopy with neutrons.

STRUCTURAL STUDIES - The study of the structure of liquids and amorphous materials is particularly well suited to the WNR/PSR because one can use the high epithermal flux to scatter at large values of Q to get excellent real-space resolution and because the inelastic contributions to the scattering are minimized. The WNR/PSR will play a significant role in the study of low-dimensional materials, because TOF methods permit one to readily integrate over irrelevant dimensions. Pulsed sources, such as the WNR/PSR, are already established as the preferred method for powder diffraction because of the constant resolution function, small d spacings, and high data rates that can be achieved and because of the advanced state of the Rietveld powder profile refinement data analysis method. They may also be revolutionary for single-crystal diffraction, in part because of the ability of TOF methods to measure twinned or multiple crystals or domains and in part because the high data rates of TOF methods may permit the use of very small crystals. These enormously simplify sample preparation requirements.

SPECIAL SAMPLE CONDITIONS - TOF methods are clearly preferred for experiments requiring limited sample access, such as high pressures, or the application of electric or magnetic fields. They are clearly advantageous for pulsed sample environments where the external stress cannot be maintained (e.g., the high intensity laser excitation of a biological sample).

There are other areas of enormous current interest in condensed matter science where the potential of the WNR/PSR needs to be explored.

BIOLOGY, POLYMERS, AND METALLURGY - Cold neutrons are essential to the application of neutron scattering in these areas because of the large scale of the structures of interest. The Rush Committee identified small angle neutron scattering and quasi-elastic scattering at 10-microvolt resolution as areas in which an urgent US effort should be generated to catch up with Europe. Estimates of instrument performance from the SNS indicate that the WNR/PSR with 200 microamperes and an optimized 20K cold H_2 source could come within a factor of two of ILL performance in these areas. In addition, these instruments will have an order of magnitude larger dynamic range than their reactor equivalents. SANS on a pulsed source will automatically provide discrimination against inelastic scattering and have superior q resolution to permit low resolution crystallographic studies of macromolecules. The pulsed source equivalent of neutron spin echo with a larger range would be particularly valuable in the study of relaxation phenomena.

POLARIZED NEUTRONS AND MAGNETISM - Full use of polarized neutrons at a pulsed source is essential for its application to magnetism. Spin modulation techniques may be required to obtain high resolution for high-energy neutrons. At short wavelengths, this will require the development of efficient methods for white beam polarization. In the

longer wavelength region, supermirror technology can be readily adapted to the WNR/PSR facility. Methods for the study of high-energy magnetic and electronic excitations need further development. They require scattering with high-energy neutrons at low q, which introduces problems of available phase space and multiple scattering. However, it is clear that pulsed sources are kinematically favored over reactors for these studies.

DYNAMIC STUDIES - The study of time-dependent phenomena such as the response of a polymer to an applied stress, needs to be fully explored with SANS methods.

The TOF method produces high data rates and large amounts of data, which has usually been regarded as a problem because of computer limitations and the lack of physical interpretation during the course of an experiment. However, with modern computer technology it is now practical to handle these data rates and to process it on line to display the results in physical terms using high-quality graphics.

There is no single number by which one can compare the performance of a pulsed source to a reactor. Direct comparison can only be carried out on an experiment-by-experiment basis. However, it has already been demonstrated that even the weak pulsed sources currently available are already superior to the best reactors for powder diffraction, liquids and amorphous materials diffraction, and vibrational spectroscopy of molecules. At the same time, there is no concept for a pulsed source instrument that will be as flexible as a triple-axis spectrometer at a reactor for the measurement of elementary excitations. A healthy US neutron scattering program will use pulsed sources and steady state sources in complementary ways.

B. WNR/PSR NEUTRON SCATTERING RESEARCH PROGRAM

At the WNR/PSR facility, we have been exploring the scientific potential of pulsed sources, developing novel time-of-flight neutron scattering spectrometers and techniques, and implementing a strong user program.

The outstanding scientific results from the WNR/PSR are in the mainstream of the Rush Committee report. The structure of the first organometallic complex that reversibly binds molecular hydrogen was determined by TOF single-crystal diffraction. This species is regarded as a long sought intermediate step in the catalytic reaction of hydrogen. After many unsuccessful attempts elsewhere, the high-pressure structure of ReO_3, a material that undergoes a compressibility collapse at 15 kbar, was determined at WNR/PSR using the geometrical advantages of the TOF method for special environment single-crystal diffraction. The first model-independent determination of the hydrogen-hydrogen pair correlation function in liquid water, showing a more ice-like structure than molecular dynamic simulations, was accomplished by low-angle scattering with epithermal neutrons and a novel isotope substitution technique. The first systematic study of the vibra-

tional spectra of short intramolecular hydrogen bonds was carried out by inelastic neutron scattering, showing trends of frequency vs. bond length that were different from those of the longer intermolecular bonds. The anharmonic force constants of metal hydrides, particularly NbH, were determined by the measurement of the shifts of high-energy harmonics of the fundamental modes. The high-energy transfer vibrational spectra of hydrogen chemisorbed on Raney nickel and coprecipitated nickel were measured for the first time. The first study of the momentum distributions of atoms in solids (e.g., the anisotropy of carbon atoms in pyrolytic graphite) was accomplished by recoil scattering with high-energy neutrons in the impulse approximation.

The development of novel time-of-flight instrumentation and techniques has also been at the forefront. The first high data rate Be-BeO Filter Difference Spectrometer was brought into operation for chemical spectroscopy and the study of dispersionless modes in solids. The nuclear resonance filter difference method was developed for electron volt spectroscopy. High-pressure single-crystal diffraction was demonstrated for the first time at a pulsed neutron source. This is possible to do with one rotation axis because of the large range in reciprocal space covered in the TOF method. The ability of TOF single-crystal diffraction to study multiple crystals and domains was demonstrated, which is particularly important in the study of phase transitions, by a study of ferroelectric domain formation above and below Tc. The Constant Q Spectrometer was developed for the study of elementary excitations in single crystal samples, with the first observation of phonon dispersion at a pulsed source. A high data rate Anger camera (400-nsec deadtime) for position-sensitive neutron detection with glass scintillators was demonstrated. A high-speed (36,000 RPM) magnetic bearing neutron chopper and control system for phasing were developed. A new instrument design concept for the suppression of sample-dependent backgrounds was developed for liquids and amorphous materials diffraction. We designed a novel two-axis goniometer specifically suited for single crystal diffraction at a pulsed source. Many benchmark experiments on the performance of target/moderator/reflector assemblies were accomplished in the WNR target #2 facility.

C. USER PROGRAM

The WNR/PSR is being developed as a national user facility for research in solid state physics, chemistry, materials science, biology, and polymers. Use of the neutron scattering instrumentation is free of charge for approved proposals from outside scientists if their results are to be published in the open scientific literature. Proprietary experiments may be scheduled with full-cost recovery according to DOE policy.

Formal proposals for experiments are reviewed twice a year by a nationally appointed Program Advisory Committee (PAC). The PAC reviews proposals on the basis of scientific excellence and optimal use of WNR/PSR capabilities. The PAC allocates two-thirds of the

neutron scattering beam time at the WNR/PSR, with the remaining third reserved for Laboratory discretionary usage, programmatic research, and instrument development.

The formal user program was initiated in 1983 with the PAC shared with the IPNS program at Argonne National Laboratory. We expect the user program to grow to approximately 200 visiting scientists per year using 8-10 instruments by 1987. Conferences and workshops are being organized to encourage external use of the facility.

It should be noted that Los Alamos National Laboratory has a long tradition in the use of its research facilities by the external scientific community. Adequate temporary housing and transportation exists for short-term visitors. The presence of a large LAMPF users program (~900 members, including 300-400 from 90 universities) provides an existing mechanism at Los Alamos to handle the expected user load on the WNR/PSR. Users find the Los Alamos area to be a very pleasant place to visit not only because of the scientific atmosphere but also because of the unique cultural, scenic, and climatic features of Northern New Mexico.

IV. WNR/PSR EXPERIMENTAL HALL PROJECT

A. DESCRIPTION

The present experimental area at the WNR/PSR high-current target was designed in 1972 to satisfy the anticipated needs of a defense and nuclear physics program. Although satisfactory for its original purpose, the experimental hall does not have adequate space to handle the requirements of the large national neutron scattering user program that will emerge in 1986 with the advent of the high neutron intensities provided by the PSR.

The present plan will dedicate the high-intensity target area to the materials science research program and shift the defense and nuclear science programs to an existing, but separate, target area.

The proposed construction project at the WNR/PSR consists of three components (refer to Figures 1 and 2), which are described below.

- Experimental Hall Expansion
- Additional Neutron Scattering Instrumentation
- Advanced Computer/Data Acquisition System

Experimental Hall Expansion - We propose to build a large (18,000 sq.ft.) experimental hall on the east side of the facility, with a 15-ton overhead crane and 20-ft. hook height, which increases the available experimental space by a factor of seven. Nine long flight paths (14 m to 50 m) will be enclosed within the hall. Two of these flight paths can be extended as far as 300 m outside the hall for ultrahigh resolution experiments. All of the flight paths can be configured to handle more than one instrument. The total number of beam holes in the biological shield will be 15. Within

this hall, large staging areas for experimental setup and "quiet" rooms for experimenters use will be provided.

We will also build a 17,500 sq.ft. three-story building directly attached to the east hall. This building will house the new data acquisition system, mechanical and electronic shops, sample preparation laboratories, cryogenic laboratories, and offices for users and personnel directly associated with the operation of the user program at the WNR/PSR.

We expect to have about six instruments on the short flight paths in the present hall after the PSR begins operation. We will renovate this area by adding two new access doors and by installing a catwalk system. These minor changes will greatly improve our physical access in this area.

Neutron Scattering Instruments - Our current plan is to develop 8-10 instruments for the WNR/PSR by 1987. Three spectrometers are already fully operational and in the user program. Two to three more are planned for development by 1986 out of existing operations and capital funds. We propose to construct the remaining instruments as part of the construction project under consideration. A description of these 10 instruments is provided in Appendix 1, along with a possible layout in the proposed experimental hall.

Computers and Data Acquisition System - Time-of-flight experiments with the PSR are expected to collect an enormous amount of data ($\sim$1 million resolution elements per instrument) at very high instantaneous data rates (up to 20 Mhz expected). On-line data reduction will be essential so that raw data can be transformed into physical terms, displayed with high-quality graphics, thereby allowing decisions on the progress of the experiment to be made. Peak data rates with the PSR will be 400 times current levels and time average data rates will be 40 times current levels. To handle these requirements, we propose to replace the present system with a modern VAX-FASTBUS system currently under development. This would include a large hub VAX computer for post-experiment data reduction and for interfacing into the ultrahigh-speed computing CRAY capabilities of the Los Alamos Central Computing Facility.

B. CAPITAL COST ESTIMATE/SCHEDULE

The total estimated cost of the WNR/PSR experimental hall project as defined above is $15.5M. These buildings would be completed on a two-year construction schedule. The experimental hall and support building construction is straightforward, not requiring significant architectural and engineering design. The scope and cost estimate of the original project was reviewed and approved in 1983 by DOE. The cost breakdown for the experimental hall project is given in Table 1.

Table 1. Cost Estimate ($K)
(cost to midpoint of construction - FY86 start)

Building Construction	8750
Spectrometers	2500
Computers	1650
20% Contingency	2600
	15500

The building construction portion does not require R&D funds or any increase in Los Alamos staff. The cost estimate for the four neutron scattering spectrometers is based on the detailed cost experience of constructing the first two spectrometers already operational at the WNR/PSR. The cost estimate for the computer system to handle the data acquisition and analysis is based on a prototype under development. To successfully design, construct, and operate the spectrometers for the national user program will require the addition of scientific and technical staff. It is estimated that two scientists and one technician per each instrument will be required for spectrometer development and for operation in the user program. All of the manpower additions have been planned for and their costs are covered in the operational costs for the WNR/PSR discussed below.

V. FACILITIES OPERATION AND DEVELOPMENT

A. WNR/PSR OPERATING COST

Since the facility is multipurpose and multidisciplinary, the costs for operating the WNR/PSR can be shared between the materials science program, defense programs, and other internal Los Alamos programs. The current plan for operating the WNR/PSR calls for 100 μA delivered from LAMPF at no expense to the materials science program for a minimum of 80% of the available LAMPF beam time (∿3500 hours/year). Two-thirds of the neutron scattering time will be scheduled for the user program as discussed earlier.

The plan presented to both Los Alamos and DOE (OBES) management in FY83 called for one-half of the operating expenses to be provided by the DOE materials science program with the other half to come from Los Alamos defense programs and internal research programs. Two-thirds of the neutron scattering research costs would be provided by the DOE materials science program (BES/DMS) with the remaining one-third coming from Los Alamos defense and other internal programs.

When the WNR/PSR is in its fully operational state providing 12-Hz, 100-μA operation, the total operating and neutron scattering research costs associated with the facility will be as summarized in Table 2.

Table 2. WNR/PSR Operations and Neutron Scattering Research Costs[a]

	Facility Operations	Neutron Scattering Research	Total
Total Costs	$5.5M	$4.0M[b]	$9.5M
LANL Programs	$2.8M	$1.3M	$4.1M
Total Costs to BES/DMS	$2.7M	$2.7M	$5.4M[c]

[a] 12-Hz, 100-μA operation, FY85 dollars

[b] Assumes 8-10 neutron scattering instruments in user program along with a staff of 30 FTEs.

[c] In FY84, BES/DMS provides $1.7M for research; total incremental costs to BES/DMS would be approximately $3.6M

B. POTENTIAL UPGRADES OF THE WNR/PSR

The LAMPF accelerator is the world's most intense, high-energy proton source and is capable of simultaneously providing beams to many experimental facilities, including the WNR/PSR.

The WNR/PSR, operating with a 12 Hz, 100 μA, 800 MeV, 270 nsec proton beam, will produce the world's highest peak thermal neutron flux of 1.7×10^{16} n/cm^2•sec. However, because of the existence of LAMPF and the PSR, there is the potential for significant upgrades in both peak and average neutron flux that could be supplied to the national pulsed neutron scattering program. The peak thermal neutron flux could be as high as 5×10^{16} n/cm^2•sec.

These potential upgrades are summarized in Table 3 along with the estimated capital costs and the associated incremental operating costs. The resulting neutron performance of these options is compared to existing sources in Table 4.

Table 3. WNR/PSR Potential Upgrade Costs (FY85 dollars)

Upgrade	Capital	Incremental Operating	
		WNR/PSR	LAMPF
24 Hz, 200 μA	∿$1.5M	$0.2M	∿$1.5M
Fission Booster with 24 Hz, 200 μA	∿$4.5M	$0.7M	zero
40 Hz, 400 μA	$10-20M[a]	$1.0M	[b]

[a] This option can be achieved via several methods that depend on the performance of the PSR and the impact on the LAMPF nuclear physics program.

[b] Incremental operational costs for this option depend significantly on LAMPF operating mode and DOE cost-sharing policy.

In addition to these intensity upgrades, the neutron scattering community has expressed interest in the availability of WNR/PSR for more than six months per year. At present LAMPF operates for approximately six months/year limited only by its nuclear physics operating budget. The accelerator is capable of operating eight to nine months/year and indeed has done so in earlier years. The total incremental costs for operating LAMPF and WNR/PSR for eight-nine months rather than six months at the 24-Hz, 200-μA level is approximately $3M.

Table 4. Pulsed Neutron Source Comparisons

	E_p (MeV)	I_{AVG} (μA)	Freq. (Hz)	Source Strength[a] (n/sec) ($\times 10^{16}$)	Peak Thermal Flux[b] (n/cm^2•sec) ($\times 10^{16}$)
LANL					
WNR/PSR (1986)	800	100	12	1.6	1.7
Potential Upgrades					
Rep. rate increase	800	200	24	3.2	1.7
Fission booster (x3)	800	200	24	9.6	5
PSR upgrade (w/o booster)	800	400	40	6.4	2
Rutherford					
SNS (1986)	800	200	50	3.2	0.8
ANL					
IPNS-1 (1984)	500	12	30	0.1	0.04

[a] Assumes depleted uranium target

[b] Average thermal flux calculated for same target-moderator-reflector configuration for all facilities
Peak thermal flux = average thermal flux/(rep rate x 30 μsec)

C. LAMPF PROGRAM AND UPGRADES

LAMPF has been operational since 1972 and achieved high intensity (∿500 μA) proton beam currents around 1975. The proton beam levels have risen continuously since that time with a record average current of 1300 μA achieved in 1983. LAMPF has clearly exceeded its design goal and is the world's most intense high-energy proton accelerator. It has the potential for providing high-current proton beams until the end of this century.

The present nuclear physics program at LAMPF is addressing important and exciting topics, and major experimental improvements being implemented will provide even more

opportunities to exploit the intense beams of protons, pions, muons, and neutrinos during the next decade. The large 900-member user program is strong and healthy.

Nuclear scientists at Los Alamos and elsewhere in the US and the world are involved in long-range planning for the 1990's for a future accelerator that would supply intense beams of higher energy protons for research with secondary beams of pions, muons, kaons, neutrinos, and antiprotons. One possibility for such an accelerator would be to take ∿100 μA of the existing 800-MeV, 1-mA proton beam from LAMPF for injection into a synchrotron/stretcher ring system that would boost its energy to 10-30 GeV. LAMPF would continue to operate under such a scenario as an injector to the PSR with all the options discussed in the previous section being unaffected.

If a new facility were not built for nuclear and particle physics, the existing LAMPF accelerator would still be capable of providing high-intensity proton beams for the WNR/PSR until the end of the century. The costs associated with the maintenance and operation of the accelerator (e.g., electrical power, klystrons, magnets, operators, technicians) would have to be borne proportionately by the materials program if the nuclear physics program were no longer present. The operating cost would depend upon exactly what level of proton current the materials science community wanted to extract from LAMPF and for how many months. The most important fact for the present discussion is that LAMPF exists and is clearly a major capital investment for the nation's scientific community and as such is a major national resource for whatever science can be pursued. Operational costs of LAMPF as a materials science accelerator would not be significantly different from a new accelerator of comparable capability.

VI. SCIENTIFIC SUPPORT SYSTEM AT LOS ALAMOS

Los Alamos National Laboratory is one of the largest multidisciplinary research and development organizations in the U.S. It has 7000 employees of which there are ∿1400 Ph.D.'s including ∿700 Ph.D.'s in physics. Laboratory scientists are involved in a variety of basic and applied research programs in physics, mathematics, chemistry, materials science, life sciences, earth and space sciences. These research efforts are supported by a large technology base in engineering, computer science, and mechanical and electronic engineering design and fabrication.

There are significant research programs at Los Alamos whose activities will support the development of a strong, diversified neutron scattering proram at the WNR/PSR. These include condensed matter research in the Physics Division, the Materials Science and Technology Division, the Electronics Division, the Dynamic Testing Division, and the Theoretical Division. Current areas of condensed matter research include electron dynamics in solids, particularly superconductivity in the actinides and rare earth elements, phase transitions induced by static and dynamics pressures, studies in metallurgy such as hydriding and structural ceramics, and research into fast, photo-

conductive devices, and superlattices. The programs in biology and medicine that are carried out in the Life Sciences Division are planning a strong interaction with the WNR/PSR scattering program and have recently hired a life scientist with neutron scattering background to initiate this effort. Interactions with the neutron scattering program are already occurring with research programs in the Chemistry Division, particularly in the area of molecular structure and dynamics, and in the Materials Science and Technology Division, particularly in actinide research.

During the past five years Los Alamos National Laboratory has established a firm commitment to a major research and development effort in materials science in support of its long-term mission in national defense and energy. Although materials research has traditionally played a key role in Laboratory programs during its 40-year history, it was recognized that significant advances in defense and energy programs during the next 20 years will require innovative solutions to challenging materials problems. Since multi-disciplinary research and development will be key to solution of many materials problems, the Laboratory formed a Center for Materials Science (A. Clogston, Director) in 1981 to provide a focus for Laboratory-wide efforts in materials research and to increase our interactions with external researchers in universities, industry, and other national laboratories.

To enhance our present capabilities in materials science, state-of-the-art tools and techniques are being developed for use by Los Alamos scientists in a variety of disciplines such as physics, chemistry, metallurgy, etc. Currently we are developing x-ray and UV beam lines at the National Synchrotron Light Source at Brookhaven. We have made modifications to our Van de Graaff accelerator laboratory to enhance its ion beam capabilities for surface science studies. We are planning to construct a major materials science laboratory that will house such instrumentation as x-ray microscopes, ion implantation devices, EXAFS, LEED, and Auger spectrometers. We are also investigating the potential of laser harmonics and free electron lasers as tunable UV sources for materials research.

In addition to the Center for Materials Science, the Laboratory has a Center for Non Linear Studies (A. Scott, Director), an Institute for Geo- and Planetary Physics (P. Coleman, Director), and a newly formed Center for Theoretical Astrophysics. These scientific centers also provide a focus for Laboratory-wide interdisciplinary research on their particular scientific theme.

In terms of scientific training, the Laboratory has had a long-standing and very successful postdoctoral program. There are both distinguished postdoctoral fellow positions (J. Robert Oppenheimer fellowship, Bernd Mathias fellowship) for outstanding young scientists and other postdoctoral positions supported either by a special Director's fund or by the scientific divisions. Currently there are 80 postdoctoral fellows at Los Alamos.

For graduate-student training, the Laboratory has interactions with both the University of California campuses and the members of the Associated Western Universities. There currently are ∿30 graduate students doing full-time research at Los Alamos. There is also a summer student program that involves both graduate and undergraduate level students in the scientific research programs. Typically there are ∿150 students in the summer program.

The Laboratory has excellent scientific research and support facilities that would provide significant opportunities for scientists engaged in neutron scattering research at the WNR/PSR. The Laboratory's Central Computing Facility (CCF) has the world's most powerful scientific computing capability, including four CRAY-1's and a CRAY-XMP. The long-range computing plan calls for two CRAY-1's in the non-classified environment by 1985 with future extensions to two non-classified Class 7 computers by 1989. In addition, the CCF supports the operational needs of a large VAX computing network at Los Alamos. The VAX is the standard research computer at most laboratory research facilities including the WNR/PSR. There are ∿50 VAX computers in use throughout the Laboratory.

In general, Los Alamos possesses an excellent and diverse scientific support capability, which already exists primarily in support of its applied programs but which is also utilized by its basic research programs. The presence of a national neutron scattering program at the WNR/PSR will greatly enhance the Los Alamos scientific effort but the users of this facility will also greatly benefit from the existence of a multi-disciplinary scientific support structure that already exists at the Laboratory.

VII. RECOMMENDATIONS

A. THE NATIONAL CONDENSED MATTER RESEARCH PROGRAM

Among the major facilities for condensed matter research, synchrotron light and neutron sources are the most versatile. While facilities for such research are expensive to construct and operate, costs for the typical experiment can be reduced to a modest level since these facilities can accommodate many experiments simultaneously and an effective user program enables them to serve a steady flow of experimenters in an orderly manner. The US has had excellent reactor neutron sources for many years. Several facilities for synchrotron light research are in operation or nearing completion and a world-class pulsed neutron facility is nearing completion at Los Alamos. However, none of these facilities are adequately staffed or sufficiently well equipped for full exploitation. We recommend that the highest priority be given to the completion and full instrumentation of those existing and developing facilities, which offer the greatest source strength and versatility for condensed matter research. More specifically, we urge the following:

- Full development and exploitation of the exciting new research opportunities in pulsed source neutron scattering at the WNR/PSR, which offers the greatest source intensity at the lowest capital and operations cost to the national materials science program.
- Addition of a neutron guide hall with instrumentation to the existing research reactor that is best suited for cold neutron research.
- Full development and exploitation of the most promising of the existing and developing synchrotron light sources by providing the resources necessary to bring them to full operational capability with a full complement of instrumentation.

The possibility of extension of neutron scattering and synchrotron light into higher intensity and new spectral ranges with entirely new facilities is extremely attractive to the scientific community. However, both spallation neutron and photon source technology are developing so rapidly at the present time, that it would be prudent to delay plans for construction of such new facilities until the most promising options can be more clearly established and the present facilities fully exploited.

In order to assure that the best options are in-hand for the next generation of sources, we recommend that the national condensed matter research program set aside a few percent of its research and operations budget for R&D on new source development.

B. THE LOS ALAMOS WNR/PSR PROGRAM

The $15.5M cost to provide the WNR/PSR with an enlarged experimental hall is a very cost-effective method to provide the US with a world-class pulsed neutron scattering capability now. Since the potential exists for considerable upgrades to the WNR/PSR neutron intensity it would be possible to maintain this preeminence until the end of the century, at a minimal cost compared to other alternatives.

We recommend the following specific funding actions to fully exploit the exciting science at the WNR/PSR:

- The earliest possible funding for the Experimental Hall Project so that the exploitation of the power of the PSR will not be delayed past its completion date in 1986.
- The initiation in FY85 of sustained funding of $2.7M for WNR/PSR operations in order that PSR tune up and operator training not delay the use of the PSR for the national user program.
- An increment of $1.0M of research funds in FY85 for neutron scattering research support at the WNR/PSR bringing the total research support from the BES/DMS to the required $2.7M level.

APPENDIX I - WNR/PSR Neutron Scattering Instruments

The selection of instruments at the WNR/PSR facility must fulfill several requirements: 1) They must meet the scientific needs of the user community. This has been discussed most recently in the Rush committee report; 2) They must take advantage of unique pulsed neutron source characteristics such as the high epithermal flux, high-resolution experiments on long flight paths, and the large dynamic range in energy or momentum transfer; 3) They must be well engineered so that the WNR/PSR can be an efficiently run national user facility, accessible to scientists who are not especially knowledgeable in neutron scattering methods. Yet the instruments must also be developmental, because only in a few areas has there been relevant experience in TOF neutron scattering research heretofore. The current plan for the first 10 instruments at the WNR/PSR, in their order of development, is as follows:

1. SINGLE CRYSTAL DIFFRACTOMETER (SCD) - Crystallographic studies of single crytal samples, with up to 20 A^{o} unit cell dimension, by the Laue TOF technique.
2. FILTER DIFFERENCE SPECTROMETER (FDS) - Inelastic neutron scattering studies of optic modes in solids and chemical spectroscopy, especially at epithermal energies, with 5% energy resolution.
3. CONSTANT Q SPECTROMETER (CQS) - Coherent inelastic neutron scattering studies of elementary excitations, such as phonons and magnons, in single crystal samples, particularly at high-energy transfers. Note that this instrument can readily be configured for polarization analysis by the use of a white beam filter and a Huesler analyzing crystal.
4. NEUTRON POWDER DIFFRACTOMETER (NPD) - A high resolution (0.1%) instrument for crystallographic studies of powder samples for analysis by Rietveld powder profile refinement methods.
5. LIQUIDS AND AMORPHOUS DIFFRACTOMETER (LAD) - Low resolution (0.7%) structural studies of liquids and amorphous materials, particularly at low scattering angles using epithermal neutrons to minimize inelasticity corrections. Also special environment powder diffraction, including the use of low angle detectors for magnetic diffraction experiments.
6. HIGH RESOLUTION CHOPPER SPECTROMETER (HRCS) - Inelastic neutron scattering studies of elementary excitations in isotropic samples, such as powders, liquids, and amorphous solids. The instrument will be initially configured to have an operating range from 0.1 eV to 1 eV incident energy with 1% energy resolution. Might later be reconfigured for higher energy electron volt spectroscopy.
7. ELECTRON VOLT SPECTROMETER (EVS) - Inelastic neutron scattering studies at 0.2 to 10 eV energy transfer, particularly studies of magnetic and electronic excitations at small Q and momentum distributions at high Q. May use a variety of techniques involving nuclear resonances to define energies.

8. SMALL ANGLE DIFFRACTOMETER (SAD) - Small Q (.001 < Q < 1 A^{o-1}) diffraction for structural studies in biology, metallurgy, polymers, and chemistry.

9. BACKSCATTERING SPECTROMETER (BSS) - Quasielastic scattering at very high resolution (1 μeV < ΔE/E < 20 μeV) for studies of diffusion, tunneling modes, spectroscopy of large scale motions in macromolecules, etc.

10. POLARIZED NEUTRON EXPERIMENT (POL) - White beam (up to 1 eV) polarized neutron experiment using nuclear polarization at mK temperatures as a filter. Can be either diffraction or inelastic scattering by the use of correlation techniques. Studies of magnetic materials, separation of coherent and incoherent scattering, or high resolution electron volt spectroscopy by spin precession.

A possible layout of 15 instruments at the WNR/PSR facility is shown in Fig. 3. Flight paths 9-11 utilize a 20K-hydrogen moderator using guide tube technology. We intend to fully exploit the potential of the WNR/PSR facility for cold neutron science. Flight paths 15, 1, and 2 will be developed on a strongly decoupled (up to 30 eV) moderator optimized for high resolution at epithermal energies. These flight paths can be extended up to 300 m. The other five instruments shown in the figure are tentative (LRCS Low Resolution Chopper Spectrometer, CMS Crystal Monochromator Spectrometer, NSE Neutron Spin Echo, SEPD Special Environment Powder Diffractometer, HRSCD High Resolution Single Crystal Diffractometer). It should be possible to place more than 15 instruments in the hall through the use of multiple collimation systems or neutron guides (both thermal and cold) in the large beam holes.

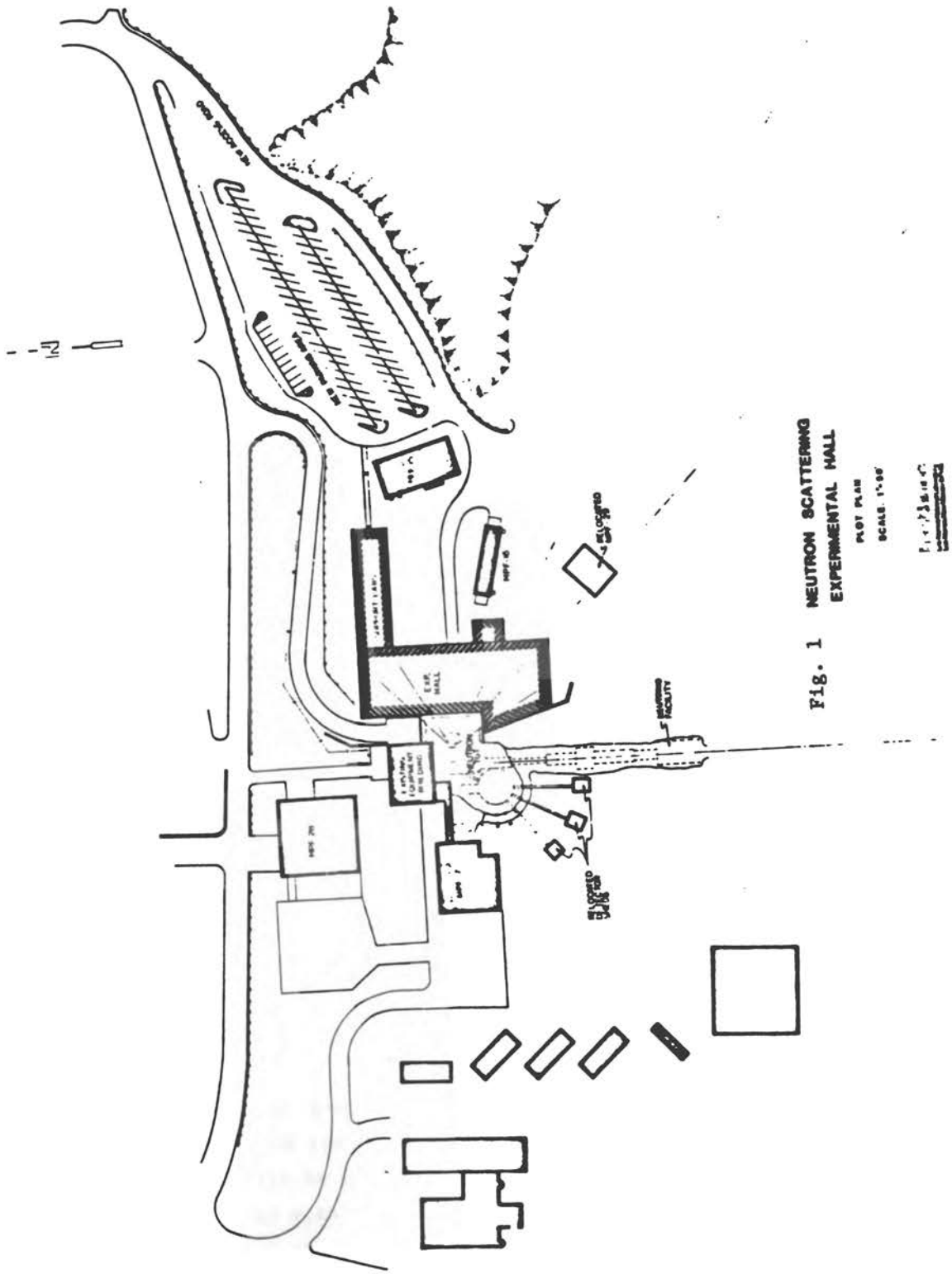


Fig. 1

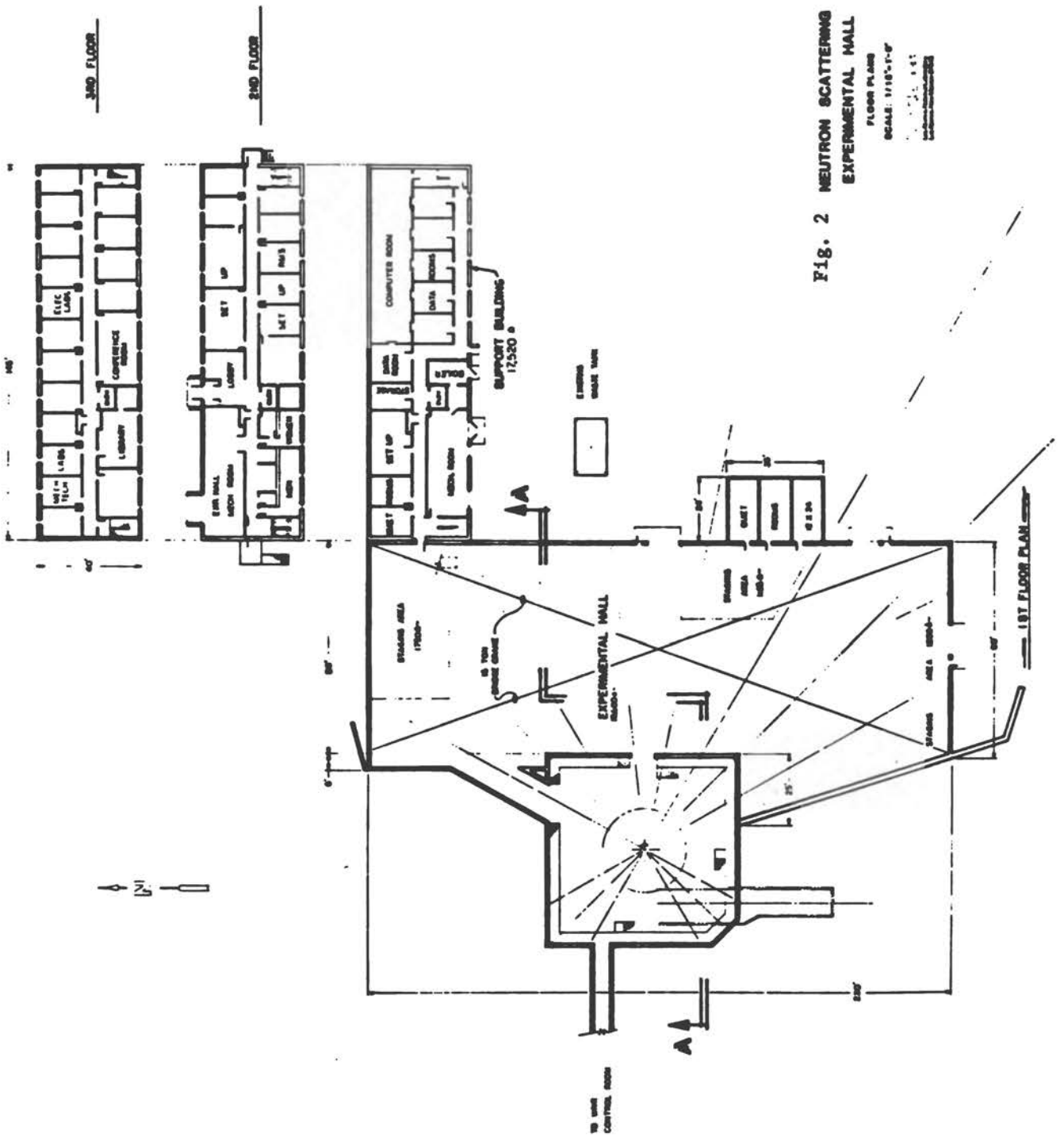


Fig. 2 NEUTRON SCATTERING EXPERIMENTAL HALL

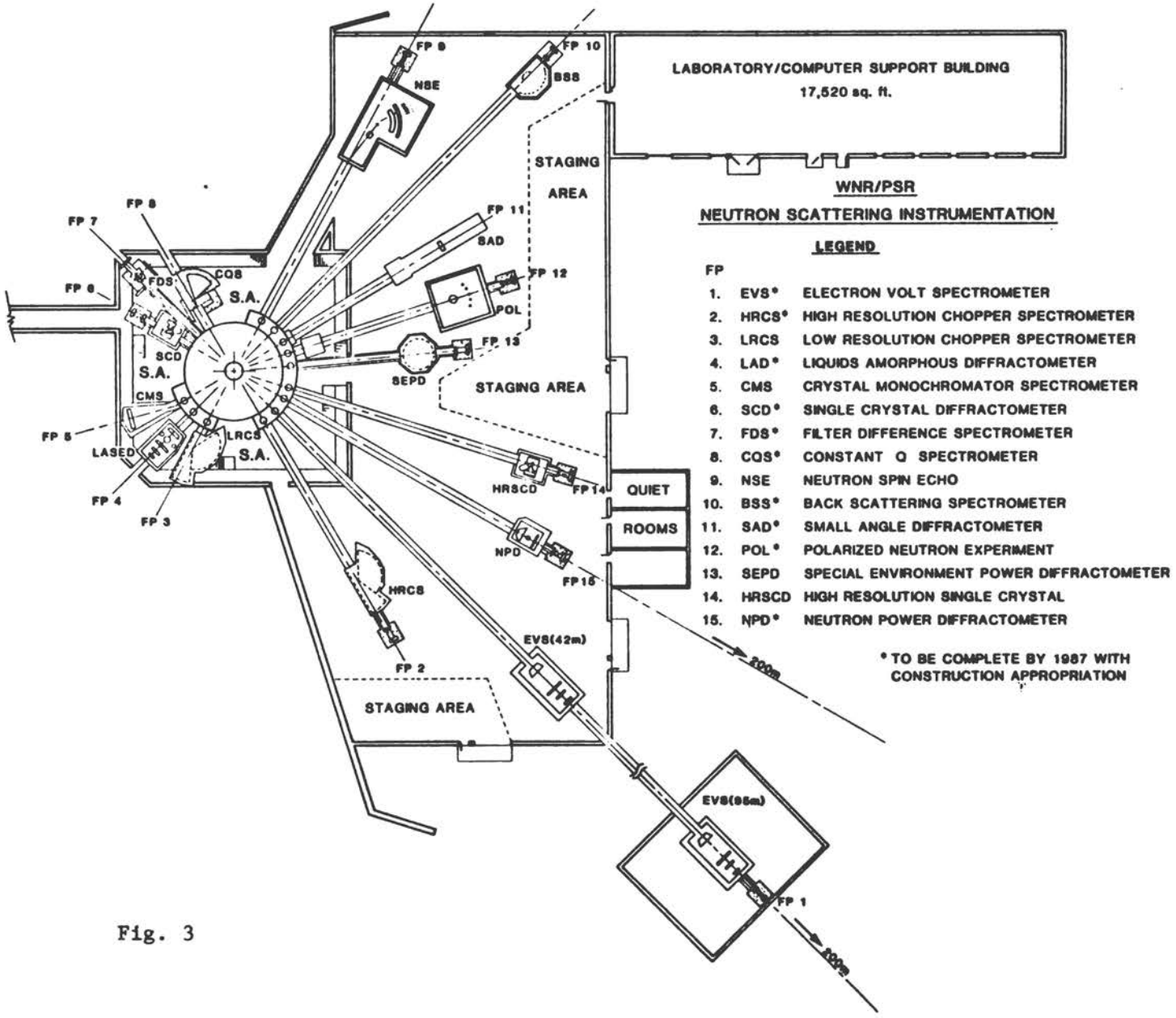

LABORATORY/COMPUTER SUPPORT BUILDING
17,520 sq. ft.
STAGING AREA
STAGING AREA
STAGING AREA
QUIET ROOMS
FP 8
NSE
FP 10
BSS
FP 11
SAD
FP 12
POL
FP 13
SEPD
FP 7
FP 9
FP 6
FDS
CQS
S.A.
SCD
S.A.
CMS
FP 5
LASED
LRCS
S.A.
FP 4
FP 3
HRSCD
FP 14
NPD
FP 15
HRCS
FP 2
EVS(42m)
EVS(85m)
FP 1
200m
200m
WNR/PSR
NEUTRON SCATTERING INSTRUMENTATION
LEGEND
FP
1. EVS* ELECTRON VOLT SPECTROMETER
2. HRCS* HIGH RESOLUTION CHOPPER SPECTROMETER
3. LRCS LOW RESOLUTION CHOPPER SPECTROMETER
4. LAD* LIQUIDS AMORPHOUS DIFFRACTOMETER
5. CMS CRYSTAL MONOCHROMATOR SPECTROMETER
6. SCD* SINGLE CRYSTAL DIFFRACTOMETER
7. FDS* FILTER DIFFERENCE SPECTROMETER
8. CQS* CONSTANT Q SPECTROMETER
9. NSE NEUTRON SPIN ECHO
10. BSS* BACK SCATTERING SPECTROMETER
11. SAD* SMALL ANGLE DIFFRACTOMETER
12. POL* POLARIZED NEUTRON EXPERIMENT
13. SEPD SPECIAL ENVIRONMENT POWER DIFFRACTOMETER
14. HRSCD HIGH RESOLUTION SINGLE CRYSTAL
15. NPD* NEUTRON POWER DIFFRACTOMETER
* TO BE COMPLETE BY 1987 WITH CONSTRUCTION APPROPRIATION

Fig. 3

NBS CENTER FOR COLD NEUTRON RESEARCH

A Presentation by The National Bureau of Standards

to the Major Materials Facilities Committee

National Research Council

National Academy of Sciences

March 18,1984

NBS CENTER FOR COLD NEUTRON RESEARCH

National Bureau of Standards
Washington DC 20234

Summary

In the past ten years, US neutron scattering facilities have fallen seriously behind those in Western Europe with respect to cold neutron research capabilities, an area that offers qualitatively new materials science opportunities. The National Bureau of Standards operates a 20 MW heavy water moderated research reactor at its Gaithersburg, Maryland site which was designed to accomodate a large volume cold source (45 cm. dia.). This volume penetrates to a region of the moderator-fuel assembly in which the neutron flux is 1.7×10^{14} n-cm^{-2}-sec^{-1}. NBS proposes to install a large cold source in this volume, which will provide a high flux of cold neutrons ($\lambda > 4$ A) to four neutron guide tubes and one beam port inside the reactor confinement building with a total area of 500 cm^2. The neutron guides will pass from the reactor hall into a new large experimental hall of dimension 240 by 130 feet. This hall will provide space for at least 15 experimental facilities, including two small angle neutron scattering facilities, two time-of-flight spectrometers, one high resolution back-scattering spectrometer, one ultra high resolution neutron spin echo spectrometer, one cold neutron triple axis spectrometer, one polarized beam spectrometer, and a quantum metrology and fundamental neutron physics facility. The beam ending in the reactor hall will be used to provide stations for neutron depth profiling and for prompt γ-ray analysis of materials. This plan leaves room for at least four more instruments to be developed in the future, and will provide world class facilities for US materials science using cold neutrons. This capability cannot be matched at any other US neutron source in the next decade, and provides for the continuing instrument and technique development essential to the success of a new source. The total facility construction cost is estimated at $24 M (FY1985), spread over three years starting in FY1986. Funding of $1.5 M is included in the Department of Commerce budget for FY1985 to initiate this project. The instruments provided by this proposal will be operated as a national user facility open to all US researchers. In addition, at least five of the instrument stations will be offered for development by Participating Research Teams which will receive 2/3 of the time available on any such instrument. Office and laboratory space will be provided for the users in the new building.

Table of contents

Scientific opportunity	1
- Physics	1
- Chemistry	2
- Materials science	3
- Biology	4
Why build this facility at NBS?	5
User policy	7
Budget and schedule	7
Appendix A - Cold source and neutron guides	10
Appendix B - Guide hall	13
Appendix C - Instruments	13
C1. High resolution small angle scattering	14
C2. Extended range small angle scattering	15
C3. Time of flight spectrometer	15
C4. High intensity time of flight spectrometer	15
C5. Cold neutron backscattering spectrometer	16
C6. Depth profiling facility	16
C7. Prompt n-Y trace analysis facility	17
C8. Cold neutron triple axis spectrometer	17
C9. Polarized beam triple axis spectrometer	17
C10.Fundamental physics and quantum metrology	17
C11.Neutron spin echo spectrometer	18
C12.Other instruments	18

Scientific Opportunity

The Solid State Sciences Committee of the National Academy of Sciences has established a subcommittee to report on the current status of neutron scattering facilities and research in the United States. Two key conclusions of this study are that the user community is growing rapidly, and that the US is currently suffering from a distinct lack of facilities for cold neutron research - that is, neutrons with wavelengths >4A. In particular, Western Europe and, more recently, Japan are taking the lead in this area of neutron research,which has led to the achievement of 1 - 5 orders of magnitude increase in resolution and sensitivity for elastic and inelastic neutron scattering research on materials. The US is currently unable to compete in the exploitation of the scientific and technological opportunities in this field. In the following sections, examples of these opportunities will be discussed briefly under the general headings of physics, chemistry, materials science and biology.

Physics

Neutron scattering has been essential to an understanding of the structure and dynamics of magnetic materials, and this will continue to be one of the most important applications of the technique. The most complete information about magnetic materials is obtained by using polarized neutrons, and observing both the spin flip and non-spin flip cross-section separately. The major obstacle to the use of this technique has been the lack of highly efficient neutron polarizers. This problem is now being redressed by developments such as focussing Heusler monochromators, polarizing supermirrors, and multi-layers. New opportunities for magnetic research will be created by an abundant supply of cold neutrons. One possible application involves polarization analysis of diffuse scattering, an almost untouched area. New types of materials such as magnetic spin glasses are characterized by very long relaxation times, an area which can be probed by the new ultra-high resolution devices, such as neutron spin echo, that have been developed for cold neutrons. NBS has for the past decade had a strong neutron program in the study of magnetic materials. Recent studies have included amorphous ferromagnets ($Fe_{80}B_{20}$), spin glasses ($Fe_{91}Zr_9$), and co-existent magnetic superconductors ($HoMo_6Se_8$). All of this work would benefit from the new instrumentation in this proposal.

In recent years, the study of phase transitions by neutron scattering techniques have led to important advances in our understanding of these phenomena. A key ingredient in these measurements is the availability of the new high energy resolution spectrometers than can be built for cold neutrons. For example, in the orientational glass system $(KCN)_x(KBr)_{1-x}$, first studied at NBS, a key question is the time scale of the relaxation process in the glass state. This time scale is too slow to be measured on any existing U.S. instrument. Similarly, the critical slowing down behavior of NO_4Br was first observed by NBS personnel, but only by use of the instruments at ILL. The two-dimensional liquid state of Rb intercalated into graphite was also studied by NBS scientists in collaboration with the ILL using a high intensity time of flight spectrometer of the type proposed in Appendix C. Recent measurements of the tunnelling of H trapped by O in Nb were first done in the US by an NBS-BNL collaboration, but the details of the temperature dependence could only be done at ILL. In many other cases, e.g. studies of complex defects and solid state diffusion, the availability

of state-of-the-art cold neutron research instruments is essential to further progress.

Finally, there is a broad range of fundamental physics problems that can best be studied using cold neutrons. For example, NBS has a program in quantum metrology which is currently centered on photon work. However, the availability of intense beams of neutrons dedicated to this work would permit entirely new areas to be explored, in which, e.g. the photon and the neutron are used together to explore the transformation properties of matter waves and new measurements of Planck's constant divided by the mass of the neutron are made by interferometric means. In addition, the possibility of producing large numbers of ultra-cold neutrons by the use of a neutron turbine and bottle would open up new areas of study in the fundamental properties of the neutron. Development of such opportunities, which build on a strong existing NBS capability, is a unique physics opportunity.

Chemistry

One specific example of the power of cold neutrons is their ability to probe intermolecular potentials by measuring the ground-state rotational tunnel splittings in molecular solids by high resolution inelastic scattering. (These tunneling splits are not observable by light scattering since they involve transitions between different spin states.) All of this work is now centered in Europe, because of the lack of cold neutron spectrometers in the US For example, at NBS the quasielastic incoherent scattering in nitromethane was measured on a triple-axis spectrometer at 4K. Although this measurement showed broadening, the tunneling spectrum could only be resolved by using the IN10 and IN13 spectrometers at ILL. The pressure and temperature dependence of the splittings revealed new details of the intermolecular potential, and were essential to the re-interpretation of other data (e.g. structure and heat capacity) on this system. Many similar problems exist and can only be addressed by the development in the US of the instrumentation in this proposal.

More generally, there are much broader classes of important research in solid state rotational dynamics and translational diffusion in chemical materials and media that cannot be addressed by current US facilities, including the diffusion of H in ordered phases of metal hydrides, the slow rotational correlations in orientationally disordered crystals, and the dynamics of molecules bound in homogeneous and inhomogeneous systems. Recent European work shows that there are broad opportunities here for in-situ studies of the low energy dynamics and diffusion of molecular species bound on or within catalysts, chemical adsorbents, and intercalated materials. Such research will provide unique information on the binding, interaction and selective release of such species. This information is critical to a fundamental understanding of mechanisms of chemical catalysis and purification. NBS has had an active research effort in all of these areas, and is well suited to further development of this area of chemical physics. Recently, a program has been initiated by the Surface Science Division to study the dynamics of molecules chemisorbed in finely divided metal catalysts. To date, this work has concentrated on high energy spectroscopy, but the availability of new instrumentation with high intensity and resolution for small energy transfers (down to 0.5 μeV) would open up entirely new research opportunities, including surface diffusion and re-orientation, and the spectroscopy of low-energy torsional modes. These

studies also require new high intensity cold neutron instruments, since they often involve the measurement of difference spectra to reveal the dynamics of low (< 1%) concentrations of molecular species.

Additional cold neutron research opportunities, currently at an early stage of exploration, lie in the area of salt solution dynamics and structure, and in studies of the growth and interaction of micelles in solution. NBS has a large group actively pursuing chemical research in this area by other methods.

Materials Science

Traditional materials science is a relatively new application of neutron scattering that has expanded greatly in the past few years. One of the most dramatic developments has been in the area of polymers, where the development of high intensity SANS facilities, coupled with the unique H/D contrast available in neutron scattering has led to revolutionary advances in understanding, settling, for example, the long standing question of the overall chain conformation in the bulk. More recently, studies of microphase separation in block co-polymers have revealed both the aggregate structure of the separated regions and the conformation of the polymers within each region. NBS has a well-established research effort in this area led by the Polymers Division, and has contributed strongly to the techniques used. Future opportunities depend critically on the development of advanced instrumentation in the US - both higher resolution and intensity SANS and ultra-high resolution inelastic scattering spectrometers. With such instrumentation, future oppotunities include the study of the short distance high frequency regime of polymer dynamics as well as the low frequency long distance dynamics, and the use of time-resolved SANS to study, for example, the kinetics of microphase decomposition and the behavior of polymer chains under dynamic external stresses.

In the general field of metallurgy, the application of SANS techniques to studies of the changes in alloy microstructure after thermal and mechanical treatment have provided new insights into both the processing and in-service degradation of new and traditional materials of commercial importance. Applications in both NDE and processing technology are only beginnning to be developed. In addition, new studies of cavity formation at grain boundaries of metals under conditions of high temperature and deformation have led to a re-evaluation of the theory of formation of such voids. However, higher flux and resolution for cold neutrons are required for this technique to be fully exploited at U.S. facilities. Additional opportunities in the study of the microstructure of new materials such as rapidly quenched metal alloys are just beginning. Preliminary studies of the evolution of density fluctuations and microstructural changes in metallic glasses have been carried out at NBS, but these measurements require higher fluxes of cold neutrons to extend sensitivity so as to allow the probing of earlier stages of transformation at higher resolution. In fact, higher fluxes are essential to allow in-situ real time studies (1 - 100 seconds) of precipitation and void formation in a wide variety of bulk structural alloys.

The beams of cold neutrons for depth profiling of near-surface impurities in semiconductors, metals and thin films, and for prompt γ-ray spectroscopic analysis of materials would provide the best capabilities in

the world for such measurements. In particular, the rapid non-destructive measurement of impurity or dopant distributions (B, Li, N, Cl) as a function of processing and annealing conditions, including three-dimensional imaging, would become possible. Such unique capabilities will be of broad scientific and technological interest to both industry and universities, as indicated by the extensive co-operative research already underway at NBS. The increased sensitivity of the prompt γ-ray analysis facility will allow the non-destructive detection of < 0.1 μg of hydrogen in metals and alloys, a critical regime for studies of embrittlement and corrosion phenomena.

Finally, the application of neutron techniques to ceramics is an area that has just begun to be explored. SANS offers a unique capability to monitor the development of microstructure in bulk samples, and the NBS Inorganic Materials Division has performed the first experiments to study the formation, density and shapes of microcracks in a ceramic. We have also developed theoretical and experimental SANS techniques to extend the method to study particle and/or void sizes of 0.001 to 10 μm. These measurement techniques, which offer a unique way to study in situ densification from green state compact to fully sintered ceramic, require the widest possible range of incident wavelengths and resolutions. These new uses of the SANS method will, of course, be much enhanced by the cold neutron capabilities in this proposal.

Biology

Since the mid-seventies, neutron scattering has made major contributions to the study of biological systems by high resolution crystallographic studies. At present, only three facilities for this work exist in the world, two of which are in the US and one of which is the joint NBS-NIH facility at the NBS reactor. The use of cold neutrons to study biological sytems is not as advanced in the U.S. as in Western Europe, but will become much more important as the coupling of high intensity sources of cold neutrons and associated instrumentation is achieved. Not only will major opportunities be opened up for US scientists in low resolution crystallographic research on large biological structures (e.g. nucleosomes and viruses), which have been initiated in recent years at the ILL, but the availability of more neutrons in the 5 - 15 A range, along with flexible wave-vector ranges, will extend applications in studies of biological assemblies in solution.

Finally, the use of low energy neutron inelastic scattering in biological research has barely begun, and the measurements are again centered in Europe because of the existence of the requisite instrumentation. Any development of this potentially exciting field, which might shed new light on the mechanisms of biological activity, must await cold neutron instrumentation of the type contained in this proposal. This will include high resolution spectrometers such as the neutron spin echo spectrometer and the lower resolution, high intensity time of flight spectrometers, which provide the sensitivity required for difference spectra measurements of the low energy chain dynamics of biological molecules in solution and other biological assemblies.

Why Build This Facility at NBS?

The NBS reactor is especially well suited to the development of a cold neutron research facility. The large volume dedicated to the cold source installation (see Appendix A) in the original design penetrates into the high flux region of the reflector ($\phi > 1.5 \times 10^{14}$ n-cm^{-2}-sec^{-1}), and allows for the optimal source design, thus providing a cold neutron flux equal to any in the US. In addition, the existing reactor biological shield penetrations are separated by 33° of arc, and three additional penetrations can be made in a removeable plug. This allows us to propose a facility with unmatched flexibility, that will serve the needs of the US materials science community by providing at least fifteen instruments, with adequate space for additional instrument development projects to provide needed expertise for future sources. This proposal will provide US researchers with internationally competitive facilities that cannot be matched in any US neutron source in the next decade.

NBS is the nation's original national laboratory, with a staff of approximately 3000 people. The mission of NBS was defined by Congress in the enabling legislation as the provision of measurement standards and services, test procedures, reliable data and research in support of the nation's efforts in Science, Technology and Commerce. NBS has a long history of cooperative arrangements with the university and industrial community, and has many mechanisms in place for guest workers, industrial research associates, visiting university faculty and students, and post-doctoral research associateships. Currently more than 500 full-time or part-time visiting scientists, guest workers and research associates participate in research at NBS. As a major part of its mission, the laboratory has a long-standing and well-defined role in materials research and measurement technology, as exemplified by the existence of a 300 person Center for Materials Science (CMS), and hundreds of other scientists working in materials-based research and analysis. In fact, almost half of NBS is engaged in research and standards work in fields whose major facilities needs are being addressed by the Seitz Committee. Moreover, this proposal has the enthusiastic support of the Department of Commerce, which has included $1.5 M in its FY1985 budget to allow advanced research and development on the cold source and instruments in this proposal. In the current fiscal year, NBS has committed incremental funds of $550 K to the installation of the D_2O cold source and to the hiring of critical scientific and technical personnel.

The Reactor Division, which includes the neutron scattering research effort, is organizationally located within CMS, and materials science has been a major driving force behind the neutron research program at NBS. Within the Center, there are four other divisions - Metallurgy, Inorganic Materials, Polymers, and Fracture and Deformation. The Polymers Division is the only major polymer research organization in the Federal or national laboratory structure. Each of these divisions uses the NBS reactor in its programs, and many of the scientific opportunities discussed above are the direct result of these interactions. In addition, many other organizations within NBS use the reactor facilities regularly in their research programs, including the Center for Chemical Physics, with strong, internationally recognized research efforts in surface science and catalysis and molecular spectroscopy; the Center for Analytical Chemistry; the Center for Absolute

Physical Quantities; the Center for Radiation Research; and the Center for Chemical Engineering. These interactions cover a broad range of materials science and fundamental physics which is reflected in the scientific opportunities. It should also be noted that NBS has several groups with major research efforts in x-ray scattering and optics, including emerging efforts in small angle x-ray scattering, which complement and enhance our existing and future neutron scattering activities.

In the field of neutron scattering instrumentation, NBS has developed one of the best small-angle neutron scattering (SANS) instruments in the U.S. for materials science. We have developed the only US facility for depth profiling and applied it to a wide variety of materials of technological significance. The filter spectrometer at the NBS reactor has the highest sensitivity of any in the world and has been used for the study of surface science and of very low-level H in metals. The NIH-NBS protein crystallography station, one of only three in the world, is based upon a new type of spectrometer, and has been used successfully in the structure studies of trypsin inhibitor, insulin, and ribonuclease. The current NBS staff has state-of-the-art expertise in the design, construction, and operation of triple-axis spectrometers, time of flight spectrometers, SANS instruments, depth profiling and prompt γ-ray compositional analysis instruments, diffractometers, and computer control systems. We are currently adding a specialist in back reflection and time of flight spectroscopy to the staff, in anticipation of our cold-neutron expansion. The NBS high resolution powder diffractometer is currently the best instrument of its kind at a US reactor.

With respect to operation as a user facility, the NBS reactor has supported 170 "hands on" users at the site in the past year (well over 200 collaborators) - 100 in neutron scattering and 70 in other neutron research - with 75 full-time or part-time guest workers and research associates. We have three long-standing participating research teams at the current facility, involving both Army and Navy laboratories, and the National Institutes of Health. In fact, half of our neutron scattering facilities were developed in this mode. In each case, researchers have been stationed permanently at NBS, and the agency involved has contributed both money and continuing manpower to the joint effort. The existing sophisticated spectrometer control and data acquisition network has been developed to be user-friendly and features a high degree of on-line data analysis and display.

As outlined above, NBS provides, perhaps more than any other laboratory, a broad scientific expertise and environment ideally matched to the major opportunities presented by a center for cold-neutron research, including high quality research groups in materials science, polymers and biology, chemical spectroscopy and catalysis, and condensed matter physics. Our growing number of part-time guest workers from universities and from the chemical, materials, electronic, aerospace and biotechnology industries attests to this, and provides a strong base for future growth and co-operation in a multi-disciplinary user facility.

Finally, NBS has in place other necessary facilities for a user-oriented facility - the central computer complex is being upgraded to a Class VI machine (CRAY-1 or equivalent); there is a large machine shop; and supporting electronics and glass shops. Our mission has always included

both cooperative research and service to the scientific community. The main NBS campus is located close to Washington, D.C., less than an hour's drive from the major airports, and in the immediate vicinity of motels, housing, restaurants, and shopping facilities. Over 100 conferences per year are run at NBS.

User Policy

The NBS center for Cold Neutron Research will be operated as a national user facility with two modes of operation. NBS will develop at least ten experimental stations for the use of the general US materials science community. Two thirds of the available time on these stations will be allocated by a Program Advisory Committee (PAC) on the basis of written proposals. The PAC will be appointed by NBS with a majority of members chosen from outside NBS. The other mode of operation will involve Participating Research Teams, which will develop 5 additional stations. These PRT's might involve NBS, although this will not be necessary. Proposals from prospective PRT's will be selected by the facility manager, with the advice of the PAC. The PRT's will be responsible for the design, construction and management of the facilities, in return for which they will be allocated 2/3 of the available time. The remaining time will be allocated by the PAC in the usual manner. For all instrumental stations, an instrument-responsible scientist will be designated to assist users in the performance of their experiments.

NBS will provide office and laboratory space to accomodate users of the facility. It will also provide standard sample environmental equipment such as cryostats, furnaces, magnets and moderate pressure systems. Any special equipment beyond these standard items will be the responsibility of the user. Standard data analysis programs will be provided for each instrument, and a means of transporting results back to the home institution in machine readable form such as magnetic tape will be available. More extensive data analysis routines will be available in some cases, but the detailed computations required to fully exploit the results will be the responsibility of the user, unless special arrangements are made.

Budget and Schedule

NBS has committed over $500 K from its reserve to this project in FY1984 for the installation and use of the first prototype source, now scheduled for the summer of 1984. This cold source will be used by two existing instruments - a small angle neutron scattering facility and a time of flight spectrometer for inelastic scattering studies. The NBS budget submitted to Congress for FY1985 includes $1.5 M for advanced research and development in cold neutron research. We plan to submit a proposal for the FY1986 budget to allow construction of the NBS center for cold neutron research. The total construction budget will be $24 M, with the profile shown in Table I below. A breakdown of the component cost is given in Table II.

In addition, NBS will request additional operating and R&D funds of $1.0, 2.0, and 3.0 M in FY1986, FY1987 and FY1988 respectively. This level of funding will be used to hire new personnel, both technical and professional, to operate the facility (including maintenance), to institute

a continuing program of investment in new instruments, and to establish cooperative projects with industry and universities. This continuing funding of both instrument research and development and cooperative programs to ensure efficient use of the facility is the first such commitment at a US neutron research center. The breakdown of these components is shown in Table III.

Table I

Component	Calendar Year 1984	1985	1986	1987	1988
COLD SOURCE					
-prototype operation					
-new source design					
-construction and testing					
-installation and operation					
NEUTRON GUIDES AND SHIELDING					
-design					
-construction					
-installation					
NEW BUILDING					
-final architectural/engineering					
-construction					
-occupancy					
INSTRUMENTS					
-conceptual design					
-detailed engineering design					
-construction					
-installation and testing					
-routine use					
FUNDING PROFILE (FY)					
-Operation and personnel ($M)	0.20[a]	1.0[b]	2.5[c]	3.5[c]	4.5[c]
-Construction ($M)	0.35[a]	0.5[b]	13.0[c]	8.0[c]	3.0[c]

a - NBS reserve funds
b - in FY1985 budget request to Congress
c - to be requested in FY1986

Table II Breakdown of construction budget ($M)

New building and associated construction (15% contingency)	11.0
New cold source and reactor confinement modifications	1.5
Guide tubes and associated shielding	1.9*
Instruments (including data acquisition computers)	8.0
Data reduction computer	0.8
Sample environmental equipment	0.8
Total	24.0

* A full complement of instruments for this facility is estimated to cost $12 M. The budget shown assumes that $4 M will come from PRT's. The actual instruments to be built with this budget item will be finalized after PRT's have been chosen.

Table III Operating budget details ($M)

	FY1986	FY1987	FY1988 and beyond
Personnel[a]	1.0	1.5	2.0
Facility costs[b]	0.5	0.7	1.0
R&D for facility[c]	0.8	1.0	1.0
Co-operative research programs[d]	0.2	0.3	0.5
Total	2.5	3.5	4.5

a Scientists, engineers, technical staff, secretarial staff

b Includes maintenance of equipment, cryogenic fluids, expendables, travel and routine replacement of components.

c This item allows for continuing development of new instrumentation and equipment. It will consist of both in-house and contract work (e.g. monochromator development and characterization, supermirror development, new instrument mockups).

d This item is intended to encourage the establishment of joint NBS, industry and university programs to ensure more efficient use of the cold neutron facility. It is expected that participating organizations will make matching contributions.

Appendix A Cold source and neutron guides

The NBS reactor was designed with a large (55 cm. diameter) volume reserved for a cold source. This volume penetrates almost to the region of maximum thermal neutron flux seen by the normal beam ports, and the flux at the innermost position of this volume is 1.7×10^{14} n-cm^{-2}-sec^{-1}. This volume is accessible through a large removeable plug in the reactor biological shield. In the existing configuration, shown in Fig. A1, two 18 cm. diameter beam holes separated by 33° view the source. This geometrical arrangement allows extraordinary flexibility in the design and operation of the cold source and any associated neutron beams. At the present time (February 1984) a D_2O ice cold source cooled to 30 K by He gas is undergoing final assembly and testing, preparatory to installation in the reactor during the shutdown from June - August 1984 for conversion to 20 MW operation. This source has the geometry shown in Fig. A1. This source has been designed with a re-entrant hole for extraction of the beams, a feature which calculations by Ageron at the ILL, and experiments at Saclay, indicate increases the cold flux by a factor of 1.6 to 2.

The performance of this source will be measured with the existing arrangement of beam holes shown in Fig. A1, which will serve two instruments, the existing Small Angle Neutron Scattering (SANS) facility, and an improved Time Of Flight (TOF) spectrometer for inelastic scattering. The expected performance of this source has been estimated by using the results of Rush et.al. (Nucl. Sci. Eng.25, 383 (1966)), which showed a gain of 20 in neutrons with $\lambda > 4A$, and is comparable to measured cold source performance in the ILL and Saclay reactors. The exact performance of the source is difficult to predict, given the different geometry of the current source and the experimental mockup. Calculations indicate that mixtures of H_2O and D_2O are even better than pure D_2O ice as a moderator (Nucl. Inst. Methods 128, 583(1975)). Therefore, in Fig. A2, we show calculated flux curves (per unit wavelength per steradian) for two different source temperatures, 40 and 60 K, after allowance for the decrease in flux with distance from the core, as illustrations of the gain expected. The higher temperature is comparable to the temperature measured by Rush. In addition, the predicted cold neutron gains are consistent with intensities measured in tests of a D_2O ice moderator in the MIT reactor. This will be confirmed by direct measurement when the source is installed. These results have been used in the estimation of neutron intensities for the proposed instruments, which will by any estimate be competitive with intensities anywhere in the world.

λ (A)

Figure A2

A comparison of the performance and capability of this source with the existing cold sources at Brookhaven National Laboratory and the Institut Laue-Langevin in France is shown in Table IV. The first line given is the flux in which the source sits, the second is the effect of the re-entrant hole, and the third is the product of these numbers. The next line gives the average size of a guide looking at the source, a parameter that gives higher intensities when focussing can be used, which is true for many instruments. The fourth line is a figure of merit including guide size. The final line gives the number of beams extracted, a measure of the number of instruments that can be accommodated.

TABLE IV COLD SOURCE COMPARISON

	NBS	BNL	ILL*
Source flux (10^{14})	1.5	2.5	4.5
Geometry	1.8	1.0	1.8
Cold neutron flux	2.7	2.5	8.1
Average guide area (cm^2)	100	30	60
Neutrons in guide	270	75	490
Number of guides	5	3	5

*Improved vertical source (to be installed in 1985)

In order to take advantage of this large source, a new shielding plug capable of extracting three large beams (17x6 cm.) whose centerlines are shown in Fig. A1 is being designed. This plug would be installed when the guide hall is ready for use, and would allow the extraction of four beams of cold neutrons into the guide hall, while the other existing beam hole would serve two instruments in the existing reactor hall. This combination of beams will provide approximately 500 cm^2 of beam area for cold neutron research. The guides themselves will be of standard construction, with Ni plated on glass, of dimension 17x6 cm. Two of the guides will have Be filters installed in the reactor hall, restricting their wavelength range to be larger than 4A, with very low fast neutron background. The guides will be straight, and thus will accept more neutrons while avoiding the usual non-uniform distribution of intensity across the guide exit for neutrons near the cutoff. These guides will be used for those instruments requiring the lowest background, and not requiring shorter wavelengths. The other two guides will also be straight, but will not have neutron filters (unless Bi proves useful for fast neutron reduction), and will be fabricated with separated Ni^{58} isotope, thus yielding a 15% increase in critical angle at all wavelengths. Such guides have been used at the Leningrad reactor, and present no problems in fabrication. These guides will be used for instruments which require the highest possible flux and the possibility of running at shorter wavelengths, down to 2 A. The layout of guides and instruments is shown in Fig. A3, and the experimental hall and instruments are described in some detail in the following appendices.

We are investigating the possibility of using a liquid D_2 cold source for the final facility. Such a source has been used successfully at the ILL and offers some advantages in simplicity of operation. Since the liquid D_2 has less γ-ray heating per unit volume, such a source would not require the Pb-Bi heat shield shown in Fig. A1, allowing the source to be placed closer to the reactor core and to be larger in diameter. The large volume available for this source would again allow the use of a re-entrant design, with the concomitant gain of 1.6 to 2 in flux. Because of its proximity to the reactor core, this source would increase the available neutron flux by approximately 20% for the guide tubes and instruments. The larger diameter would also allow the use of higher guides in the three new penetrations.

Appendix B. Guide hall

A new building will be erected adjacent to the existing reactor confinement building to accomodate the neutron guides and instruments. This building will be 72x40 m. square (240x130 ft.), with a 12 m. (40 ft.) high roof to allow installation of a 1000 kg. (20 ton) crane with a floor to hook clearance of 8 m. (25 ft.). This crane will be able to access the entire experimental area, running longitudinally along rails and transversely by trolley. The building is designed for a floor loading of 85 kg/m^2 (2000 lb/ft^2) at any point, and the guide tubes and associated shielding will be supported by individual support structures running along the length of the guides. These supports will themselves be supported by pilings driven to rock, in order to minimize both settling and deflection when the floor loading is changed as experiments are installed and changed. The general floor plan of the experimental level is as shown in Fig. A3. This level of the new building will have the same elevation as the existing floor in the reactor confinement building, thus simplifying interchange of sample environmental equipment. Personnel and light equipment access to this building will be from the existing building at two points, one near the entrance to the reactor confinement building and the other from the existing office wing. Large equipment access will be by a truck entrance which will allow a tractor trailer to back under the crane on the main floor. A limited amount of office and laboratory space is provided on the main floor and on a mezzanine level for the use of the technical staff and users. The building is designed to maximize the amount of natural lighting on the experimental floor by the use of large windows, since this area will not be part of the reactor confinement.

In addition, there will be a lower level consisting of offices, laboratories and storage space. Each office will be on an exterior wall, well above grade, allowing the use of windows. The main local data analysis computer will also be situated in this area, as will be terminal rooms for users. This computer will be linked to the main campus computer.

A detailed architectural/engineering study of this building has been performed by Kidde Consultants. This study includes soil tests and borings, a detailed structural design, and all necessary changes to existing structures, utilities and other facilities. The final report of this study will be available in April 1984.

Appendix C Instruments

The cold source, experimental hall and guide layout have been described in appendices A and B. As shown in Fig. A3, the guides will be well shielded from the reactor face to the guide hall, including passing through an existing 8 m. concrete wall at the reactor confinement building. This wall will be penetrated by 40 cm. diameter holes, and the guides will be surrounded by water shielding as they pass through these holes, thus avoiding any cracks in the shielding. The beams entering the experimental hall will thus be clean and well-collimated, especially G3 and G4 which will be filtered by cooled Be to remove fast neutrons. Since G1 and G2 will not be filtered, there will be fast neutrons in the guides, but the distance from the reactor core implies a natural collimation much higher than for normal beam ports. Nonetheless, good shielding will be required whenever a

monochromator is inserted into the guide. The relevant guide parameters required for instrument design are given below.

G1 and G2 - Ni^{58} coating, γ_c=0.00204 radians/A, 17x6 cm. cross-section straight, no cutoff wavelength.

G3 and G4 - normal Ni coating, γ_c=0.00174 radians/A, 17x6 cm. cross-section, Be filter, $\lambda \geq 4A$

Each instrument will be connected to its own local computer and data display terminal. All local computers will be connected into a general Local Area Network which will include a main data analysis computer with extended data analysis and display capabilities. This computer will be connected to the main NBS computer complex, a Class VI machine, which is currently being acquired.

C1 High resolution small angle neutron scattering instrument

This instrument will be installed at the end of G4, utilizing 6x6 cm. of beam. The incident beam will be monochromatized by either of two mechanical velocity selectors with resolution $\Delta\lambda/\lambda$ of either 10% or 25%. The total flight path available for this instrument is 30 m., divided equally between the incident and scattered beam. The incident flight path will have three fixed lengths of 15, 10, or 5 m. Fig. C1 shows the calculated flux on the sample for various minimum values of the momentum transfer, all obtained at 15 m. with varying incident wavelengths and $\Delta\lambda/\lambda$ = 25%. For minimum Q's below 0.0016 A^{-1}, the sample size would be 7.5 mm. diameter, so that this design makes use of the focussing collimator design used successfully at the current NBS SANS facility to allow the use of sample areas of 3 cm^2, which requires a sample diameter of 2.5 cm. The fluxes shown in the figure have been corrected for various losses such as velocity selector transmission, and are consistent with extrapolation from the existing instrument. They will be checked experimentally when the cold source is installed.

The collimation may, of course, be relaxed by shortening the flight paths in order to increase the available flux. However, experiments with Q_{min} close to 0.01 A^{-1} would be better performed on the extended range SANS facility described below. The detector, which will be of the ORNL Borkowski-Kopp design, similar to the one in use at the current NBS facility, will be able to be moved continuously from a distance of 2 m. to 15 m. inside the vacuum flight path. The estimated cost of this instrument is $0.9 M, based on the cost of the existing facility.

C2 Extended range small angle scattering instrument

This instrument is optimized for measurements at somewhat larger momentum transfers than the high resolution instrument, and will be installed on G1 at the end of the guide. It will have a variable length flight path before the sample of up to 8 m., with standard pinhole collimation, and two velocity selectors with $\Delta\lambda/\lambda$ = 10% and 25%. The final flight path will be 5 m. long, and will be able to rotate about the sample to an angle of 30° from the incident beam. This instrument will allow greatly enhanced capabilities in, for example, real-time SANS studies and medium to low resolution biological structure studies. As currently designed, the minimum Q will be 0.01 A^{-1} and the maximum Q will be 0.7 A^{-1} with an incident wavelength of 5 A. With this minimum Q, the number of neutrons incident on the sample will be in excess of 10^7/sec and even higher for more relaxed collimation. This implies very high data rates, and will require a different detector design. Two possibilities exist currently - either a composite design similar to the one in use at the University of Missouri, or the detector in use at the ILL. Other schemes can be envisioned, and the final design has not been chosen. The current estimate of the cost of this facility is $700 K.

C3 Time-of-flight spectrometer

This spectrometer will be based on the existing NBS instrument, which has an evacuated flight path of 2.5 m. and a range of scattering angles from -20° to 140°. The instrument will be installed on G1 which has no filter, and so can be used for wavelengths as small as 2A. The incident beam will be obtained by reflection from a pyrolitic graphite monochromator, curved to focus the beam onto the sample position. This monochromator will utilize 11 cm. of beam height, focussed vertically onto an image size at the sample of 6 cm. The remaining 6 cm. of beam will pass directly down the guide to the extended range SANS instrument at the end of this guide. The guide width will be 6 cm., a value inconveniently wide for a TOF spectrometer. This width will be reduced to 3 cm. at the sample by means of a tapered super-mirror snout, yielding an increase in flux at the expense of horizontal divergence (which is unimportant for the measurements to be done at this instrument). The chopper will be a simple Fermi type as is the case in the existing NBS TOF spectrometer. The incident energy will be variable from 2.3 meV to 14 meV, with energy resolutions from 40 μeV to 400 μeV, yielding pulsed monochromatic fluxes of 3×10^3 to 3×10^4 n-cm^{-2}-sec^{-1} for samples as large as 18 cm^2. The estimated incremental cost of this spectrometer is $400 K.

C4 High intensity TOF spectrometer

This instrument will be similar to the one described in C3, except that the monochromator will be of the multiple crystal time focussing type. It will be installed on the guide G4, which is Be filtered, thus restricting the incident energy to be less than 5 meV. In addition, the flight path and detector system will be more elaborate in order to accomodate more solid angle at the detectors. The principle of time focussing is quite simple, and requires that the sweep time of the chopper be chosen so as to have all neutrons reflected from different monochromator crystals (each set for a slightly different energy) arrive at the detectors at the same time for elastic scattering. Of course, this focussing breaks down for large energy

transfers, but the sweep time can be adjusted to account for this to some extent for a given energy transfer. The net effect of the arrangement is to increase the energy width of the incident beam without affecting the resolution. The required chopper speeds are quite reasonable for neutrons with $\lambda > 4$Å, and the chopper presents no problems in fabrication. The maximum pulsed flux at the sample (again assumed to be 6x3 cm.) will be approximately 10^5 n-cm^{-2}-sec^{-1} with an energy resolution of 150 μeV at an incident energy of 5 meV. The estimated cost of this instrument is $1.1 M, a large fraction of which will go into the monochromators and detectors.

C5 Cold neutron back-scattering spectrometer.

This instrument is intended for high resolution inelastic studies, and will feature energy resolutions of 0.3 to 2 μeV. The basic concept of this instrument is that the contribution of the angular divergence to the energy width of a Bragg reflected beam goes to zero as the Bragg angle is increased to 90°, so that for a perfect crystal, the energy width is given by the Darwin width of the crystal. In order to have useful neutron intensities, the condition of exact back-scattering is somewhat relaxed, but the energy resolution is as high as $\Delta E/E = 1.4 \times 10^{-4}$. The instrument will be similar in concept to the existing IN11 instrument at the ILL, but will incorporate some design features which have been proposed to improve that facility. It will be installed on G4, and will use the top 12 cm. of the guide, while allowing the rest of the beam to pass undisturbed to the high resolution SANS facility at the end of the guide. The use of this geometry in itself allows a substantial increase in sample flux, since the guide height does not have to be increased to accomodate a neutron switch. The beam size resulting from such a large guide area (12x6 cm^2) is too large to be used directly, but the beam can be reduced to 3x3 cm. by the use of a tapered supermirror snout without substantially changing the overall angular resolution of the machine, which is dominated by the large angular acceptance of the focussing analysers. In addition, the use of a rotating deflector crystal as proposed by B. Alefeld can provide another factor of two in intensity, although it requires a large amount of pyrolitic graphite and the use of a second phased chopper. Incorporating all of these factors, the estimated flux on the sample will be approximately 5×10^4 n-cm^{-2}-sec^{-1}. The cost of construction of this instrument will be of the order of $1.1 M.

C6 Depth profiling facility

This technique utilizes the activation cross section of a number of elements (e.g. B, He^3, Li) that decay by charged particle emission to non-destructively probe the near surface distribution of small concentrations of these elements, e.g. in thin films, semiconductors and coatings. The depth profile is derived from the energy spectrum of the emitted particles, which is a direct measure of the depth from which they were emitted. The current facility at NBS is installed on a thermal neutron beam hole, and can achieve sensitivities as high as 7×10^{13} atoms-cm^{-2} for B with a depth resolution of order a few nanometers (sample dependent). The basic limit on the technique is the available flux and its energy distribution. The angular distribution of the incident beam is unimportant. A new facility for these measurements and for the prompt γ-ray facility will be installed on the cold neutron beam in the reactor hall. The beam will be filtered by a Bi single crystal cooled to 77K to remove γ-rays and fast neutrons and will be 6x6 cm^2 when it leaves the main shield. This beam will be reduced to 2x2 cm^2 by the use of

a super mirror snout, thus increasing the flux by increasing the angular divergence. Since the measurement does not depend on angular collimation, this flux gain is all useable. This will result in a gain in neutron flux of more than an order of magnitude over the current facility, and in addition, the longer average wavelength will increase the sensitivity by another factor of five. These combined factors will necessitate improvements in sample arrangements, data acquisition hardware and other support equipment as well as allowing entirely new types of measurements to be performed. The estimated cost of these improvements is $500 K.

C7 Prompt n-γ trace analysis facility

At present, a prompt γ-ray analysis facility for compositional analysis of materials is installed in a vertical facility at the NBS reactor. As was discussed in C6, it is possible to increase the sensitivity by two orders of magnitude by installing this facility downstream of the depth profiling facility. This will be sufficient to allow the detection of < 0.1 μg of H. The beam will be used after it has passed through the depth profiling station, which will remove less than 10% of the beam. This facility will also need some upgrading to handle the higher data rates, for an estimated cost of $300 K.

C8 Cold neutron triple axis spectrometer

This type of instrument is by now well defined, and needs little discussion. The basic design will be of the Tanzboden type to allow maximum flexibility for future changes. The monochromator will be 11 cm high, vertically focussed pyrolitic graphite with an image height of 3 to 6 cm, depending on incident wavelength. It will be installed on G1, and so will have a range of incident energies from 2.3 to 15 meV, with energy resolution for the monochromator from 25 to 500 μeV, depending on energy and collimation. The calculated flux on the sample will vary from 3×10^5 to 5×10^6 n-cm^{-2}-sec^{-1} for incident energies from 2 to 5 meV. The estimated cost of this spectrometer is $600 K.

C9 Polarized beam triple axis spectrometer

This instrument will be based on the triple axis design above, plus polarizing elements such as supermirrors, neutron guide fields and polarization flippers. The use of a Tanzboden design for the triple axis simplifies this arrangement. The estimated cost of this spectrometer is the basic of a triple axis spectrometer ($600 K) plus another $200 K, which allows for the development of the necessary extra equipment.

C10 Quantum metrology instrument

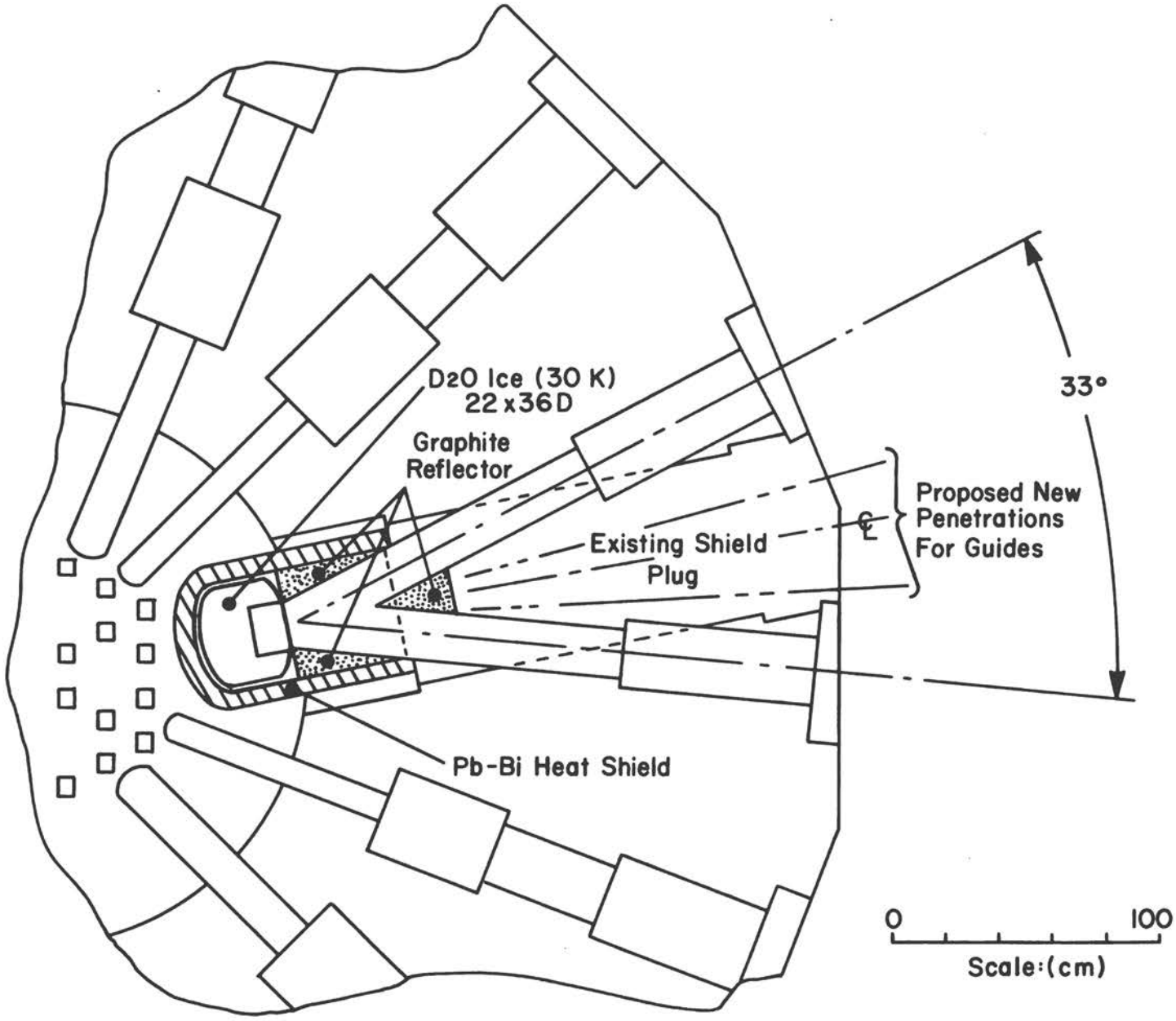
This instrument will be used to study the fundamental properties of neutrons and to establish a common measurement scale for photons and neutrons. It will be installed at the end of G2, where the useful range of neutron wavelengths will be 2 - 12 Å. The design of this instrument has not yet been finalized, but a preliminary estimate of the cost is $500 K.

C11 Neutron spin echo spectrometer

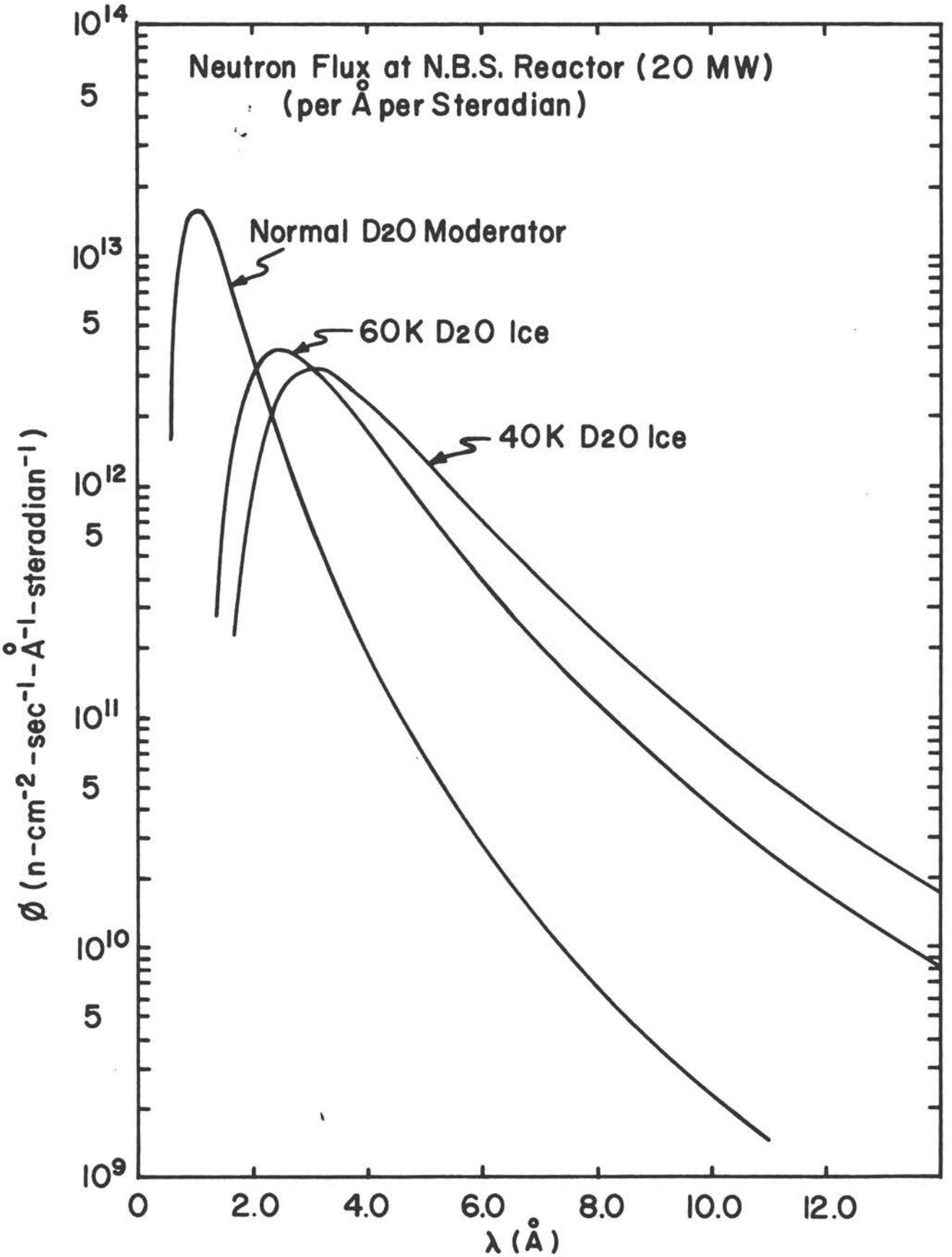
This spectrometer is intended for ultra high resolution studies of quasielastic scattering. The high energy resolution is achieved by utilizing a broad band of incident energies, and "tagging" the velocity of each incident neutron by the number of precessions an initially polarized neutron makes in a long magnetic field. The polarization is measured after scattering at the sample and passage of the neutrons down another field in which the neutrons precess in the opposite direction. By this technique, the resolution is achieved with a useful neutron intensity. The principles of design and operation of these spectrometers is now well-established by the successful operation of the IN11 spectrometer at ILL. The resolution of this instrument is currently of the order of 80 neV (20 MHz) at 8 A incident wavelength. There are possible changes to the instrument to improve this by an order of magnitude. Although this instrument design has not been carried to a point allowing precise cost estimates, it is estimated that an instrument with capabilities similar to the IN11 spectrometer could be built for approximately $1.1 M.

C12 Other instruments

The instruments described above do not exhaust the possibilities for useful neutron research, and other instruments are foreseen, depending on the interest of possible PRT's. These would include, but not be limited to,an ultra cold neutron facility for fundamental physics studies, diffuse scattering spectrometers, a low resolution biological diffraction instrument, and a triple axis spin echo spectrometer. Other possibilities will arise in the future, and this proposal is intended to be flexible enough to allow such opportunities to be pursued. In fact, considerable effort will be devoted to a continuing program of new instrument development at this facility, which will make a major contribution to the long-term development of cold neutron research on materials in the US.



Geometry of Current N.B.S. Cold Source


Neutron Flux at N.B.S. Reactor (20 MW)
(per Å per Steradian)
Normal D2O Moderator
60K D2O Ice
40K D2O Ice
Ø (n-cm⁻²-sec⁻¹-Å⁻¹-steradian⁻¹)
λ (Å)
10¹⁴
5
10¹³
5
10¹²
5
10¹¹
5
10¹⁰
5
10⁹
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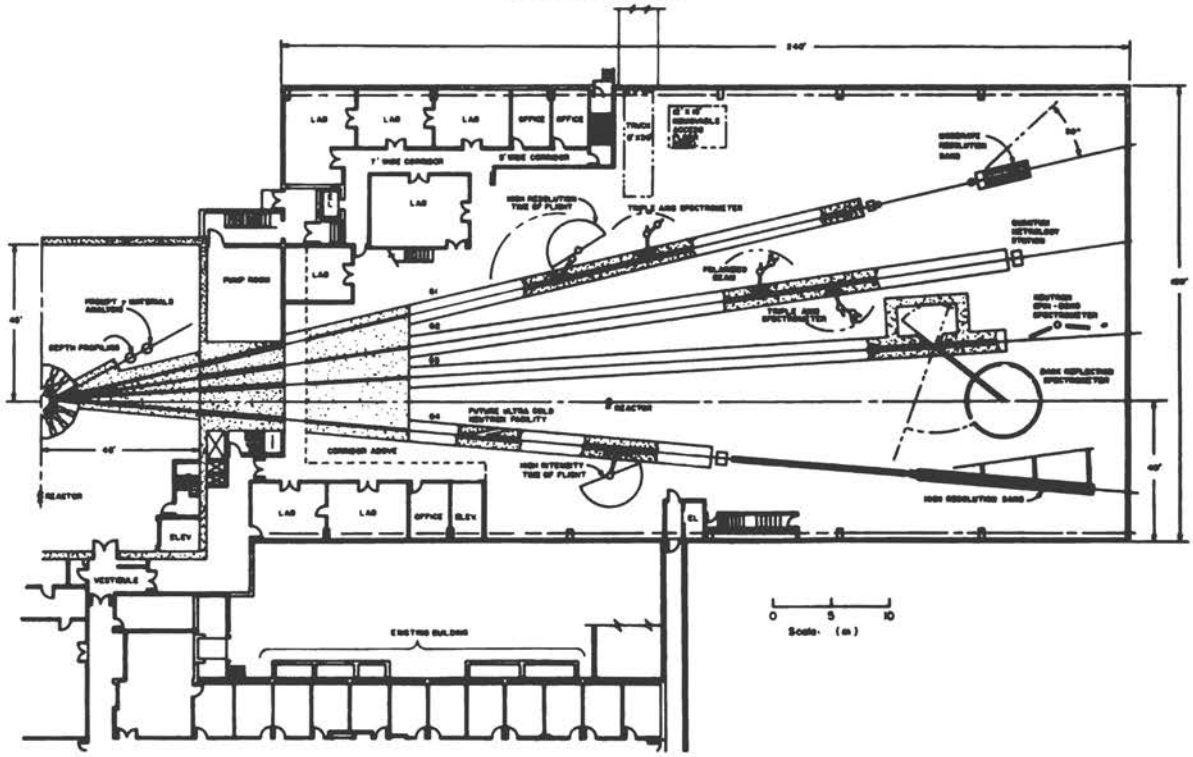
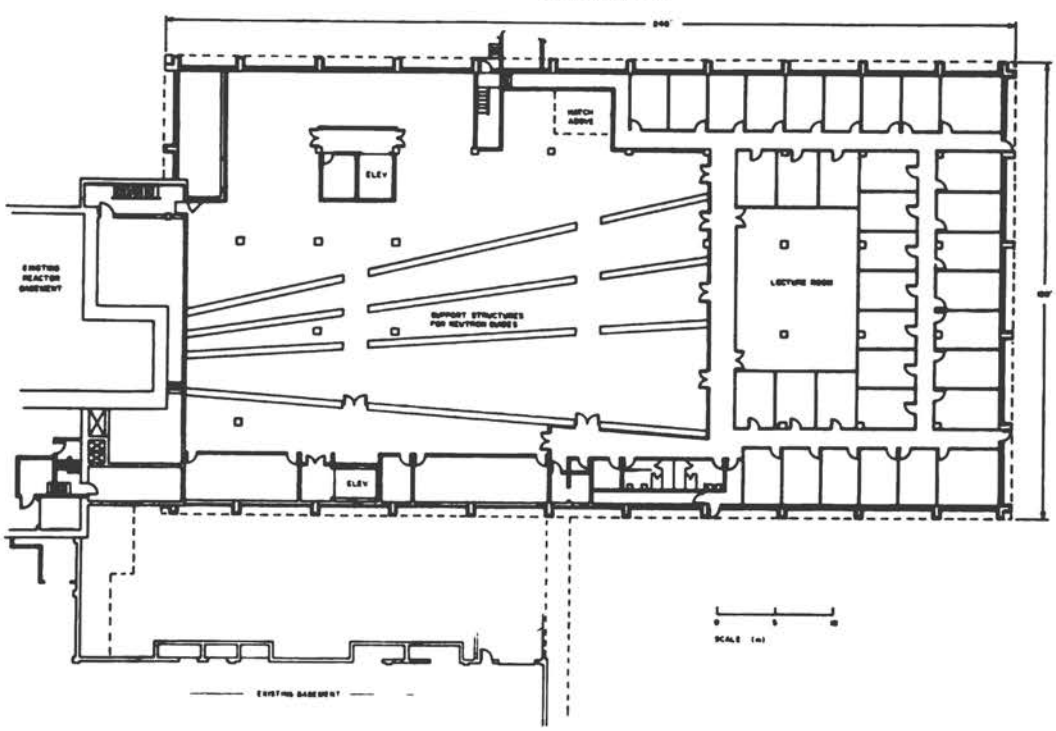
12.0

NBS CENTER FOR COLD NEUTRON RESEARCH
EXPERIMENTAL FLOOR



OFFICE FLOOR



ORNL PRESENTATION
to the
MAJOR MATERIALS FACILITIES COMMITTEE
of the
NATIONAL RESEARCH COUNCIL

FEBRUARY 26, 1984

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Contract No. W-7405-eng-26

Oak Ridge National Laboratory
operated by
Union Carbide Corporation
for the
Department of Energy

CONTENTS

I.	INTRODUCTION	1
II.	SCIENTIFIC JUSTIFICATION	2
III.	USER PROGRAM	6
IV.	REACTOR DESCRIPTION AND PERFORMANCE	8
V.	EXPERIMENTAL FACILITIES	13
VI.	COSTS AND SCHEDULE	16
VII.	SCIENTIFIC SUPPORT SYSTEM	17
	REFERENCES	18

SUMMARY

In the belief that an improved high-flux reactor best meets the total long-term needs of the U.S. in the areas of neutron scattering, isotope production, and materials irradiation, ORNL is beginning an effort to produce the world's best research reactor. Because we have worked on this project for only a short time, our plans and cost estimates are still preliminary, but our objectives are firm. We expect to achieve a peak thermal flux in a D_2O reflector of 5×10^{15} n/cm^2 sec. Through improved beam tube design and focusing monochromators, the number of neutrons incident on the sample could be increased by an order of magnitude over the best now available in the U.S. for many experiments. The reactor would be fully equipped with two cold sources, a hot source, and about 30 advanced instruments. The six cold guides would have a potential scientific value six times greater than the comparable facilities at the Institut Laue-Langevin. Our initial efforts have been focused on a major upgrade of the High Flux Isotope Reactor (HFIR) for which the preliminary cost estimates in FY 84 dollars are as follows:

Conceptual design, R&D, preliminary safety analysis	$24M
Engineering design and construction	
Reactor and Building	$128M
Experimental facilities	$71M
Annual reactor operating cost	$12M
Annual neutron beam research from all sources	$10M

The neutron beam facilities will be a national users' resource with user policies determined by an independent committee. ORNL has demonstrated its ability to design and operate research reactors, and has a broad scientific support system with particular strengths in detector development and design of data acquisition systems. Finally, the construction of a new or modified research reactor would be politically acceptable to the citizens of Oak Ridge.

I. INTRODUCTION

At ORNL we have started a project aimed at the design and construction of the world's best research reactor. Our primary motivation is to provide U.S. scientists with unexcelled facilities for neutron scattering research. As further motivation, we hope to provide unequaled facilities for some nuclear physics experiments and improved, flexible facilities for isotope production and radiation damage studies. Neutron scattering, which was born as a by-product of the U.S. investment in research reactors, has provided unique and fundamentally important information for a wide variety of scientific disciplines: condensed matter physics, chemistry, biology, materials science, and polymer science. At issue is the long-range future of neutron scattering in this nation. We believe the scientific value of this technique is such that the U.S. should have the best possible neutron source to replace its aging sources currently in use (see Table 1). We must not be content with a plan to partially catch up with our friends in Europe; the ORNL plan will put the U.S. significantly ahead of the rest of the world. Because of the long lead time for the design and construction of a major neutron source, we must begin <u>now</u> to have a new source by the mid '90s.

Table 1. Age of U.S. Research Reactors

	Started Operation	Age in 1994
ORR	1958	36
MITR	1958	36
HFBR	1965	29
HFIR	1966	28
MURR	1968	26
NBSR	1969	25

We have focused on a reactor rather than a pulsed source in the belief that a steady-state source best meets the national long-term needs, particularly in the important area of long wavelength, cold neutron research. There has been a substantial world-wide investment in pulsed sources in recent years; it is now appropriate to have a period for developing experimental techniques using these sources and for critical evaluation of the scientific results obtained through these techniques. There is no doubt of the value and reliability of reactors as neutron sources. In our opinion, pulsed sources will remain a valuable supplement to, but not a substitute for, high-intensity steady-state sources.

In undertaking this design effort ORNL is responding to repeated calls from the scientific community for work to begin on a new neutron source. Beginning in 1974 with a letter to the Director of Physical Research of the AEC,[1] continuing through the 1977 NRC report on neutron scattering,[2] the 1980 Brinkman report,[3] and the 1984 Rush report,[4] the U.S. scientific community has issued a series of urgent pleas for the design of advanced neutron sources. It is appropriate, both politically and historically, for ORNL to initiate work on a reactor. The world-wide, popular fear of reactors, which

has been a contributing factor to recent emphasis on spallation sources, is not a significant factor in Oak Ridge. The city of Oak Ridge owes its existence partly to the need for the X-10 Graphite Reactor, where the foundations of neutron scattering were solidly laid by E. O. Wollan and C. G. Shull. Since those early days, ORNL has had a variety of research reactors and the local populace has developed a more sophisticated, less alarmed attitude toward them than has the general public.

We have challenged our reactor design team to produce a thermal flux in a large D_2O reflector of 5×10^{15} n/cm^2 sec. At least as important as this higher flux is the opportunity to fully incorporate the advances in neutron technology which have occurred since the present generation of neutron sources was constructed. By combining higher source strength and improved beam tube design, we hope to achieve an order of magnitude increase in the number of neutrons incident on the sample for many experiments. The planned cold sources and beam guides should have a potential scientific value six times greater than the comparable facilities at the Institut Laue-Langevin (ILL).

II. SCIENTIFIC JUSTIFICATION

In this section we focus primarily on the need for more intense neutron sources. Our response to your questions on recent accomplishments and the ORNL involvement in them is contained in Table 2 at the end of this section.

General Background. It is likely that it will take the best part of a decade to bring a new reactor into operation. It is extremely difficult to anticipate specific research problems which then will be of great interest. However, we are absolutely confident that neutron beams will be essential in gaining fundamental understanding of the new materials sure to be developed in the next and succeeding decades. The growth and diversity of neutron scattering has been firmly based on the unique properties of the neutron as a probe of condensed matter. Basic information on structure and dynamics of materials can be obtained with neutrons that is not obtainable by any other technique. Building more intense photon sources of any energy is not going to change this fact. The only potential conflict is in measuring excitations in the eV range where scientists at spallation neutron sources are reaching up in energy transfer and scientists at synchrotron sources are striving to develop high-resolution techniques in energy transfer. Synchrotron sources offer no competition to neutrons in the thermal and sub-thermal energy ranges below 100 meV where reactor sources are so valuable.

Need for Higher Flux. Our discussion will be biased in the direction of our past scientific experience, but it is certainly true that all scientific disciplines now using neutron scattering would benefit from higher intensities. A more comprehensive review of scientific opportunities is contained in the Rush report.[4]

Many beautiful examples of lattice dynamical examinations of materials by neutrons are in the literature; particularly impressive is the new work on the phonon dispersion curves of the A15 compounds. A complete lattice dynamical examination has been carried out for the low T_c superconductor Nb_3Sb. Unfortunately, large crystals of the high T_c superconductors Nb_3Sn or Nb_3Ge are not available so that a similar study of them is now impossible. It is clear that a study of the electron-phonon coupling should not be limited to only the acoustic modes because the many nearly flat optical modes contribute to the superconducting phenomena. The proposed reactor would make such a study possible. Indeed, this problem is typical; the materials of interest are frequently available only in very small crystals. In fact, lattice distortions that result in a high T_c may prevent the attainment of large crystals for many important superconductors.

Lower dimensional phenomena are always interesting for comparison with theoretical models. Neutron scattering techniques have been used to study the dimerization in $MEM(TCNQ)_2$ that results in the spin Peierls transition. The LA phonon branch has been measured in this material, but the transverse branch, whose softening leads to the transition, has not because of the small sample size and the necessity of high resolution measurements. We believe that this branch could be measured with the proposed reactor and knowledge of its behavior near the transition would be of great importance in the understanding of such transitions. The study of other lower dimensional phenomena, such as solitons and one-dimensional superconductors, would benefit greatly from higher neutron fluxes. Intercalated graphite, which has two-dimensional features, has been the subject of some excellent neutron investigations. Structural information has been obtained for the intercalant layers, phonons propagating normal to the layers have been observed, but studies of phonons propagating within the layers are not available because of the small effective sample size. Higher flux would make these studies possible.

Exfoliated graphite provides us with the possibility of studying surface phenomena. Studies have been performed for rare gas atoms, diatomic molecules, and hydrocarbons on graphite. Elastic scattering measurements have been performed to determine the overlayer structures and phase transitions. Particularly notable are the measurements of the commensurate-incommensurate and melting transitions. Unfortunately, details of these phase transitions have not been entirely established, and higher flux will have a large impact in this area.

Biological specimens are quite often available only as small crystals. Protein crystallography is a very important area where neutrons have provided new information. Higher flux would permit large gains in this area allowing high-resolution diffraction studies of proteins of higher molecular weight and of smaller samples.

Neutrons are unexcelled for obtaining detailed information about magnetic systems. The neutron studies of magnetism and superconductivity in the reentrant superconductor $ErRh_4B_4$ have established the coexistence of ferromagnetism, sinusoidal modulated magnetism with a wavelength of about 100 Å,

and superconductivity in a narrow temperature range near 1 K. Studies on the small single crystal available suggest that near the transition, ferromagnetic fluctuations take place in the superconductor, in contrast to the theories which specify that the fluctuations should be associated with the modulated wave vector. The proposed reactor would make a detailed study of the fluctuations possible, enhancing our understanding of superconductivity. Itinerant magnetism is one of the most challenging theoretical problems, and neutrons must be used to gain understanding of the problem. Of great interest at this time are Moriya's efforts to unify classes of itinerant magnets in terms of spin fluctuation theory. Measurement of the excitation spectra of the weak itinerant magnets like $ZrZn_2$ would do much to assess the effectiveness of the spin fluctuation theory. Small crystals are available, but efforts at the ILL to examine the magnetic excitations have failed. The proposed new reactor would make this investigation possible. Triple-axis polarization-analysis experiments would be particularly valuable for this and a wide variety of magnetic problems.

The quantum solids and fluids ^3He and ^4He have always been subjects of considerable interest. The effective sample size of ^3He is small because of its high absorption. The momentum distribution in ^4He has received considerable attention at a number of neutron scattering centers. With the new reactor source we can measure the momentum distribution in the Fermi liquid regime for ^3He. Pulsed spallation sources will also contribute greatly to this effort, but moderate energy neutrons may have to be used to obtain sufficient momentum resolution. Additional neutron flux would also greatly aid the study of both the paramagnons and phonons in ^3He. Higher resolution is particularly needed to separate more convincingly the paramagnon from residual elastic scattering from the sample holder.

Critical ingredients of the proposed reactor are hot and cold sources built into the reactor reflector and optimized for maximum neutron intensity. The hot source would be very valuable for measuring high-energy excitations in single crystals, for instance, the magnetic excitations in transition metals. Spallation sources are particulary valuable in this range also and would be complementary. Great gains in low-energy neutron fluxes would be provided by the cold sources. Indications are that cold neutron intensities about six times higher than at the ILL could be achieved. This intensity increase would make a wide variety of new experiments possible. Low-energy spectroscopy of chemical systems would be greatly improved, making possible studies of the details of rotation and diffusion of molecular species. Significant improvements could be made in all areas of small-angle scattering. The already important field of investigation of polymers could be greatly enhanced and extended to time-dependent effects. Important theories of polymer dymamics and relaxation could be checked in a definitive manner.

Additional flux would allow important studies of kinetics in materials science. Time-dependent effects of decomposition of solid solution alloys and microstructure changes induced by heat treatment or mechanical strain could be examined. The time scales of importance are seconds to minutes; higher flux means that shorter time duration phenomena could be observed. It

would be particularly valuable to study changes in cluster arrangements which occur at short times after a change in temperature.

This technique of real-time diffraction is certainly not limited to materials science applications. There are exciting opportunities in polymer dynamics, biology, chemical reactions, and liquid crystals. In view of the energy-time relationship in scattering theory, this technique can be considered a pathway to new ultra-low energy regimes. At ORNL we are now constructing, in collaboration with the Japan Atomic Energy Research Institute, a real-time diffraction instrument featuring a wide-angle (130°) position-sensitive detector and a sophisticated data acquisition system. High intensity will be a key factor in extending the range of application of this diffractometer to short time phenomena.

Finally, the enhancement of cold neutron intensity would make possible great improvements in studies of basic neutron properties and in the use of neutron interferometers and neutron optics. A possible application of a very intense cold neutron source is a neutron microscope. This would have great potential for biological investigations as living samples could be examined in air. Neutrons, of course, provide good contrast for elements in biological materials and deuterated tracers could be used. Using modern microlithography, it is possible to build a Fresnel lens with a diameter of 1 cm and a focal length of 1 m for 20 A neutrons. Such lenses are f/100 which is comparable to electron microscope lenses. Stringent beam collimation is needed so counting rates would be low. Nevertheless, with an advanced source it appears that such a device would be practical.

Space limitations prevent further discussion of these topics, but it is clear that present reactor sources have made great contributions to the field of neutron spectroscopy and that more neutron flux is the key to more interesting and important experiments. The reactor has firmly established itself as the central ingredient in neutron scattering studies.

Recent Accomplishments. Oak Ridge has a rich heritage in neutron scattering and has continued a leadership role in the field of neutron scattering. Following is a table of important recent areas of neutron scattering research and development. One * indicates ORNL participation in the area. Two ** indicate a leadership role.

Table 2. Recent Accomplishments in Neutron Scattering

Magnetism

Excitations in transition metals**, rare earths**, and amorphous materials**; excitations and form factors of mixed-valent materials**, magnetic superconductors**, properties of spin glasses*, phase transitions in random fields*, phase transitions in lower dimensional magnets*, solitons, magnetic ordering of nuclei**.

Table 2 (Contd.)

Structures and Phase Transitions

Intercalated graphite*, incommensurate-commensurate phase transitions*, overlayers on exfoliated graphite, protein crystallography.

Lattice Dynamics and Chemical Spectroscopy

Electron-phonon interaction in superconductors**, lattice dynamics of mixed-valent materials**, low-energy spectroscopy of molecular species, dynamics of low-dimensional systems*, phonon-defect interactions**, polymer dynamics.

Quantum Fluids

Momentum distributions in ^{4}He**, excitations in ^{3}He.

Small-Angle Scattering

Chain configuration in polymers**, polymer blend compatibility**, micelles*, flux-line lattices in superconductors**, nucleosome structures**, ribosome structures, membrane studies, microstructural changes in solids.

Neutron Interferometry and Optics

Tests for equivalence in the quantum limit, spinor behavior of the neutron, neutron Fizeau effect, neutron Aharonov-Bohm effect.

Development of Instrumentation

Position-sensitive detectors**, high-resolution spectroscopy, high-resolution powder diffraction and profile refinement, multilayer monochromators, supermirrors, time-of-flight instrumentation, correlation choppers**, interferometers, extreme sample environments (low temperature**, high pressure*).

III. USER PROGRAM

At present the user program associated with the neutron scattering facilities at ORNL includes the program of the National Center for Small-Angle Scattering Research (NCSASR), and a DOE-sponsored program for the other facilities at HFIR (described below) which includes a nearly continuous research collaboration with Ames Laboratory and a U.S.-Japan Cooperative Program in Neutron Scattering.

NCSASR. This is a user-dedicated facility sponsored by NSF through an interagency agreement with DOE. Facilities of the Center include full-time use of the NSF-funded 30-m small-angle neutron scattering (SANS) instrument at HFIR and a fraction of time (~30%) on four DOE-funded instruments; two

small-angle x-ray cameras, a 5-m SANS instrument at ORR, and a high-resolution double-crystal SANS instrument at HFIR. Beam time on the various instruments is assigned on the basis of proposals submitted in advance. All proposals, including those from the ORNL staff, are reviewed by an external Program Review Committee, and all are rated on the basis of scientific merit. The 30-m SANS instrument is usually booked about four months in advance. The performance of the Center is reviewed by a Policy Committee consisting of an external panel of scientists appointed by NSF and ORNL. As shown in Table 3(a), the 30-m SANS instrument has been saturated with users from the beginning, indicating unsatisfied demand for this type of facility.

Table 3. User Participation at ORNL Neutron Scattering Facilities

	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983
(a) National Center for Small-Angle Research					
Experimenter personnel					
University			42	31	37
Industry			9	15	11
ORNL			6	11	11
Other national Laboratories			5	4	0
Others			5	5	2
Total			67	66	61
Use ratio, %					
University			72	72	62
Industry			14	14	13
ORNL			5	8	17
Other national laboratories			5	3	0
Others			4	3	8
(b) DOE Neutron-Scattering Facilities					
Experimenter personnel					
University	3	8	13	19	20
Industry	0	0	0	0	1
ORNL	12	16	13	14	15
Other national laboratories	4	8	8	7	6
Others	5	7	6	6	17
Total	24	39	40	46	59
Use ratio, %					
University	7	10	17	23	21
Industry	0	0	0	0	1
ORNL	75	71	65	61	55
Other national laboratories	8	10	10	9	6
Others	10	9	8	7	17

DOE Program. The other neutron scattering facilities at HFIR, which include three triple-axis spectrometers, a polarized-beam triple-axis spectrometer, a time-of-flight spectrometer, a four-circle diffractometer, and a powder/liquid diffractometer with a linear position-sensitive detector, have always been available to a broad community of users on an informal basis. However, to insure the most effective utilization of these ORNL-DOE facilities by scientists outside ORNL a formal users' program was established in January 1982. A brochure describing the ORNL facilities and a booklet giving policies and procedures have been prepared and distributed to over 200 outside scientists who had previously expressed an interest in our user program. Written proposals are reviewed by a committee of ORNL staff members, and there is a waiting period of about three months in scheduling the experiments. An Advisory Committee, composed of outside scientists, is available to act in an appellate capacity for rejected proposals. The Advisory Committee also reviews the users' program periodically and advises ORNL management.

The Ames Laboratory neutron program relies primarily on their instrumentation installed at the ORR, but the Ames staff are also heavy users of the HFIR facilities. In addition, the U.S-Japan Cooperative Program in Neutron scattering is resulting in significant use (two person-years) of the HFIR facilities by Japanese scientists. These two groups of experienced neutron scatterers provide a nearly continuous stream of outstanding research proposals, which are reviewed as a part of the DOE users' program. As shown in Table 3(b), the number of users of the DOE facilities has grown substantially in recent years. Nearly 50% of the available beam time is now assigned to user experiments. Since it is necessary for the ORNL staff to carry out its obligations to the in-house DOE programs, it is unlikely that this user program will grow much beyond its present size unless the ORNL staff is increased and until additional spectrometers are constructed.

Since the proposed reactor will be a national research facility, a National User Policy Committee, with representatives from the user community, would be established to formulate policies for use of the reactor. We would advocate that some reasonable fraction of the time (~25%) be reserved for instrument development and research by the in-house staff. As detailed in the Rush report,[4] the experience in Europe and in the U.S. is that when new, user-oriented neutron instruments are provided, they become saturated with users rather quickly. We anticipate the same user response to our proposed facility which should accommodate about 450 users per year.

IV. DESCRIPTION AND PERFORMANCE OF REACTOR

Goals. The primary objective of the research reactor design effort is to produce a higher thermal neutron flux with minimal contamination by fast neutrons in a configuration which facilitates use as a source for neutron scattering experiments. The associated requirements are that the reactor be designed for both safety and simplicity of operation and maintenance. This helps in obtaining the required approval for operation from the appropriate

agencies and insures a high on-line availability for experimentation. At the same time, the reactor should be cost-effective with regard to research and development requirements, capital cost, and operating costs including staff, maintenance, and component replacement, especially the fuel elements. The fundamental physical constraints on meeting these requirements involve the material strength of fuel and structural materials as a function of temperature and irradiation history, the heat removal capability of the fuel-clad-coolant combination, and the stability of the fuel element to the rate of coolant flow. Other important limits are the requirements for reactor control, for a reasonable operational core lifetime, and for simple fuel handling.

Current Approach. The fundamental approach of the current design effort is to start with the strength of the current HFIR system, which was designed primarily for isotope production, and work toward an improved source for all users of the reactor. At the same time, the technology base available from the current HFIR is being pushed to a limit which is prudent for obtaining the required institutional approvals and realistic in terms of the operational simplicity and system cost. This approach is intended to capitalize on the success of the existing HFIR system and to utilize the technology which makes this possible. At the present time, the HFIR system has both an outstanding availability (~92% over many years) and an exceptional power density as indicated by Table 4. The preliminary power density proposed for the new design concept is also included for comparison.

Table 4. Comparison of Reactor Power Densities

Reactor	Average Power Density (kW/l)
Commercial high temperature gas-cooled	8
Commercial boiling water	54
Commercial pressurized water	98
Liquid metal cooled	411
HFR (ILL)	1140
HFIR	1930
HFIR-II (preliminary)	3030

Although many other reactor types were briefly considered, and some alternate concepts are still under consideration, there does not appear to be another system which offers the combination of high flux, high operational safety, and reliable, economic operation. Some comments on specific reactor types follow.

1) Gas-cooled reactors offer high inherent safety but low power density, and therefore, low neutron source levels.

2) Commercial pressurized water systems involve increased capital cost, operational complexity, and a reduced safety margin.

3) Commercial boiling light water systems have a significantly reduced safety margin, especially with regard to fuel melting temperatures.

4) Liquid metal cooled systems would require a significant R&D effort to attain the same flux levels, have higher capital and operational costs, and increase safety concerns and operational approval complexity.

5) Multi-loop and separate cores are still under investigation but they appear more expensive in capital and operational cost, more difficult to control, and to require more total power to attain the same reflector flux level.

It is desirable to retain the basic concept of an "in-pool" reactor, even with a D_2O system inside the pressure vessel, in order to facilitate fuel handling and inherent system safety. Also, the highly automated reactor control system concept used in HFIR should be retained since it results in ease of operation, high safety and availability, and reduced staff requirements. It is especially desirable to continue the use of aluminum-based alloys as the fuel dispersion medium and basic constituent for the core, with austenitic stainless steel for the primary cooling system. We estimate that a change from an aluminum-based fuel element to stainless steel would increase core costs by a factor of five and that zirconium-based core costs would increase by a factor of ten. Since the new design concept will probably have a shorter fuel cycle lifetime than the current HFIR (more cores/year), this is a major consideration in operational costs. For example, adoption of a zirconium-based core might lead to an annual fuel cost of $24M.

As an initial basis for comparison, some operating characteristics of existing research reactors are shown in Table 5. Based on this information

Table 5. Operating Characteristics of Existing Research Reactors

	HFR (ILL)	HFBR (BNL)	HFIR (ORNL)
Power (MW)	57	60	100
Coolant	D_2O	D_2O	H_2O
Reflector	D_2O	D_2O	Be
Height/diameter (cm)	80/39	53/51	51/43
Average power density (kW/l)	1,145	705	1,930
Peak unperturbed thermal flux in reflector (neut/cm^2·sec)	1.5×10^{15}*	1.05×10^{15}	1.3×10^{15}*

*These results came from recent ORNL calculations for the beginning of the fuel cycle. Slightly different values can be found elsewhere, and the values also vary over the fuel cycle.

and on the perceived limits in the current HFIR design, the following parameters are being investigated to attain a peak thermal neutron flux in the reflector of ~4–6 x 10^{15}: coolant composition (D_2O, H_2O), reflector composition, core height-to-diameter ratio, metal vs coolant volume fraction in the core, and power density and coolant flow velocity to accommodate system power levels up to 200 MW.

Summary of Core Calculations. An initial set of one-dimensional calculations was performed for scoping purposes. The results are given in Table 6 and indicate significant potential gains in thermal flux in the reflector region from an all-D_2O system at the expense of a heavier fissile loading. This study was followed by a fairly thorough parametric study (~40 cases) performed in two-dimensional r-z geometry and following the neutron flux levels through the full reactor core burnup. Roughly one-third of the calculations were H_2O cooled, primarily with a D_2O reflector, while the rest were D_2O cooled and reflected. Peak and average power densities, fissile loading requirements and consumption, and the peak thermal flux in the reflector were obtained for each case.

Table 6. Preliminary Survey for HFIR-II Core (100 MW, Spherical Model)

Coolant	Reflector	Critical U-235 Loading (kg)	Peak Reflector Flux (10^{15} n/cm^2-sec)
H_2O	C	1.7	1.5
H_2O	Be	1.8	1.6
H_2O	H_2O	3.5	0.9
H_2O	D_2O	2.0	1.8
D_2O	D_2O	3.0	3.0

The general conclusions resulting from the 2-D parametric study are summarized below.

1) An all D_2O system provides ~40% more thermal flux than an H_2O cooled core with a D_2O reflector.

2) By utilizing radially variable fuel loading and burnable poison to flatten the power density, it appears possible to significantly increase the average power density while keeping the peak power density (and thus the peak fuel temperature) roughly constant.

3) The reflector thermal flux peak increases as the system power increases above 100 MW, but cooling requirements will limit the attainable power density and thus constrain the thermal flux.

4) A greater core height-to-diameter ratio tends to increase the thermal neutron flux in the reflector and to decrease the fissile loading, but increases the pressure drop over the core.

5) Reducing the core metal volume fraction reduces the core pressure drop and lowers the fissile loading requirement.

Best Case Results. The results of the parametric study led to the definition of the current reactor core design concept which is presented in Table 7. It should be emphasized that this is a preliminary concept and will

Table 7. Preliminary Reactor Core Concept

- All D_2O system, 2.5-m diameter reflector
- 150 MW (100 MW)*
- Peak power density 4.8 MW/1 (4.4 MW/1)
- Average power density 3.0 MW/1 (1.9 MW/1)
- Metal volume fraction 0.4 (0.5)
- Split annular core, inside radius 13.5 cm, outside radius 24 cm (6.5 cm, 21.6 cm)
- Internal control and safety elements (external)
- Core height 60 cm, core diameter 48 cm (50.8 cm ht, 43 cm diam.)
- Peak unperturbed thermal flux in reflector 4×10^{15} (1.3×10^{15})
- Fissile core loading 9.0 kg (9.4 kg)
- Fuel cycle time 16 days full power (23 days)
- Peak fast flux in central region, $E > 0.15$ MeV ~ 1.5×10^{15} (1.2×10^{15})
- Axial thermal flux variation in the core ~50% (~50%)
- Radial thermal flux variation in the reflector ~ factor of 2 out to 70 cm (~ factor of 5 in beryllium reflector)
- Coolant velocity 60 ft/sec (51 ft/sec)
- Core pressure drop ~150 psi (110 psi)

*Current HFIR values given in parentheses

undoubtedly change as our work progresses. A diagram of the core configuration is shown in Fig. 1. A central D_2O region is surrounded by a cylindrical control plate which is, in turn, surrounded by two annular fuel assemblies, separated by a D_2O region. The two-piece core provides access for possible placement of additional control elements or, potentially, access to a high-energy flux region for material irradiation samples. Having two separate core sections also greatly simplifies fuel handling by reducing concerns regarding criticality safety. The D_2O reflector results in a fairly broad, flat thermal neutron flux distribution in the radial reflector, as shown in Fig. 2. Flux plots for the ILL and the existing HFIR are also included for comparison. Coupled with a relatively small (~50%) axial flux variation in the core, this concept provides a large volume of high-intensity neutrons for the placement of cold and hot sources, and associated beam guides, beam tubes, and material irradiation facilities.

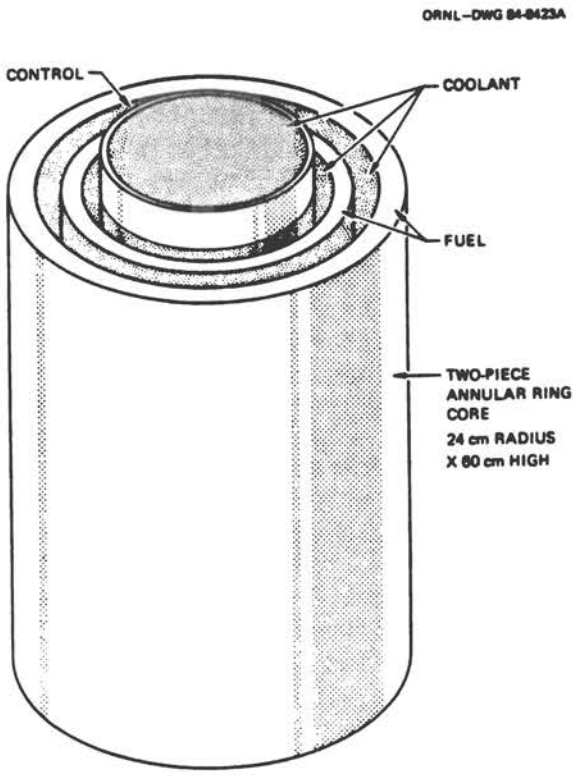

Fig. 1. Preliminary HFIR-II core concept.

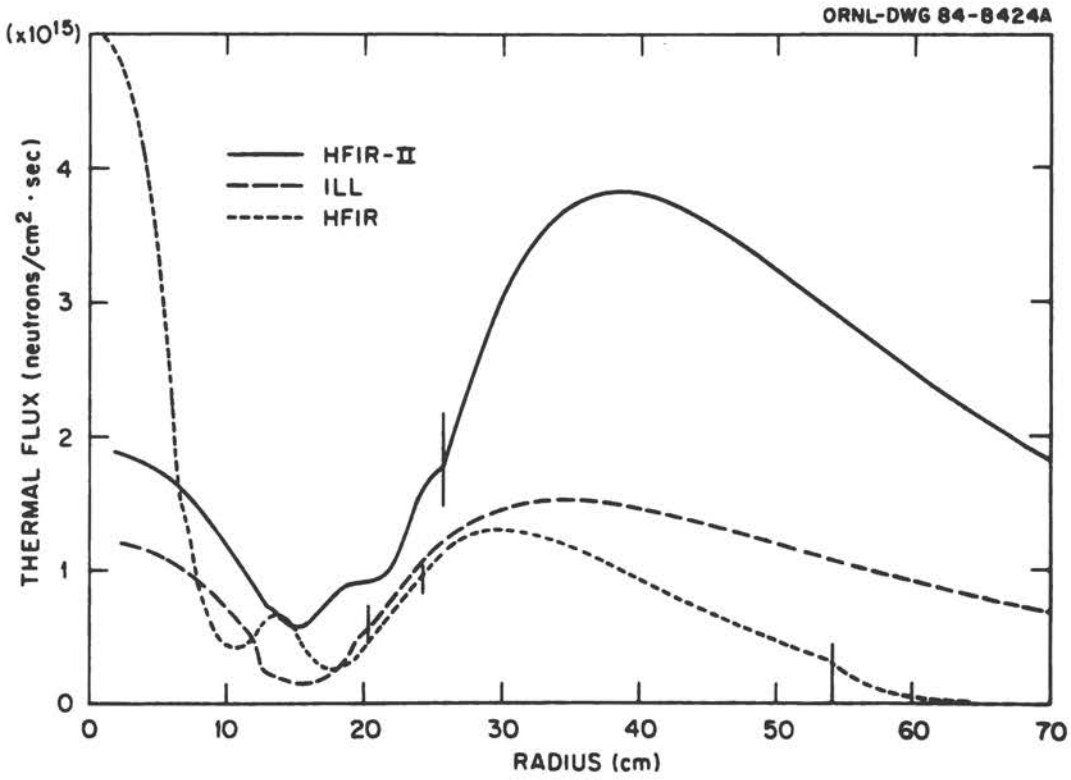

Fig. 2. Thermal neutron flux level vs radius at the core mid-plane. Vertical lines indicate start (and end) of reflector region. All results are from recent ORNL calculations for fresh, unperturbed systems.

Future Efforts. While the preliminary design concept presented in Table 7 represents a distinct advance over the performance of the current HFIR core for neutron scattering, there are indications that the performance might still be increased significantly, and a peak thermal neutron flux of 5–6 x 10^{15} in the reflector appears attainable, provided that the physical stability of the fuel plates proves to be sufficient. In particular, the ability of the new core element to withstand the increased coolant flow required for higher power densities appears to be significantly greater than initially estimated. Increased performance will, of course, come at the expense of higher fissile loadings and increased coolant pumping power and heat dissipation capacity.

V. EXPERIMENTAL FACILITIES

The first step in our study is an evaluation of a major HFIR upgrade. Since we have not progressed past this first step, we are not yet in a position to offer concepts of an entirely new facility.

The two major current problems with the HFIR are the limited number of horizontal beams (4) and the limited floor space for experimental apparatus. We are working on a concept which solves these problems by creating a large experimental guide hall (210' x 200') with eight beam guides, enlarging the existing experimental space in the beam room, and adding three more horizontal beams. The guides exit the reactor on the side not presently used for beam tubes, pass under the storage pool in a transition region which can be used for bending the guides, and then enter the new guide hall. The concept is illustrated in Fig. 3. Two cold sources in the D_2O reflector supply cold neutrons to six guides, and there are two thermal guides. A hot source feeds two horizontal beams in the enlarged beam room. Four slant tubes (2 thermal, 1 hot, 1 cold) deliver neutrons to an experimental area on the floor above the beam level floor. The array of beams is summarized in Table 8. It is anticipated that the thermal and hot tubes will see source fluxes of

Table 8. Proposed Beam Lines

Type	Energy	No.	Dimensions (cm)
Horizontal Tube	Thermal	5	10 x 15
	Hot	2	10 x 15
Slant Tube	Thermal	2	10 diam.
	Cold	1	10 diam.
	Hot	1	10 diam.
Horizontal Guide	Cold	6	4 x 15
	Thermal	2	4 x 15

GROUND FLOOR BEAM PLAN

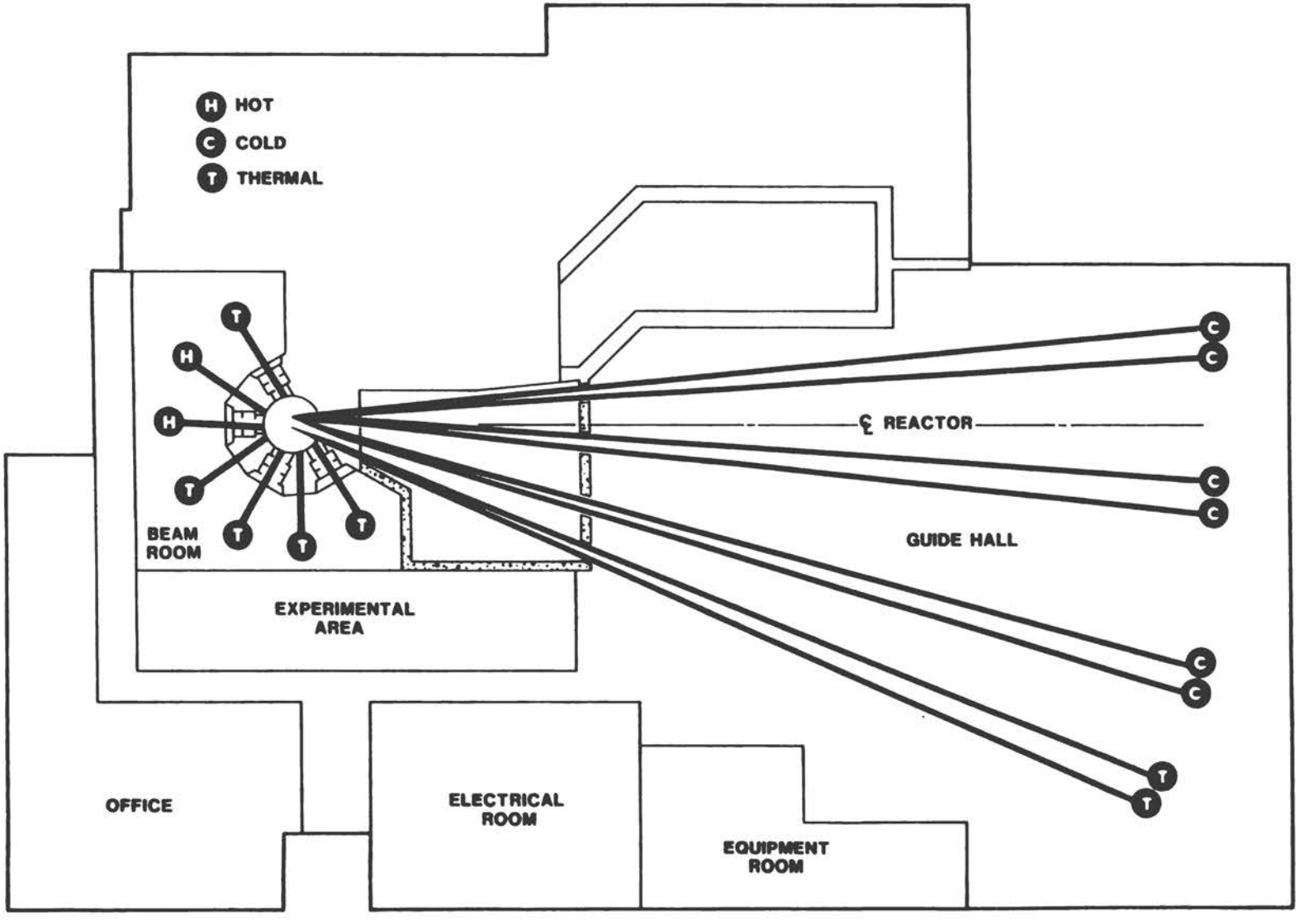

Fig. 3

4–5 x 10^{15} n/cm^2 sec and the cold source will be placed in a region where the thermal flux is about 3 x 10^{15} n/cm^2 sec.

The heat removal problem associated with the two cold sources is a challenging engineering task on which we are just beginning to work. If liquid D_2 is used we must have a large He refrigeration plant of about 50 kW capacity and may have to use forced circulation of the D_2. Assuming that satisfactory cold source operation can be achieved, it is of great interest to compare the potential scientific value of the cold neutron facility with similar facilities, both existing and proposed. We suggest that one reasonable figure of merit is simply the total number of cold neutrons delivered to the guide hall. For some experiments a more meaningful figure of merit is the neutron intensity delivered by the guides, in which case one can leave the guide cross-sectional area out of consideration. Acknowledging either ignorance or equality of such factors as the guide coating material, degree of illumination of the guide by the source, attenuation between source and guide, and efficiency of moderation of the source, a partial figure of merit (M_T) based on the total number of cold neutrons can be obtained by the product of the unperturbed flux at the cold source position, the area of each guide, and the number of guides. An alternate, intensity-based figure of merit (M_I) ignores the guide area. The appropriate numbers for several facilities of interest are given in Table 9 where the partial figures of merit have been normalized to the installation at the ILL. There are two important points to be made with regard to Table 9. First, the NBS and BNL proposals, while valuable as first steps, will not come close to putting the U.S. on a par with the ILL, let alone surpass its capability. A plan which fails to look beyond these proposals is unsatisfactory in the long term. Second, the ORNL proposal has the potential to produce the world's best cold neutron facilities by a wide margin.

Table 9. Potential Scientific Value of Various Cold Neutron Facilities

Location	Flux (10^{14}n/cm^2 sec)	Av. Guide Area (cm^2)	No. Guides	Partial Relative Merit M_T	Partial Relative Merit M_I
NBSR(NBS)*	1.7	102	5	0.4	0.24
HFBR(BNL)*	3	22	3	0.1	0.26
HFR(ILL)	5	63	7	1	1
HFIR-II(ORNL)*	30	63	7	6	6

*Proposed

At the present time we are planning to install a hot source even though a case can be made that this experimental regime should be left to the spallation sources. We believe that important results on the structure of liquids and amorphous materials and on high-energy excitations could be obtained with an intense, reactor-based hot source. Probably, the hot source

will be a block of graphite located in the D_2O reflector and heated to around 2000 K. It should produce hot neutron beams with intensity four times greater than those at the ILL.

For many experiments, significant intensity gains with little loss of resolution can be achieved by relaxing the vertical collimation in the beam tubes. Examples are triple-axis spectrometry, powder diffraction, and diffuse scattering. Two methods for providing greater vertical divergence are to increase the height of the beam tube at the source or to use vertically focusing monochromators. The first method is used at Chalk River where the beam tubes are elliptical with axes of 3 7/8" and 8 7/8". In a vertically focusing monochromator the reflecting planes are curved to form a cylindrical surface so that an image of the source is formed at the sample position. While vertically focusing monochromators are in widespread use, the existing arrangements of beam tube, collimator, shutter, and post-monochromator collimation have not been designed to take full advantage of the possible gains. The essential point to remember is that for vertical focusing the intensity at the sample position is proportional to the height of the monochromator; while for a conventional, flat monochromator the central intensity at the sample is proportional to the height of the source. Possible gains are summarized in Fig. 4 which shows the total number of neutrons incident on a sample as a function of sample height. The source-monochromator-sample separations correspond to an existing HFIR spectrometer. At the present time we are restricted to a source height of 4" and a monochromator height of 2.5". For the new reactor we are considering elliptical or rectangular beam tubes 4" wide and 6" high with vertical collimation which would allow 6" high monochromators. This proposed design would allow gains of 2.4 for small samples and 3.6 for large samples over the best now obtainable at HFIR in addition to the gain achieved by higher source flux. With a flux of 5×10^{15} n/cm^2 sec in the reflector, this would result in gains of a factor of 12–18 in neutrons incident on the sample. For small samples it would be desirable to have the capability to decrease background with no loss of intensity from the sample by adjusting the effective source height.

Approximately 30 instruments of diverse purpose would be constructed. The selection of instrument types will be made after careful consultation with the user community. As a first step in this process, a workshop will be held on May 30, 1984.

In this report we have naturally placed all our emphasis on neutron scattering, but it should be remembered that research reactors serve many purposes. In the new reactor there would be facilities for isotope production, materials irradiation, neutron activation analysis, and nuclear physics research. We will also consider facilities for γ-ray diffraction, positron production, depth profiling, and neutron radiography. The HFIR was designed to produce a very high thermal flux in the central flux-trap region for production of transuranium isotopes. However, we now know that the production of certain important isotopes, like ^{252}Cf, ^{254}Es, and ^{257}Fm, would benefit from a harder neutron spectrum. For example, the production of ^{254}Es from ^{252}Cf increases by a factor of five when Cd is used as a thermal neutron filter and

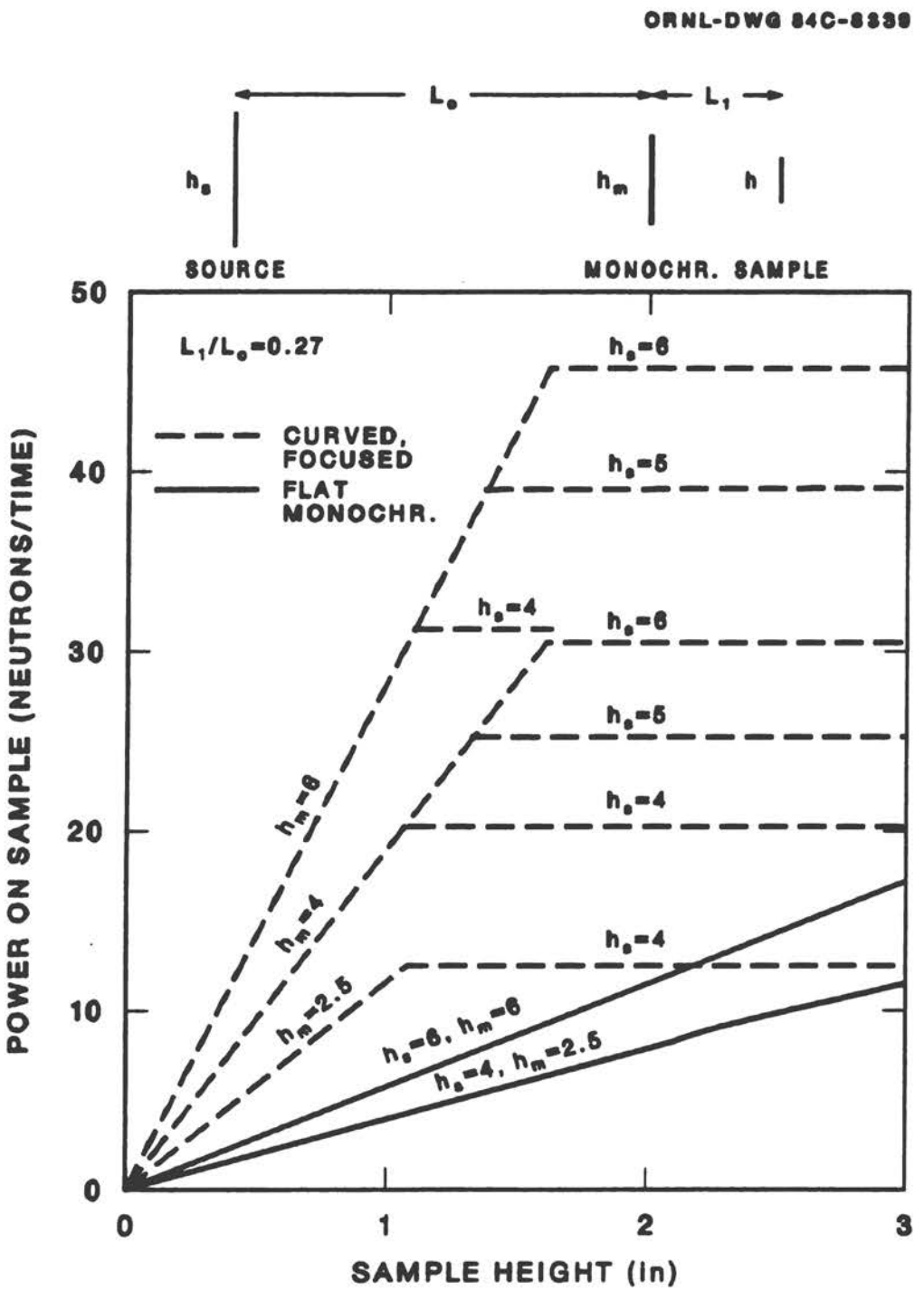

Fig. 4. Neutrons incident on sample as function of sample height for various combinations of source height (h_s) and monochromator height (h_m). Dimensions are in inches. The proposed HFIR-II design would allow operation on the $h_m = 6$, $h_s = 6$ line. At present we are limited to $h_m = 2.5$, $h_s = 4$.

the sample is exposed to only epithermal neutrons. In HFIR-II we will try to provide more flexible isotope production facilities so that the neutron spectrum can be adjusted to maximize productivity of certain isotopes. The fusion reactor materials program could also benefit from a major HFIR modification. Their needs are for a lower thermal flux, a higher fast flux, a capability to adjust the flux spectrum to meet experimental requirements, a larger sample volume, and the ability to properly monitor and control the sample environment during irradiation. Every effort will be made during the design phase of HFIR-II to maximize the value of the reactor to all user programs.

VI. COSTS AND SCHEDULE

Please remember that we are at the beginning of a lengthy design process so that our estimates of the costs are uncertain. A reliable cost estimate will not be available until completion of the conceptual design. We are assuming that the facility will be designed to meet NRC standards but will not be subject to licensing procedures by the NRC. There would be a significant impact on cost and schedule if NRC licensing is required. Our current cost estimates, summarized in Table 10, are based on a 200 MW reactor with the facilities described in the preceding section including up to 30 experimental instruments. We have assumed replacement of essentially all the HFIR equipment including, of course, the core and pressure vessel. Only the pool and building remain, with extensive modifications and additions to the building. At the present level of accuracy, the estimate for an entirely new facility would be close to the values in Table 10. The research and development funds are needed for work on fuel development, cold and hot sources, heat transfer, structural mechanics, and criticality and control. Based on operating experience with the HFIR we estimate the annual reactor operating cost as $12M ('84 dollars). The major assumption is a factor of two increase in the fuel cost over the current HFIR fuel. It should be noted that the total operating cost of the HFIR and the ORR was $10M in 1983.

Table 10. Estimated Costs for Design, Development, and Construction. Contingency not included.

FY	Activity	Cost '84 M$
86	Begin conceptual design, safety analysis, R&D	4
87	Issue Conceptual Design Report, continue safety analysis, R&D	8
88	Complete R&D, issue Preliminary Safety Analysis Report	12
89-93	Engineering design and construction	
	Reactor and building modifications	128
	Experimental facilities	71
	(Beam tubes, guides, shutters, cold and hot sources, spectrometers)	
94	Begin operation	

In order to use the experimental beam facilities efficiently and to assure strong interaction with users, we recommend a research budget of $10M per year. This is based on a research staff of 60 scientists, not all of whom need be permanent employees, 15 technicians, and 3 engineers.

VII. SCIENTIFIC SUPPORT SYSTEM

The Oak Ridge National Laboratory has all of the scientific support systems one would expect at a major research laboratory. There are broad-ranging experimental and theoretical research programs in the Biology, Chemistry, Metals and Ceramics, Physics, and Solid State Physics Divisions. There is a large support staff of design engineers, electronic engineers, instrument technicians, and craftsmen for the development, construction, and maintenance of experimental equipment and instrumentation. Sophisticated sample preparation and characterization facilities are available within the research divisions. The Computer Sciences Division provides assistance with data acquisition and analysis along with access to their computing facilities which consist of two IBM 3033 computers and a DEC PDP-10 with five parallel processors.

Aside from these essential, but general, support systems there are specific features of the ORNL organization which would provide additional scientific advantages to the construction of HFIR-II.

1) Neutron Scattering Experience. Research programs in neutron scattering exist in the Chemistry and Solid State Divisions at ORNL. The personnel within these research groups provide valuable expertise regarding the desired experimental facilities at the new reactor.

2) Detector Development. The detector development group of the Instrumentation and Controls Division has pioneered the design of position-sensitive detectors, several of which have been built and installed at ORNL neutron diffractometers. This expertise will be of great value in the instrumentation of the new reactor.

3) Data Acquisition and Control Systems. Also within the Instrumentation and Control Division are groups devoted to the development of computer-based systems for control of experimental apparatus and data acquisition. They already have extensive experience with neutron spectrometers.

4) Reactor Design Expertise. ORNL has a long and successful history in reactor design. One of the more recent examples of their success is the HFIR which has produced the highest thermal neutron flux in the world for the past nineteen years with a reliability factor in excess of 90%. The ORNL staff has the capability to design and operate the HFIR-II.

REFERENCES

1. Letter to John Teem, Director, Division of Physical Research, from Julius Hastings, October 25, 1974.

2. "Neutron Research on Condensed Matter: A Study of the Facilities and Scientific Opportunities in the United States," National Research Council, 1977.

3. "Report of the Review Panel on Neutron Scattering," Ames Laboratory IS-4761, UC-25, 1980.

4. "Current Status of Neutron Scattering Research and Facilities in the United States," Subcommittee on Neutron Scattering, Solid State Sciences Committee, National Research Council, 1984.

THE ROLE OF NATIONAL LABORATORIES IN MATERIALS SCIENCE RESEARCH

H. Postma

Transcript of a Talk Presented to the Seitz Committee of the National Research Council Washington, D. C.

April 16, 1984

The materials research roles of the National Laboratories encompass a variety of activities besides the operation of major facilities. I would like this morning to point out some of those other activities (summarized in Figure 1) and examine how they interrelate. Your committee is trying to get a clear picture of National Laboratory materials sciences research, and this makes it essential to see how the relationships between the major facilities and these other programs or efforts operate, and how they strengthen the overall effort.

One of our major activities is to support the national missions in fusion, fission, fossil, and solar energy, as well as energy conservation through the technological development of new materials. I should also include in the list of Figure 1, at least for the Oak Ridge National Laboratory, support activities for the Nuclear Regulatory Commission, which has large materials efforts, as well. I will talk about those later.

A second major activity involves basic research in support of the technologies. This is basic research that is more or less targeted: we might say, all right, we would like to have a new kind of ceramic that might do so-and-so, without specifying exactly the characteristics, or, we would like to incorporate waste in a particular kind of media--please see what you can do.

Then, there is long-term multidisciplinary basic research in which you do not know what the outcome is going to be: and finally there is the construction and operation of major facilities, which is basically what your panel is addressing.

The national labs provide a framework for carrying out all these activities, and I am going to talk about that framework -- how we integrate these activities into a coherent effort -- this morning. As a concrete example, I am going to talk primarily about Oak Ridge. I will also talk about some work at Argonne. I asked all the laboratories, aside from their defense parts, to send me some suggestions three weeks ago, so I could incorporate it in the talk, and Argonne was kind enough to respond. I appreciate that.

To give just one example of an integrating framework, Oak Ridge manages a fossil-energy materials program to achieve certain results for the fossil materials people (Figure 2). One aspect involves the Lab doing the

planning -- the technical planning -- for the materials R&D needs. The actual research implementation turned out to involve $8.8 million in FY 1983, of which about 24 percent went for in-house research and the balance was subcontracted -- 27 percent to universities, and 49 percent to industrial research centers and to other government and other national laboratories.

We interface this programmatic research with the basic energy-sciences work. Let me show you how that works and follow the thread through. If you scan through the activities of the entire fossil-energy program at Oak Ridge, which include liquidification R&D, enhanced oil recovery, etc., you come to the panel on Figure 3 termed "materials." You will note that related basic energy sciences research involves about $1.5 million. Among the BES research activities that interface to the materials technology is our iron-nickel aluminide work, on which I will concentrate. But I should note some other interfaces: in BES solid-state research they study ion implantation for improved ceramics and they also carry out surface investigations. All of these different activities intertwine, and that is one of the things that National Labs expedite: the integration of those activities.

Now let's see what that means in practice. We subcontract, as I said, 76 percent. We go to the institutions shown in Figure 4 for various purposes. This is rather sketchy in the sense that I do not give the specific science or technology that is being looked at, but you can see from the figure what is being studied at a variety of schools, industries, and at other national laboratories. So that is one example of how the National Labs integrate diverse activities.

Now, the fossil energy people are hunting for good structural materials that have the kinds of qualities listed in Figure 5: high-temperature strength, corrosion- and erosion-resistance, ductility, and in general, structural materials that do not use a lot of strategic materials. One of the approaches we followed to meet these requirements involved the iron-nickel aluminides. If you look at Figure 6, you will be reminded that single crystals of nickel aluminide are ductile, but in polycrystalline form the material is extremely brittle. I am going to pass around a particular sample (Figure 7) in which a little boron was added, about 500 parts per million. Note its flexibility.

This new material came about through a suggestion for in-house seed money, as we call it, where we invest a little bit of the laboratory overhead money to try out promising ideas. We found out that the procedure worked. The basic energy sciences people then proceeded to fund it for further investigation.

All of a sudden, the fossil energy and the conservation and other people thought it was a desirable alloy for their purposes, so we put together an effort to develop the alloy more fully. That occurred about two years ago. At the present time there are nine industrial companies that are taking this technology and doing something with it, including making commercial-size heats.

Now why is this material interesting? It is now ductile, so you can fabricate it -- take the foil and wiggle it around and compare with what the pure iron-nickel aluminide looked like. You find if you look at Figure 9 that nickel aluminide with boron has favorable high temperature characteristics compared to stainless steel and hastelloy, one of the superalloys, and the waspalloy, which is a cast used in turbines. And the advanced aluminides, which are now a step beyond what I am passing around, and which incorporate hafnium and traces of other elements, are very, very much stronger at high temperatures, and that is what is now being commercially looked at by commercial teams.

So now we have nine companies who are actually interested in taking over, and their proprietary work will lead to the ability to actually make those commercial heats. We feel that this is a very successful transition in a very short time from seed-money investigation, to funding by basic-energy science, to incorporation within the total complex of the Department of Energy, to the actual transfer of that technology, again, all in a fairly short time.

Another kind of research addresses the fact that we really do not understand why boron or hafnium or other additions play the role in ductility that they do. But now, because the technology has made this advance, there are people at General Electric who are looking at the bonding mechanism, the sharing of electrons between boron and the other members of the structure. It is not unusual to have the science lead the technology, but in this case the process -- and Oak Ridge is also working with the universities to see if from the fundamental understanding you can make further advances -- was reversed.

In another area, we are looking at the fracture toughness of alumina containing 20 percent zirconia doped with yttria, and you can see in Figure 10 that by concentrating on high uniformity and high purity, you can actually create a ceramic that is very much better than results from conventional techniques.

You can also make stronger materials by using silicon carbide whiskers to reinforce ceramics. Figure 11 is just a picture of a whisker-reinforced ceramic, and some of its properties are shown in Figure 12.

So these whisker-reinforced and dispersed-particle composites now exhibit potential for improved high-temperature strength over conventional silica carbide and, therefore, they are of some importance, because the conservation people are interested in ceramic heat engines. In this case, again, the technology is leading the science.

I also want to talk about the Nuclear Regulatory Commission program, because frequently we forget the way diverse activities can interrelate. The heavy-section steel program looks at materials, develops analytical methods for calculating the point at which things break and actually carries out structural testing (Figure 13).

The problem is this: In a reactor, you are very much worried that the containment might be breached. You worry about fractures that may exist in the reactor vessel, particularly under high pressure conditions that occur in reactor operations (140 megapascals can be reached at approximately 300-or-so degrees C). When a reactor vessel is quenched, you worry that any preexisting fractures may propagate and grow. If the pressure vessel breaks, then you have a bad release.

In order to investigate this possibility, what people normally do is -- and it has been going on for a number of years -- to calculate how fractures actually propagate, lock the results and the computer code in a safe, and then "run" the experiments later. Not many people like this approach, but that is one of the realities of the program. You perform a test to make the sample vessel break and then dig out the code and see what happened.

Recently we were able to use a combination of pressure and temperature cycling -- and this involves the major facility shown in Figure 14, but it is not a major facility under your consideration, because it is not, science directed, but it is a technology which is driving the science in trying to understand fracture mechanics -- to try and understand how fractures are initiated and how fractures are arrested.

This very large facility lets us test sample reactor vessels under actual conditions. We made an important discovery: The NRC or the ASME code is about a factor of two too conservative, because the cracks are arrested very much sooner than one would have thought from the computer code development. That may be because of three-dimensional effects or it may be because of a misunderstanding of fracture mechanics, but in any event measurements made in a precise way led to the discovery.

What does it mean? There are a number of reactors whose containment vessels have been investigated because the NRC is concerned that their lifetime is about over. The lifetime would be about 17 years, according to the present code.

According to our new results, that lifetime can be extended to 39 years. Well, that is quite an important economic repercussion from materials science, or from materials technology. In fact, that one little experiment alone could pay in savings for the entire materials program in the United States. That is just one example, but you can find others if you look around with that in mind.

Such things occur because at a national laboratory you have the people that can put together a big facility, that can understand both the science and the technology and work together -- mechanical engineers, metallurgists, and solid-state physicists, in this case.

Another example, this time at Argonne, involves the study of radiation-induced segregation that is illustrated in Figure 15. Selective transport of certain elements occurs as shown in Figures 16 and 17 causing elemental

redistribution in the material when it is irradiated. Why this happens is a good scientific question, and one that was not predicted.

Of course, the phenomenon has ramifications because the technology people are very much worried about what happens when materials are irradiated for a very long time. Radiation induced segregation occurs and it leads to embrittlement. So the technology concern is, do these low-swelling alloys that were created about a decade ago actually lose resistance at the very high radiation dose.

As another example, surface modification -- these activities use what we might call minor, rather than major facilities -- involves a multidisciplinary approach to trying to develop new materials, in this case through laser annealing and through ion implantation. I will give you the two examples mentioned in Figure 18. A few years ago (again, this is the second case of such a story) some people came to me and asked for some seed money to try to look at the effects of ion implantation and laser annealing, because they thought they could create supersaturated alloys. They could blast the surface, have rapid melting and rapid quenching, and wind up with a different phase that was scientifically very interesting. The work also happened to have some practical repercussions, which is what I will talk about now -- I will not talk about the science, which is another area that would take a fairly long time itself.

In short, we are now able to create solar cells (Figure 19) by implanting material with a glow discharge rather than doing ion implantation -- this is now being done by Helionetics, a private company in California -- and then laser-annealing the damage out, yielding solar cells that have about 16-1/2 percent efficiency and that can be fabricated through mass-production (Figure 20).

This was a sort of spinoff from a technique that was developed mainly as a scientific pursuit that then evolved into this. As a final example of surface modification, people from The University of Alabama in Birmingham came to us, because we have a users facility (I am going to give you some users statistics in a minute), to find out how to use this facility for improving artificial hip joints. You say, well, what is going on?

Hip joints are made out of titanium. When in the body, they corrode through electrolytic action. If you rub your fingers over the sample I'm passing around (Figure 24) you can feel the roughness in the normal titanium alloy, and the smoothness or lack of corrosion in the ion-implanted alloy. By surface-implantation of nitrogen you can increase the protection of this surface by a factor of 400 or 500, which means now that your hip joint may last 1000 years instead of 4 years. That is pretty significant. If you could only get the rest of you to last that long, I think you would be in good shape.

The actual hip joint, planted in a polyethylene socket looks like the rendition in Figure 23. This is titanium that was initially very well polished and after it sits in your body for a few years, it begins to take the form of that rough surface you felt a moment ago.

The ion-implanted joint is now before the FDA for approval and several companies are involved. The additional cost of implantation is about 1 percent of the cost of the hip joint, to start with, so that means the company will probably charge about $3000 for the hip joint instead of $1500.

Well, what has happened? The major thing that has happened, is that the interrelationships in the national laboratory between the science and technology have, as expected, yielded a lot of benefits. They are easy to recount and easy to understand.

Another very important and new thing that has happened is that the laboratories have opened up their facilities for a wide variety of uses. In this surface modification case, you can just look at Figure 25. In this particular ion surface modification laboratory we have over 40 companies--and universities--that come in to use this facility to study new phenomena scientifically.

In fact, we had to double the size of the laboratory and then add a new accelerator in order to be able to handle the work load. If you look across the entire DOE complex and ask what kinds of facilities are being used by the communities (DOE came out with a summary book recently -- Figure 26 shows a list of those that are related to materials science) you find that a lot of people all over the country are coming to utilize these unique facilities. Figure 27 provides usage profiles of some major facilities similar to the ones you are considering. You see that roughly 50 percent of the usage, in most cases, is by universities and industries, the remainder by in-house and other DOE and government laboratories, and a fair fraction by foreign groups. So these are the kinds of facilities that are attracting national and international attention.

In one example Schlumberger uses -- in a proprietary way -- a DT neutron source (Figure 30) in oil wells to try to understand what is in the well -- to identify what hydrocarbons are present. To calibrate the device, they went to the intense pulsed-neutron source at Argonne to make the measurements summarized in Figures 28 and 29. Again, here is a utilization of a scientific facility which has a practical repercussion.

About a year-and-a-half ago Roger Whiteley and I wrote an article for Research Management on user facilities. About six months later it appeared in Business Week (Figure 31) and it outlined How Business is Using the Government Laboratory. If you read that article, you will find that it deals with precisely the kinds of large unique facilities that you are making decisions about: facilities which represent unique capabilities in this country, and perhaps in the world, that permit industry to gain a toehold in a proprietary way, and science to advance immensely.

About two weeks after that article came out, there was an Exxon ad in which Exxon was bragging -- I think you have seen a lot of these ads -- about how the small-angle neutron scattering facilities at Oak Ridge and at the National Bureau of Standards were being used for polymer research (Figure 32); again, an industrial use, carried out, in this case, in an open way.

Industry has been having a hard time creating useful new polymers, and so they have been looking at new ways to combine old polymers and trying to understand how those polymer blends will work. Small-angle neutron scattering is a tool for seeing whether these things are compatible (Figure 33) in which case those blends may actually have some use. These neutron-scattering studies of polymer blends have been done by the variety of institutions listed in Figure 34, including the University of Massachusetts by themselves, and also in cooperation with Xerox and Exxon, and proprietary research done by DuPont, Firestone, and Kodak. So that is a hot field.

I have taken you through alloys fast, ceramics fast, polymers, and composites, but all of these materials sciences come together around a lot of major facilities that are necessary for the research.

What does it take? As Figure 36 illustrates, building and constructing facilities, major ones such as those as you are deliberating, is only one step. You have to identify the driving scientific requirement or the technological requirements. The users look to the facility scientists to tie the new instrumentation together. They look to us to provide a good reliable and high availability operation, to ensure continued funding, and we, the facility's management, has to look to the users for identifying the needs.

There are a lot of ancillary facilities (Figure 37) that are provided, that are absolutely necessary, and you heard some of those particularly emphasized by Los Alamos yesterday: computers, engineering, maintenance, all of these things, in order to ensure that these things will operate, as Ralph Moon says, with better than 90 percent on-line time, so that the users, when they go, know that they will have something to work with.

I should add number nine to Figure 37, because nine, in the case of reactors, has got to be tanks and machine guns and other things that are required nowadays and that, of course, pose a serious problem, particularly at university research reactors.

What have we learned from the past (Figure 38)? Adequate funding is crucial. With marginal funding you just cannot realize the full potential of the machines. Construction-related R&D is needed. You have got to allow for state-of-the-art instrumentation, initially in the construction phase. I think NBS yesterday also indicated that that is a crucial element. And you have got to get funding for the new instrumentation.

There is a belief that there is a sum-zero game; that is, if you do anything new, it comes out of the hide of everything that exists (Figure 39). I think, if you look, you will find that large new facilities mainly come at the expense of existing large facilities in terms of operating.

It is new money -- so-called construction funds -- that builds new machines. It is unrealistic to expect that those construction funds would be turned into operating funds by Congress, so you have to consider the construction funds separately.

What usually happens is that any time there is a large new facility, an old one gets shut down. You find that the discoveries made in large facilities really open up entirely new areas of science, new fields appear and, in fact, the whole area of science progresses as a result. Consequently, large materials facilities will create overall growth in materials science.

I believe that the high-energy physicists who were bold enough to propose a Desertron at a cost of somewhere between $1-5 billion are bold enough and probably will succeed. I hope that the materials scientists will not be too timid to try to get a number of major facilities that represent only 10 percent of that cost, that will yield science and technologies that are as important in their own right as high-energy physics is in its; but that will yield, in addition to new understanding, something that is of direct consequence and benefit to the country, things like solar cells or hip joints or new alloys or new ceramics.

My final point deals with quality and quantity. The quality of basic-energy sciences and materials research was looked at a couple of years ago by a very extensive study (Figure 40). There are about 1200 projects in the Department of Energy. One hundred twenty-nine of them were randomly selected for review. A peer review was done by 180 people, of whom 85 were from universities and others were divided between industry, the national laboratories, and other groups, such as not-for-profits. That evaluation indicated -- it studied some 30 percent of DOE's materials research -- that the programs are well managed, and provide high-quality science and long-range mission support (Figure 41). Materials sciences have remained strong. All these reviewers said that the laboratory and non-laboratory materials programs were comparable in quality, and that, in fact, the large-dollar projects rated higher than the smaller projects (Figure 43); that is, those things associated with large facilities yielded better science than the smaller ones.

Ninety percent of BES materials projects were rated good or above, with no important deficiencies. Figure 43 shows you some of these ratings. The numerical scale rating of 10, like Bo Derek, is the best. Below 5 indicates that DOE ought to pay some attention to it -- 5 was sort of a threshold.

For projects between $100K and $350K, the study found that, in general, the laboratory projects were better, but there were at nonlaboratories more projects that were rated excellent at the high end, so you pays your money and takes your choice in that interpretation. For those who want to follow this up, I think you will find that, as usual, there are a lot of DOE reports around. This is a report from March, 1982, an Assessment of the Basic Energy Sciences Programs and it is done across the board, not just in materials sciences.

I think you will find the report very interesting, because one of your concerns is not just new projects, but also how well old ones have been done and how well the new ones are likely to be done.

NATIONAL LABORATORIES' ROLES IN MATERIALS RESEARCH

presented by

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OAK RIDGE NATIONAL LABORATORY

to the

MAJOR MATERIALS FACILITIES COMMITTEE

COMMISSION OF PHYSICAL SCIENCES, MATHEMATICS, AND RESOURCES OF THE NATIONAL RESEARCH COUNCIL

MARCH 19, 1984

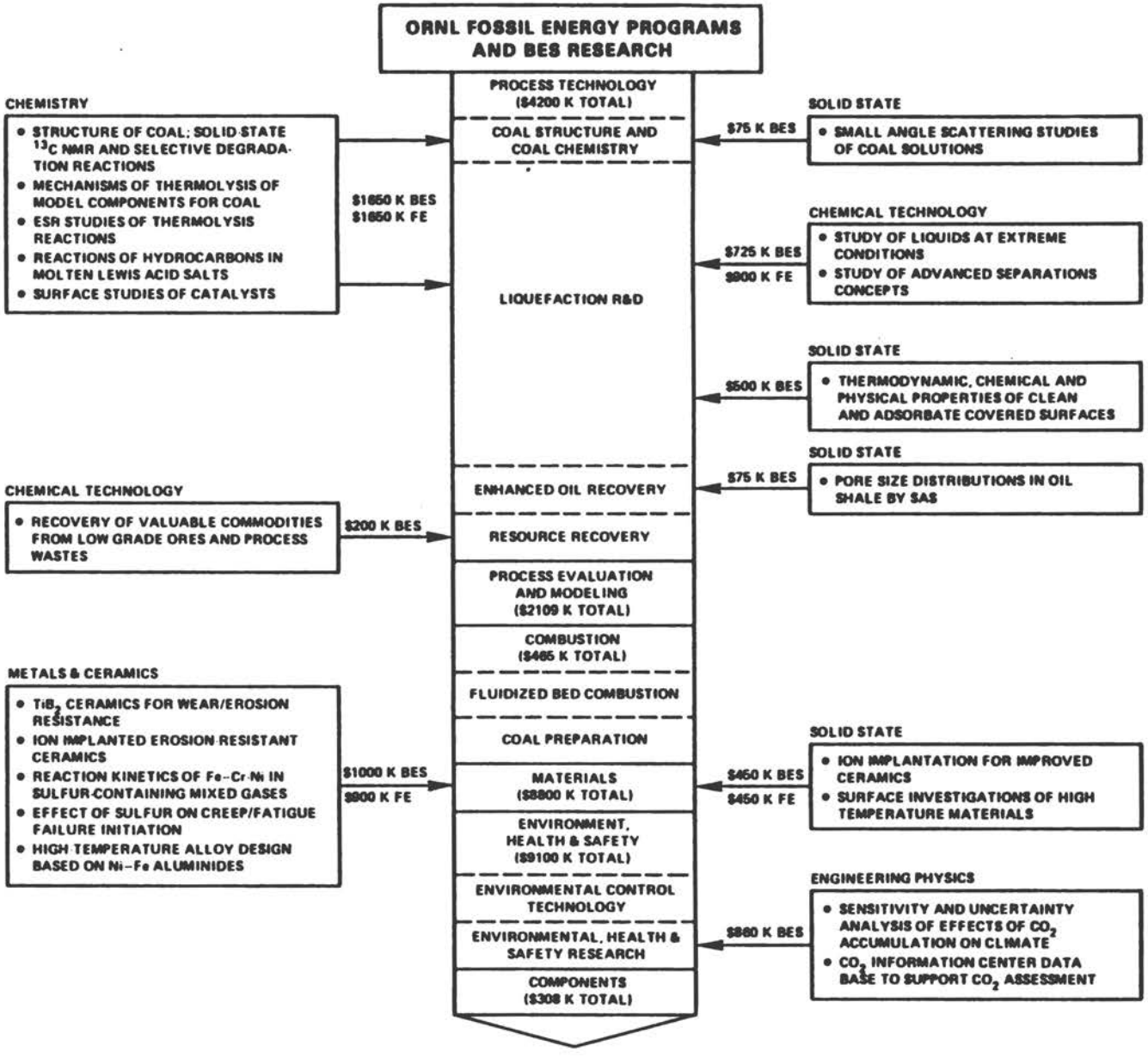
MATERIALS RESEARCH ROLES OF THE NATIONAL LABORATORIES

- TECHNOLOGY DEVELOPMENT IN SUPPORT OF NATIONAL PROGRAMS (FUSION, FISSION, FOSSIL ENERGY, CONSERVATION, SOLAR, etc.)
- BASIC RESEARCH IN SUPPORT OF TECHNOLOGIES
- LONG TERM OR MULTIDISCIPLINARY BASIC RESEARCH
- CONSTRUCTION AND OPERATION OF MAJOR FACILITIES
- NATIONAL LABORATORIES PROVIDE A FRAMEWORK FOR INTEGRATING THESE ACTIVITIES

NATIONAL LABORATORIES PROVIDE LEAD ROLES IN ENERGY-RELATED MATERIALS RESEARCH AND DEVELOPMENT

AS AN EXAMPLE, ORNL MANAGEMENT OF THE FOSSIL ENERGY MATERIALS PROGRAM (ADVANCED RESEARCH AND TECHNICAL DEVELOPMENT, GASIFICATION COMPONENTS) INVOLVES:

- PLANNING OF R&D NEEDS
- IMPLEMENTATION OF R&D ($8.8 M IN 1983 FROM FOSSIL ENERGY)
  - IN-HOUSE (24%)
  - SUBCONTRACTS (76%)
    - UNIVERSITIES (27%)
    - INDUSTRIAL RESEARCH CENTERS (14%)
    - OTHER GOVERNMENT AND NATIONAL LABS (35%)
- CONTROLLING/REPORTING
- INTERFACING BES AND FOSSIL ENERGY MATERIALS RESEARCH


ORNL FOSSIL ENERGY PROGRAMS AND BES RESEARCH
PROCESS TECHNOLOGY ($4200 K TOTAL)
COAL STRUCTURE AND COAL CHEMISTRY
LIQUEFACTION R&D
ENHANCED OIL RECOVERY
RESOURCE RECOVERY
PROCESS EVALUATION AND MODELING ($2109 K TOTAL)
COMBUSTION ($465 K TOTAL)
FLUIDIZED BED COMBUSTION
COAL PREPARATION
MATERIALS ($3800 K TOTAL)
ENVIRONMENT, HEALTH & SAFETY ($9100 K TOTAL)
ENVIRONMENTAL CONTROL TECHNOLOGY
ENVIRONMENTAL, HEALTH & SAFETY RESEARCH
COMPONENTS ($308 K TOTAL)
CHEMISTRY
• STRUCTURE OF COAL: SOLID STATE ^{13}C NMR AND SELECTIVE DEGRADATION REACTIONS
• MECHANISMS OF THERMOLYSIS OF MODEL COMPONENTS FOR COAL
• ESR STUDIES OF THERMOLYSIS REACTIONS
• REACTIONS OF HYDROCARBONS IN MOLTEN LEWIS ACID SALTS
• SURFACE STUDIES OF CATALYSTS
$1650 K BES
$1650 K FE
CHEMICAL TECHNOLOGY
• RECOVERY OF VALUABLE COMMODITIES FROM LOW GRADE ORES AND PROCESS WASTES
$200 K BES
METALS & CERAMICS
• TiB_2 CERAMICS FOR WEAR/EROSION RESISTANCE
• ION IMPLANTED EROSION RESISTANT CERAMICS
• REACTION KINETICS OF Fe-Cr-Ni IN SULFUR-CONTAINING MIXED GASES
• EFFECT OF SULFUR ON CREEP/FATIGUE FAILURE INITIATION
• HIGH TEMPERATURE ALLOY DESIGN BASED ON Ni-Fe ALUMINIDES
$1000 K BES
$900 K FE
SOLID STATE
• SMALL ANGLE SCATTERING STUDIES OF COAL SOLUTIONS
$75 K BES
CHEMICAL TECHNOLOGY
• STUDY OF LIQUIDS AT EXTREME CONDITIONS
• STUDY OF ADVANCED SEPARATIONS CONCEPTS
$725 K BES
$900 K FE
SOLID STATE
• THERMODYNAMIC, CHEMICAL AND PHYSICAL PROPERTIES OF CLEAN AND ADSORBATE COVERED SURFACES
$500 K BES
SOLID STATE
• PORE SIZE DISTRIBUTIONS IN OIL SHALE BY SAS
$75 K BES
SOLID STATE
• ION IMPLANTATION FOR IMPROVED CERAMICS
• SURFACE INVESTIGATIONS OF HIGH TEMPERATURE MATERIALS
$450 K BES
$450 K FE
ENGINEERING PHYSICS
• SENSITIVITY AND UNCERTAINTY ANALYSIS OF EFFECTS OF CO_2 ACCUMULATION ON CLIMATE
• CO_2 INFORMATION CENTER DATA BASE TO SUPPORT CO_2 ASSESSMENT
$860 K BES

ADVANCED RESEARCH AND TECHNICAL DEVELOPMENT (AR&TD) FOSSIL ENERGY MATERIALS PROGRAM INVOLVES A WIDE VARIETY OF ACTIVITIES AND INSTITUTIONS

ALLOY AND JOINING DEVELOPMENT

COMBUSTION ENGINEERING
COLORADO SCHOOL OF MINES
OAK RIDGE NATIONAL LABORATORY
PENNSYLVANIA STATE UNIVERSITY
UNIVERSITY OF CALIFORNIA AT BERKELEY
UNIVERSITY OF CINCINNATI
UNIVERSITY OF CONNECTICUT
UNIVERSITY OF TENNESSEE

MECHANICAL PRDPERTIES OF ALLOYS

ARGONNE NATIONAL LABORATORY
CORNELL UNIVERSITY
IDAHO NATIONAL ENGINEERING LABORATORY
OAK RIDGE NATIONAL LABORATORY
UNIVERSITY OF CALIFORNIA AT SANTA BARBARA
UNIVERSITY OF ILLINOIS
WESTINGHOUSE ELECTRIC CORPORATION

CORROSION OF ALLOYS

ARGONNE NATIONAL LABORATORY
AERODYNE RESEARCH, INC.
GENERAL ELECTRIC COMPANY
METAL PROPERTIES COUNCIL/IITRI
OAK RIDGE NATIONAL LABORATORY
PACIFIC NORTHWEST LABORATORY
UNIVERSITY OF PITTSBURGH

EROSION AND WEAR

ARGONNE NATIONAL LABORATORY
BATTELLE COLUMBUS LABORATORIES
LAWRENCE BERKELEY LABORATORY
METAL PROPERTIES COUNCIL/IITRI
NATIONAL BUREAU OF STANDARDS
OAK RIDGE NATIONAL LABORATORY
UNIVERSITY OF NOTRE DAME

CERAMIC POWDER AND FIBER SYNTHESIS

LOS ALAMOS NATIONAL LABORATORY
OAK RIDGE NATIONAL LABORATORY

FABRICATION DEVELOPMENT

LOS ALAMOS NATIONAL LABORATORY
OAK RIDGE NATIONAL LABORATORY

STRUCTURAL CERAMIC TESTING AND CHARACTERIZATION

NATIONAL BUREAU OF STANDARDS
OAK RIDGE NATIONAL LABORATORY

CORROSION AND MECHANICAL PROPERTIES OF REFRACTORIES

ARGONNE NATIONAL LABORATORY
IOWA STATE UNIVERSITY
MASSACHUSETTS INSTITUTE OF TECHNOLOGY
NATIONAL BUREAU OF STANDARDS
PENNSYLVANIA STATE UNIVERSITY
VIRGINIA POLYTECHNIC UNIVERSITY

ADVANCED FOSSIL ENERGY CONVERSION SYSTEMS REQUIRE STRUCTURAL MATERIALS HAVING

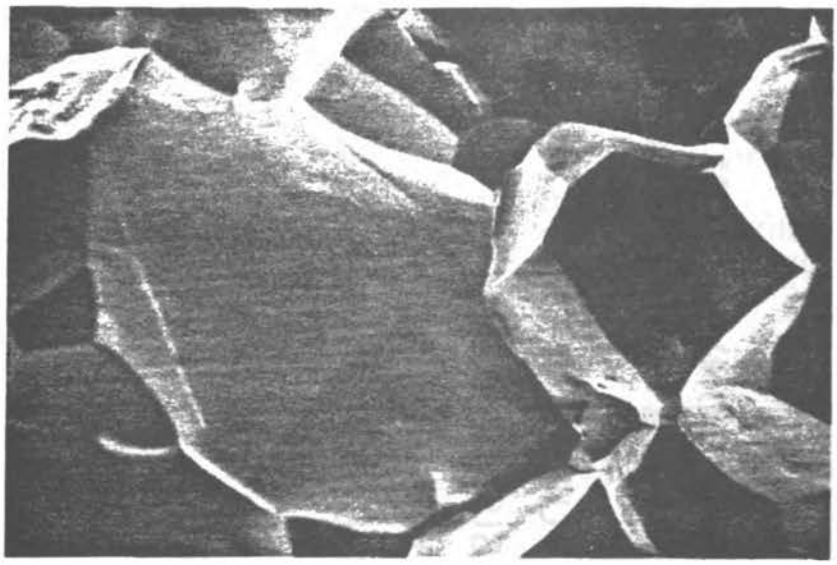
- GOOD HIGH TEMPERATURE STRENGTH
- GOOD CORROSION RESISTANCE
- GOOD DUCTILITY AND FABRICABILITY
- MINIMAL USE OF CRITICAL STRATEGIC ELEMENTS

Fe, Ni ALUMINIDES WITH THESE PROPERTIES WERE DEVELOPED IN THE BASIC RESEARCH PROGRAMS

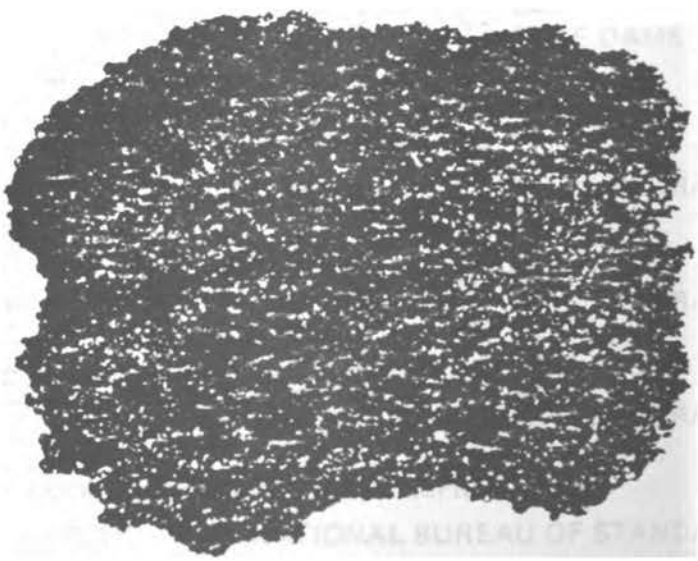
3/84

POLYCRYSTALLINE Ni_3Al SHOWS POOR DUCTILITY AND BRITTLE GRAIN-BOUNDARY FRACTURE

- SINGLE CRYSTALS OF Ni_3Al ARE DUCTILE
- POLYCRYSTALLINE Ni_3Al IS EXTREMELY BRITTLE BECAUSE OF GRAIN-BOUNDARY WEAKNESS



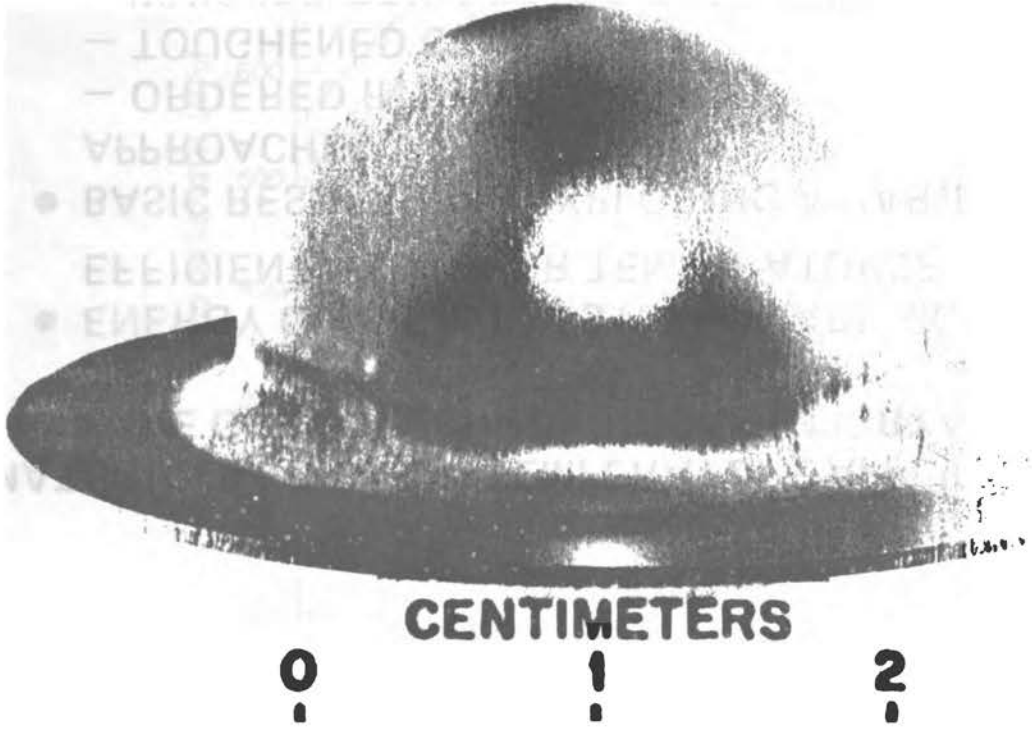
BRITTLE GRAIN BOUNDARY FRACTURE AT ROOM TEMPERATURE



EXTENSIVE CRACKING ALONG GRAIN BOUNDARIES IN Ni_3Al CAST INGOT HOT ROLLED AT 1200°C

DUCTILITY AND FABRICABILITY OF Ni_3Al CAN BE DRAMATICALLY IMPROVED BY MICROALLOYING WITH B AND Mn

- Ni_3Al ALLOYS MICROALLOYED WITH B AND Mn WERE READILY COLD FABRICATED INTO SHEETS, FOILS, RODS, AND WIRES
- MICROALLOYED Ni_3Al EXHIBITED A TENSILE DUCTILITY OF 50% AT ROOM TEMPERATURE
- CUPS OF MICROALLOYED Ni_3Al WERE SUCCESSFULLY FABRICATED BY DEEP DRAWING AT ROOM TEMPERATURE

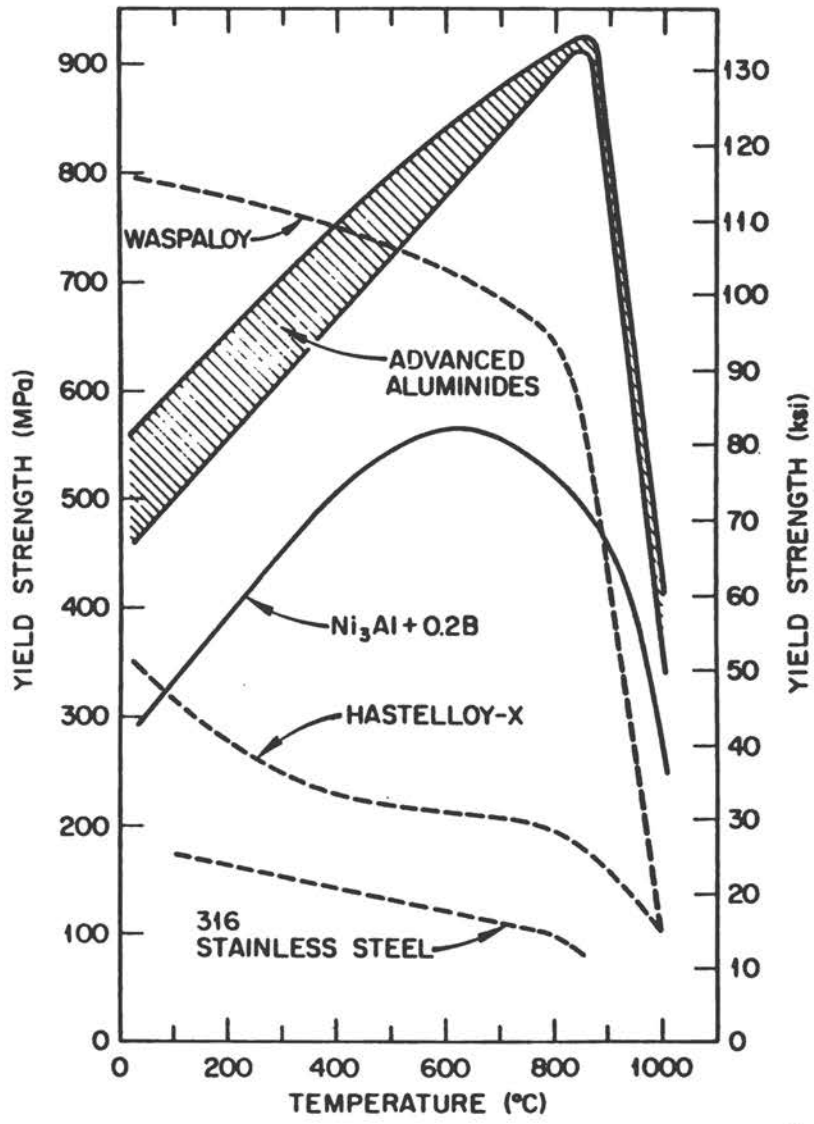


IN COMPARISON, MANY STAINLESS STEEL BLANKS WERE CRACKED DURING THIS FORMING OPERATION

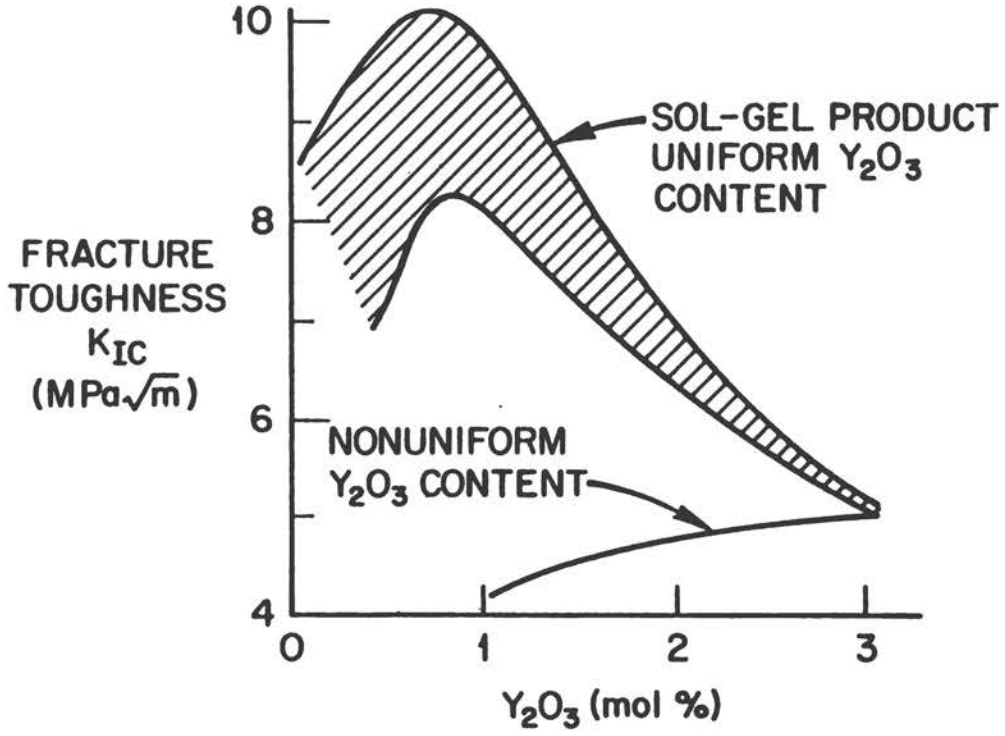
MATERIALS FOR HIGH TEMPERATURE APPLICATIONS HAVE GREAT TECHNOLOGICAL IMPORTANCE

- ENERGY CONVERSION SYSTEMS ARE MORE EFFICIENT AT HIGHER TEMPERATURES
- BASIC RESEARCH IS EXPLORING A VARIETY OF APPROACHES, e.g.,
  - ORDERED INTERMETALLICS
  - TOUGHENED CERAMICS
  - WHISKER REINFORCED COMPOSITES

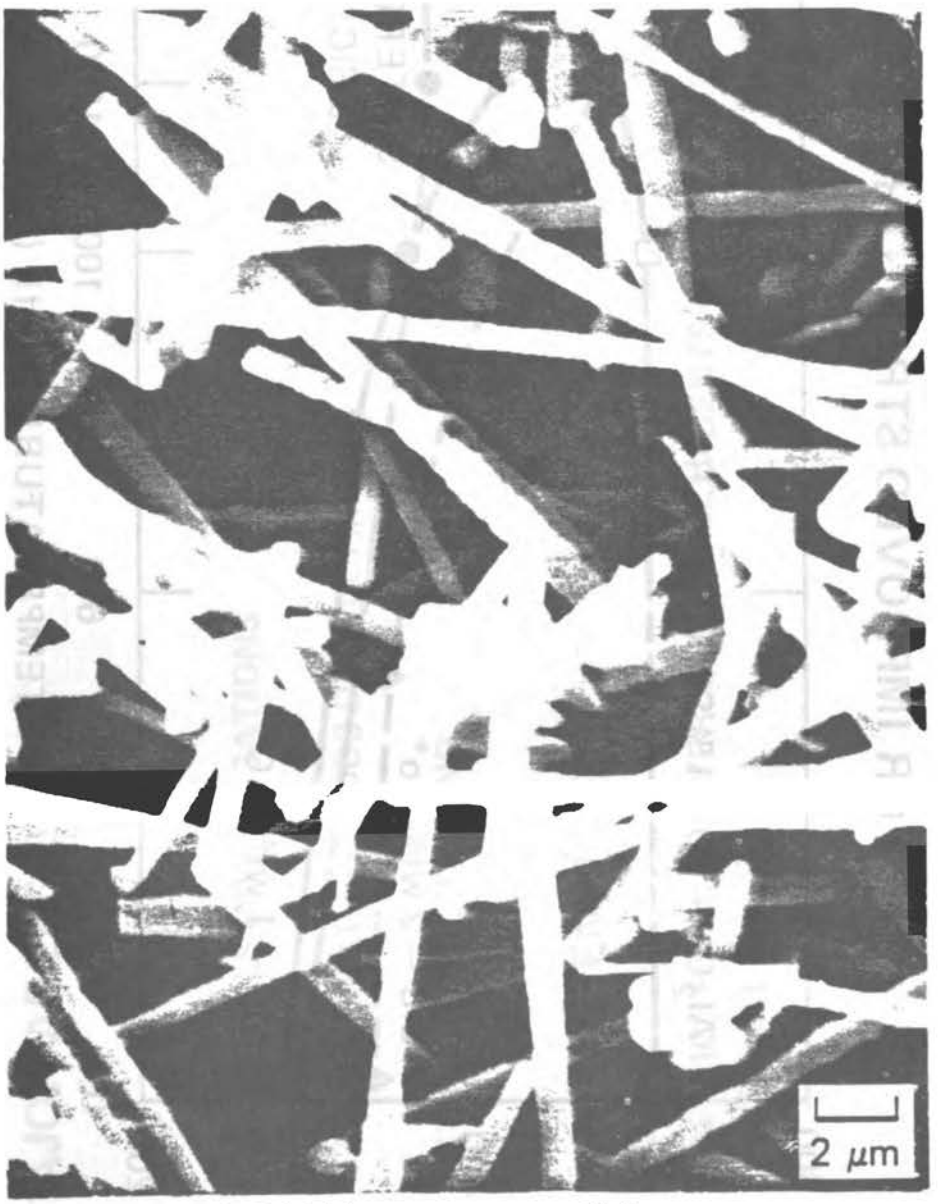
ADVANCED ALUMINIDES ARE STRONGER THAN COMMERCIAL ALLOYS AT ELEVATED TEMPERATURES BECAUSE THEIR YIELD STRENGTH INCREASES WITH TEMPERATURE



FRACTURE TOUGHNESS OF ALUMINA CONTAINING 20% ZIRCONIA DOPED WITH YTTRIA IS VERY SENSITIVE TO THE AMOUNT AND DISTRIBUTION OF THE YTTRIA

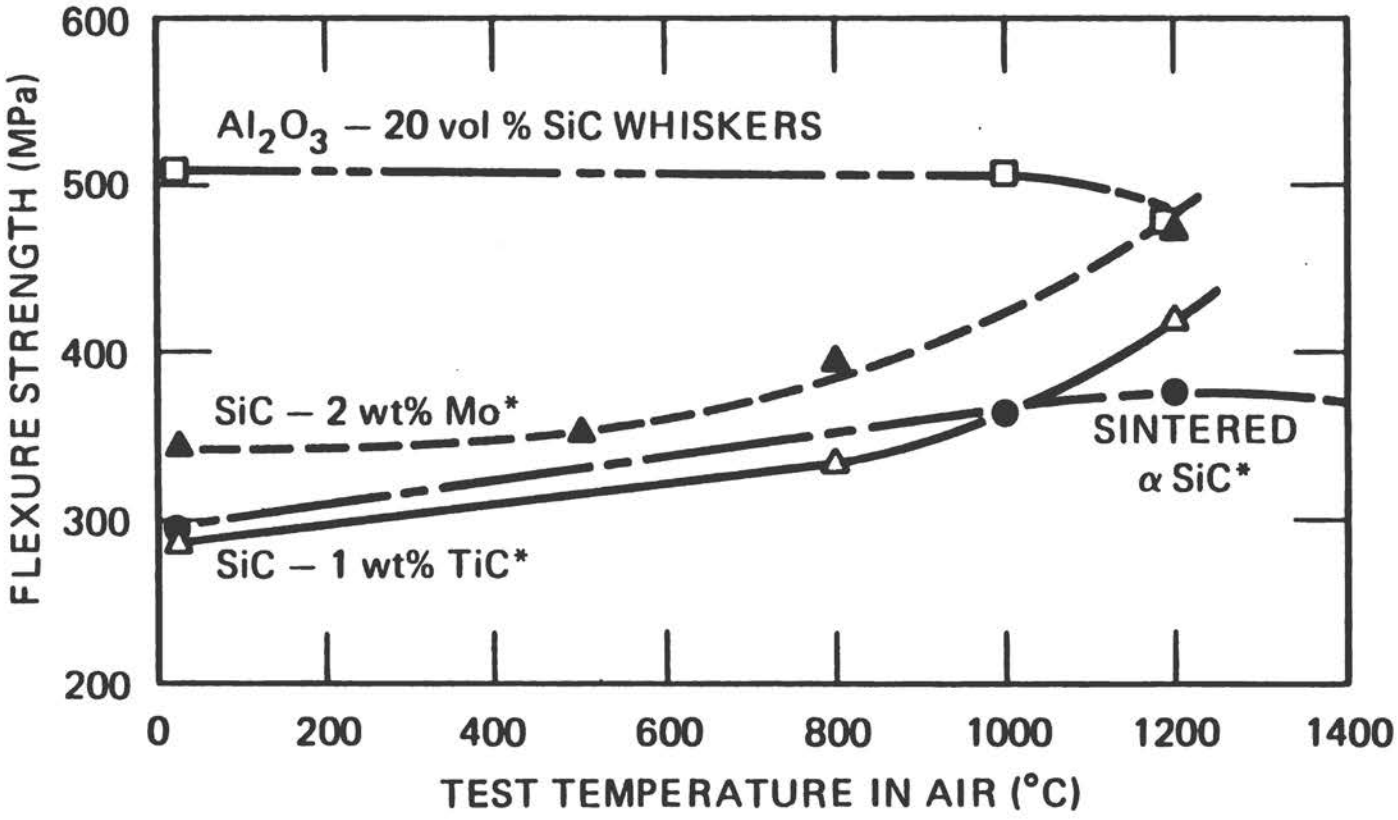


ARCO SiC WHISKER IS USED IN FABRICATION OF SiC-WHISKER REINFORCED CERAMICS



• AVG DIAM	0.6 μm
• LENGTH	10–80 μm
• AVG L/D	75
• PARTICLE CONTENT	10–20 wt %

DISPERSED PARTICLE AND WHISKER REINFORCED COMPOSITES EXHIBIT POTENTIAL FOR IMPROVED STRENGTH



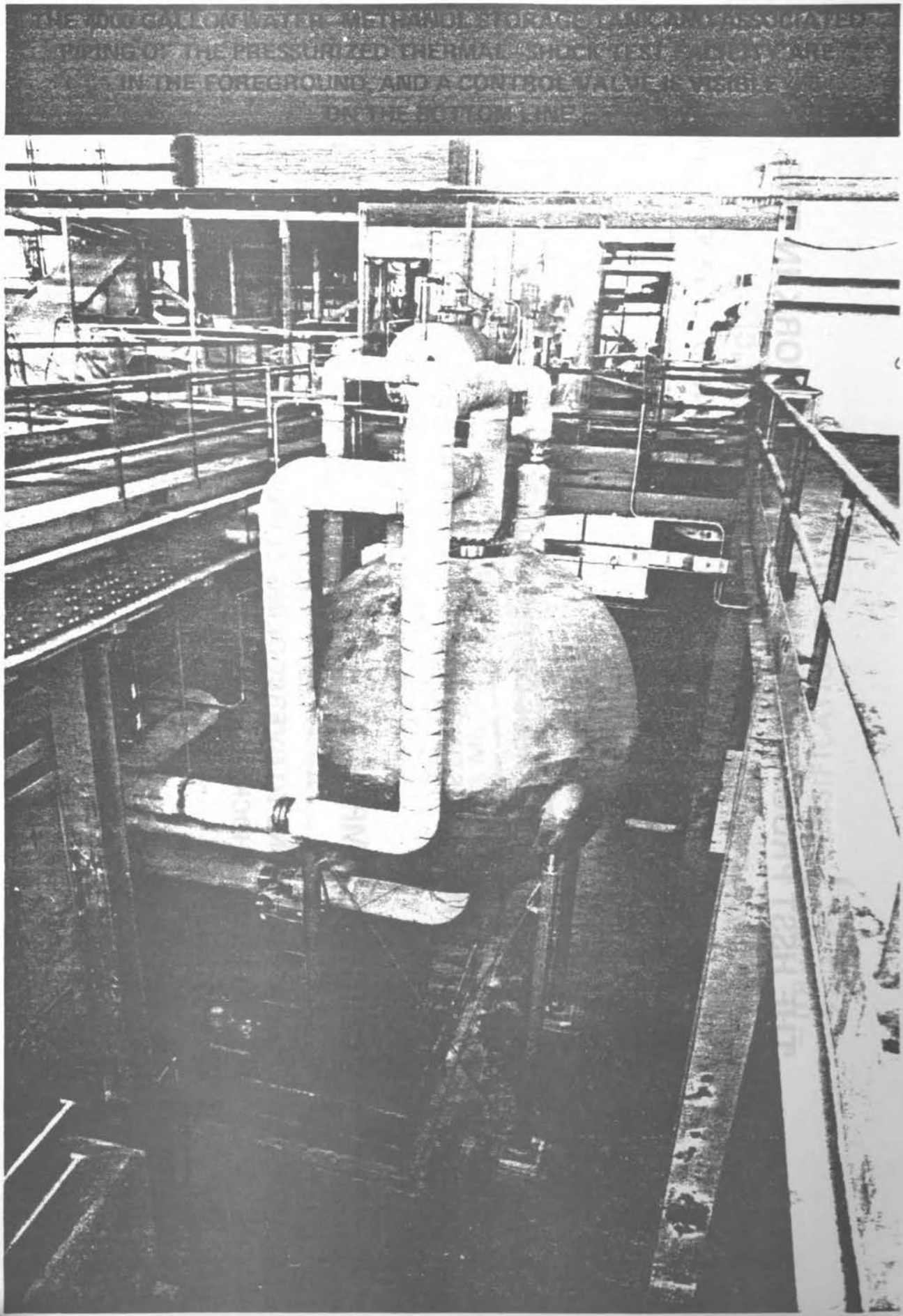
*~ 0.8 wt% B
~ 2 wt% C
} DENSIFICATION ADDITIVES

THE HSST PROGRAM SCOPE INCLUDES WORK IN THE MAJOR AREAS OF

- MATERIALS INVESTIGATIONS
- ANALYTICAL METHODS DEVELOPMENT
- STRUCTURAL TESTING

CURRENT EMPHASIS

- APPLICATIONS TO OVERCOOLING ACCIDENTS (PRESSURIZED THERMAL SHOCK)



ARGONNE NATIONAL LABORATORY IS STUDYING RADIATION-INDUCED SEGREGATION

- SELECTIVE TRANSPORT OF CERTAIN ALLOYING ELEMENTS CAUSES PRECIPITATION AND PHASE REDISTRIBUTIONS IN MATERIALS UNDER IRRADIATION
- RESULTING MICROSTRUCTURAL CHANGES PROFOUNDLY AFFECT IN-SERVICE PERFORMANCE OF IRRADIATED COMPONENTS
- GRAIN BOUNDARIES BECOME EMBRITTLED
- LOW SWELLING ALLOYS LOSE RESISTANCE AT HIGH RADIATION DOSES

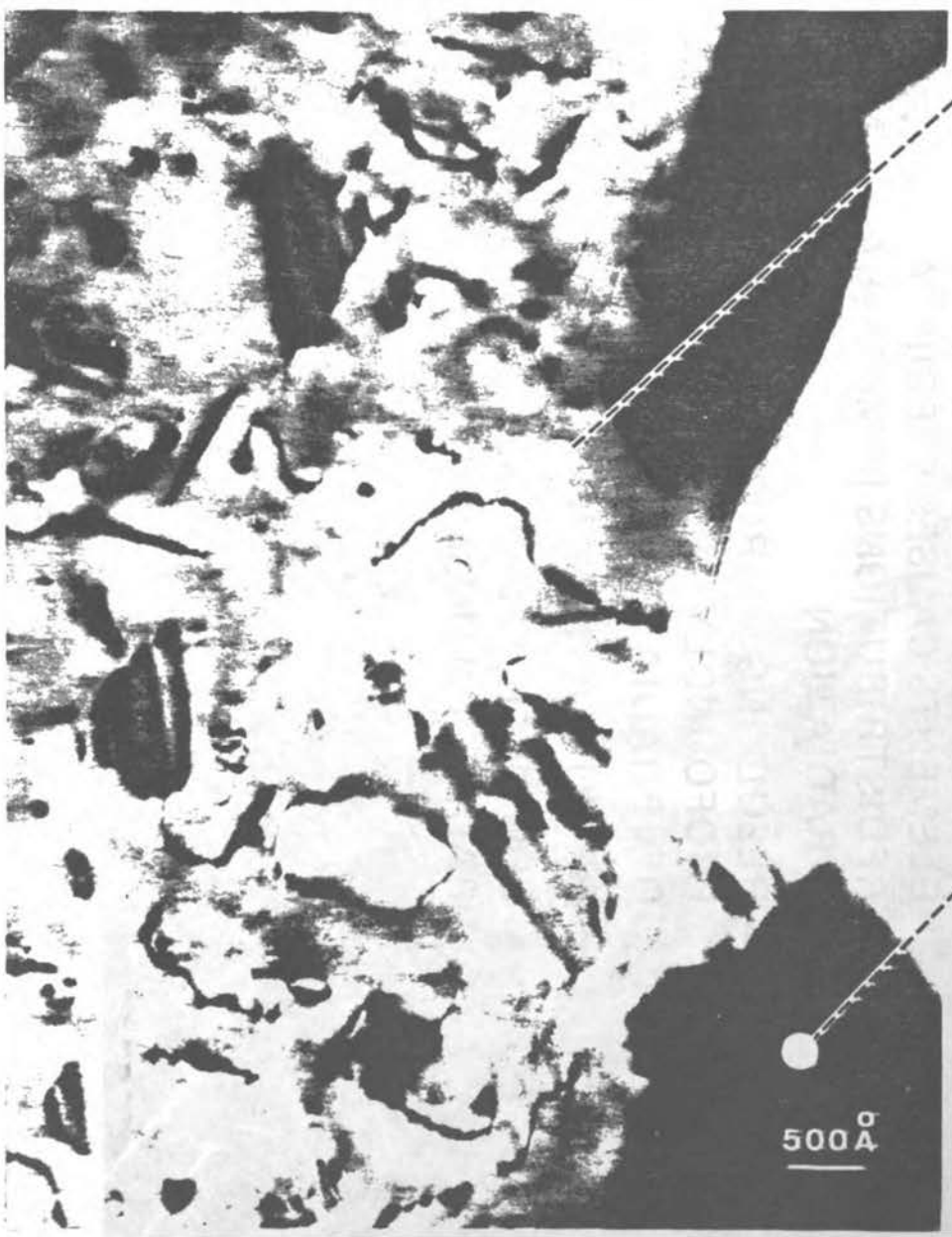
3/84

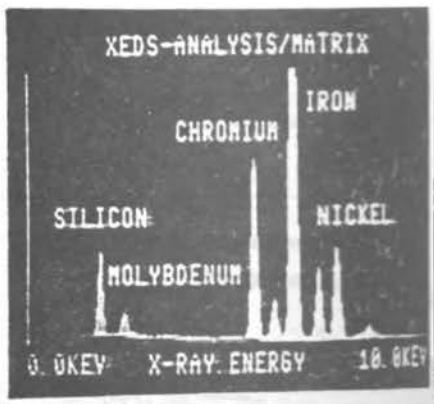
STATE-OF-THE-ART ANALYTICAL ELECTRON MICROSCOPY

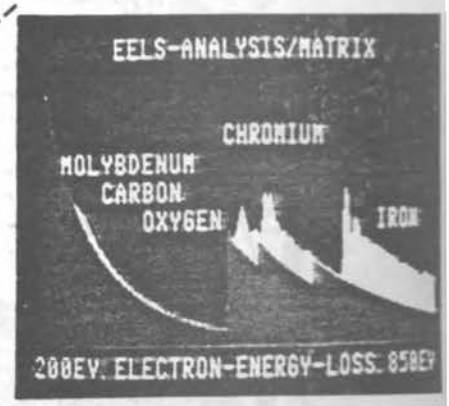
ELEMENTAL REDISTRIBUTION DURING IRRADIATION

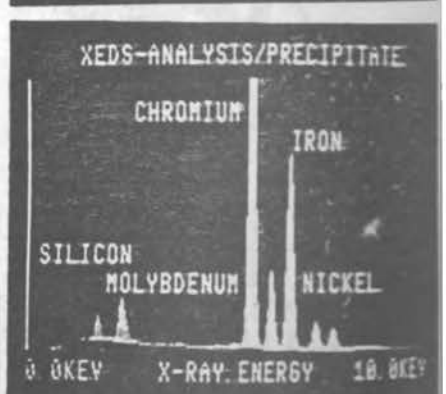
Material: 316 Stainless Steel
Solution Annealed and Aged - 10 hrs 800 ^{0}C

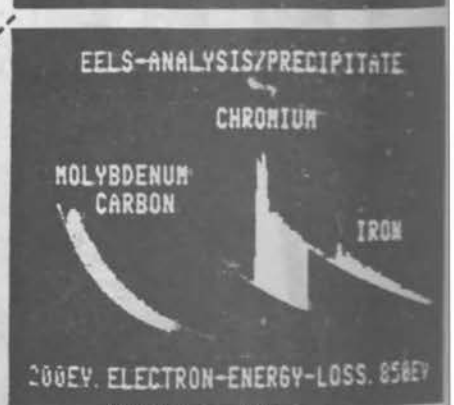
Irradiation: 40 appm He^{+} with 3 MeV Ni^{+}, 8 dpa 621 ^{0}C

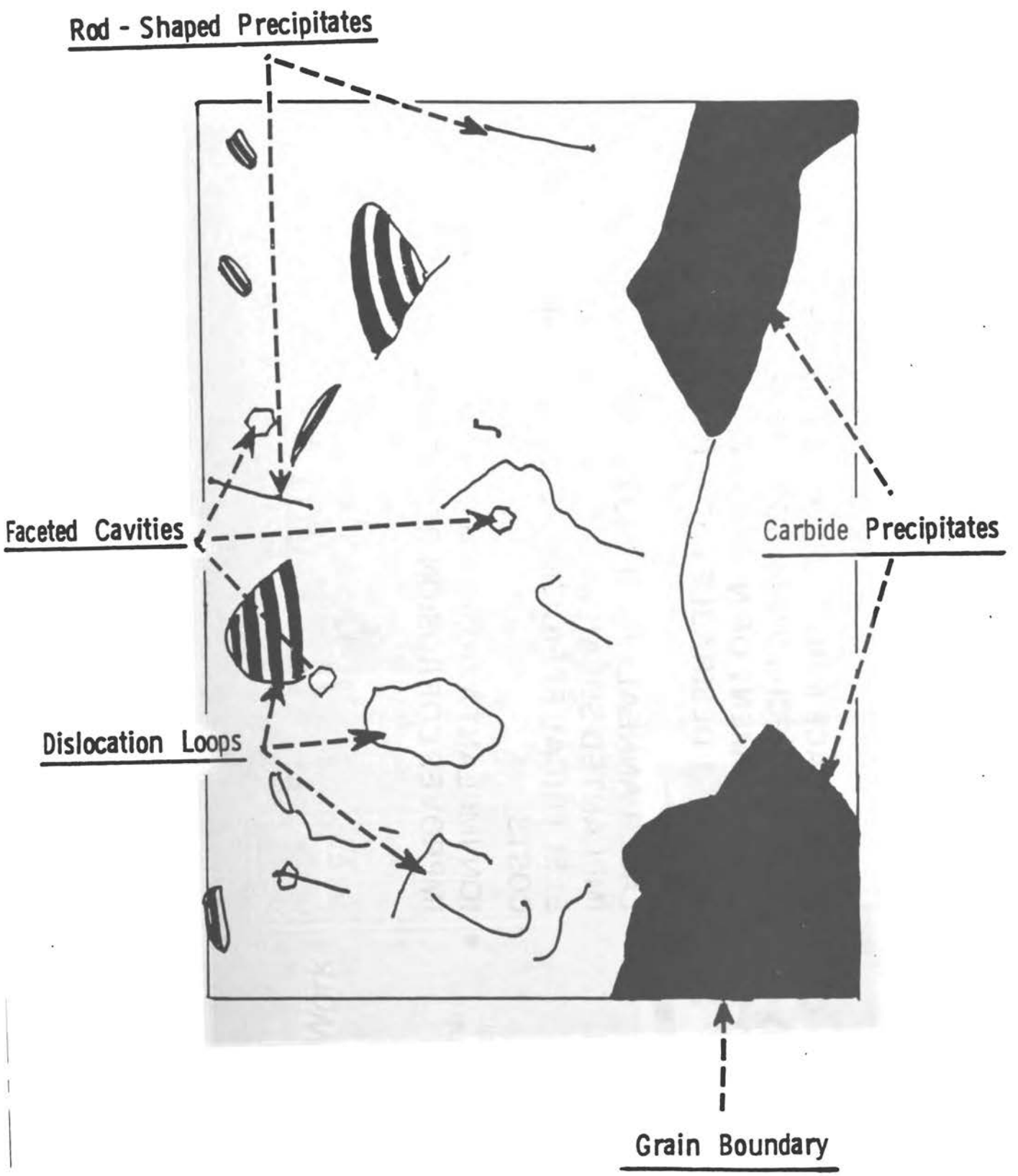











Rod - Shaped Precipitates
Faceted Cavities
Carbide Precipitates
Dislocation Loops
Grain Boundary

SURFACE MODIFICATION INVOLVES A MULTIDISCIPLINARY APPROACH TO THE DEVELOPMENT OF NEW MATERIALS HAVING DESIRABLE PROPERTIES

- LASER ANNEALING OF GLOW DISCHARGE ION-IMPLANTED SOLAR CELLS RESULTS IN HIGH ELECTRICAL EFFICIENCIES, LOW FABRICATION COSTS
- ION IMPLANTATION OF ARTIFICIAL HIP JOINTS IMPROVES CORROSION RESISTANCE

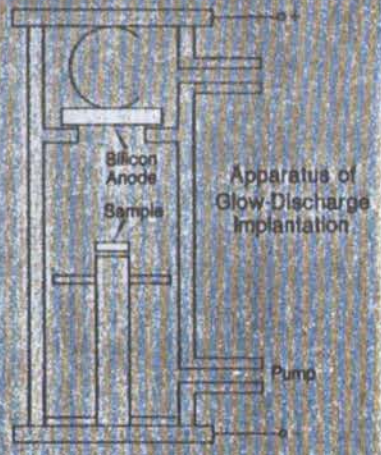
3/84

High-Efficiency Si Solar Cells by Beam Processing

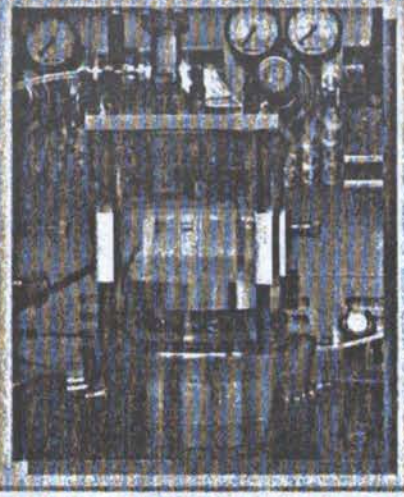
Oak Ridge National Laboratory

Present Work

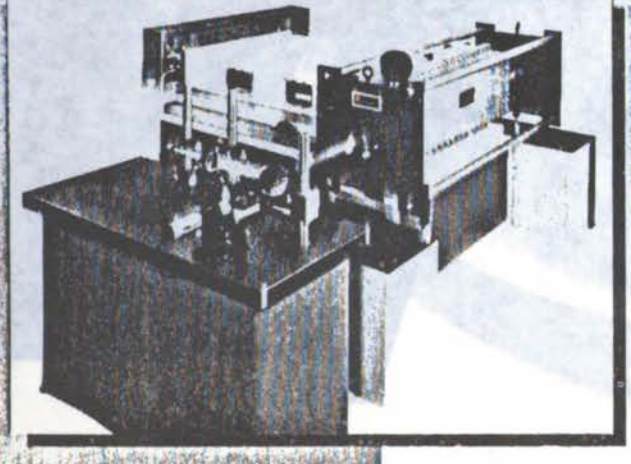
- Low Cost
- Gas Discharge
- Implantation



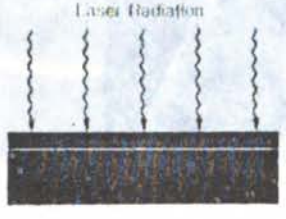
Apparatus of Glow-Discharge Implantation



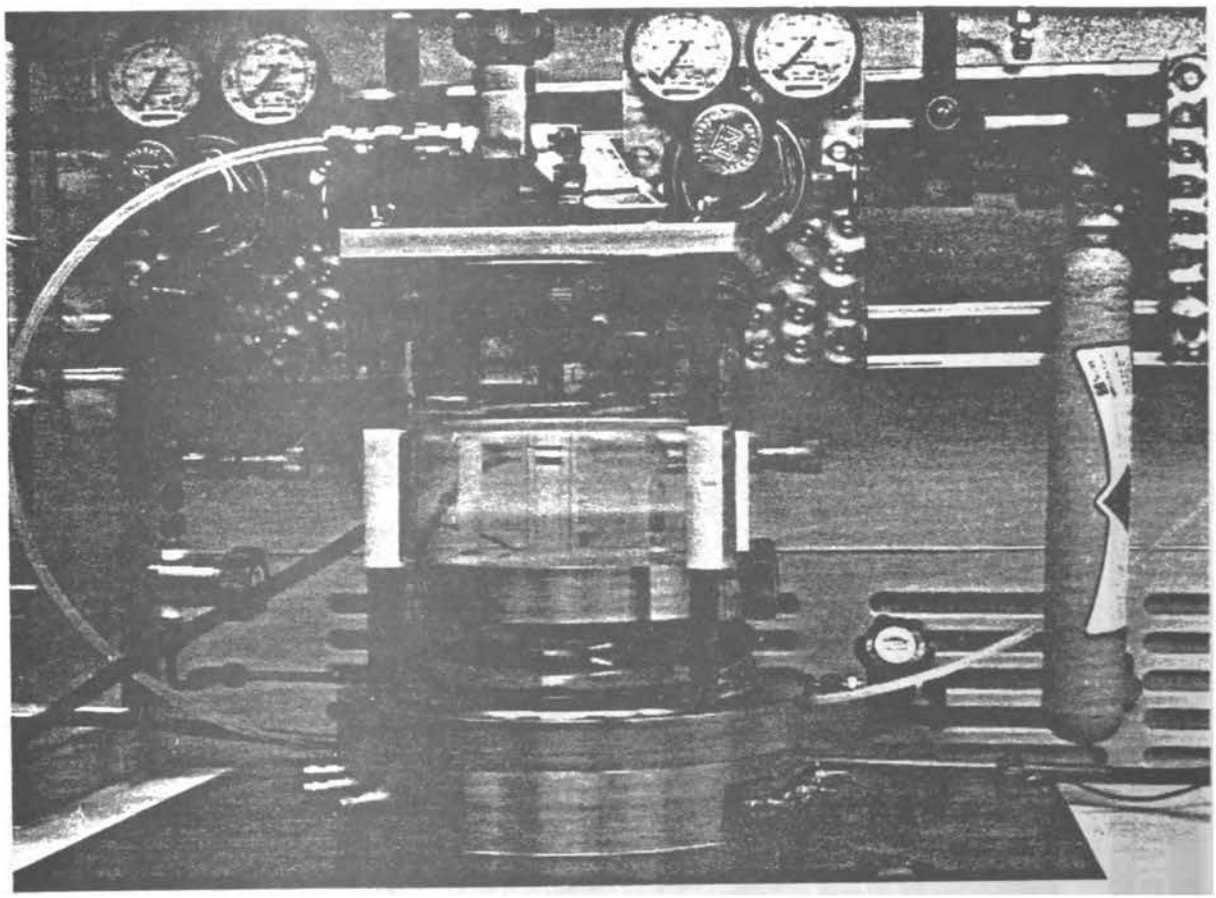
Source: BF_3 or PF_5
Chamber: 8" ID × 8" high
Pressure: 1×10^{-3} mm
Voltage: 0.5–5 kV
Current: 0.05–0.1 mA/cm²

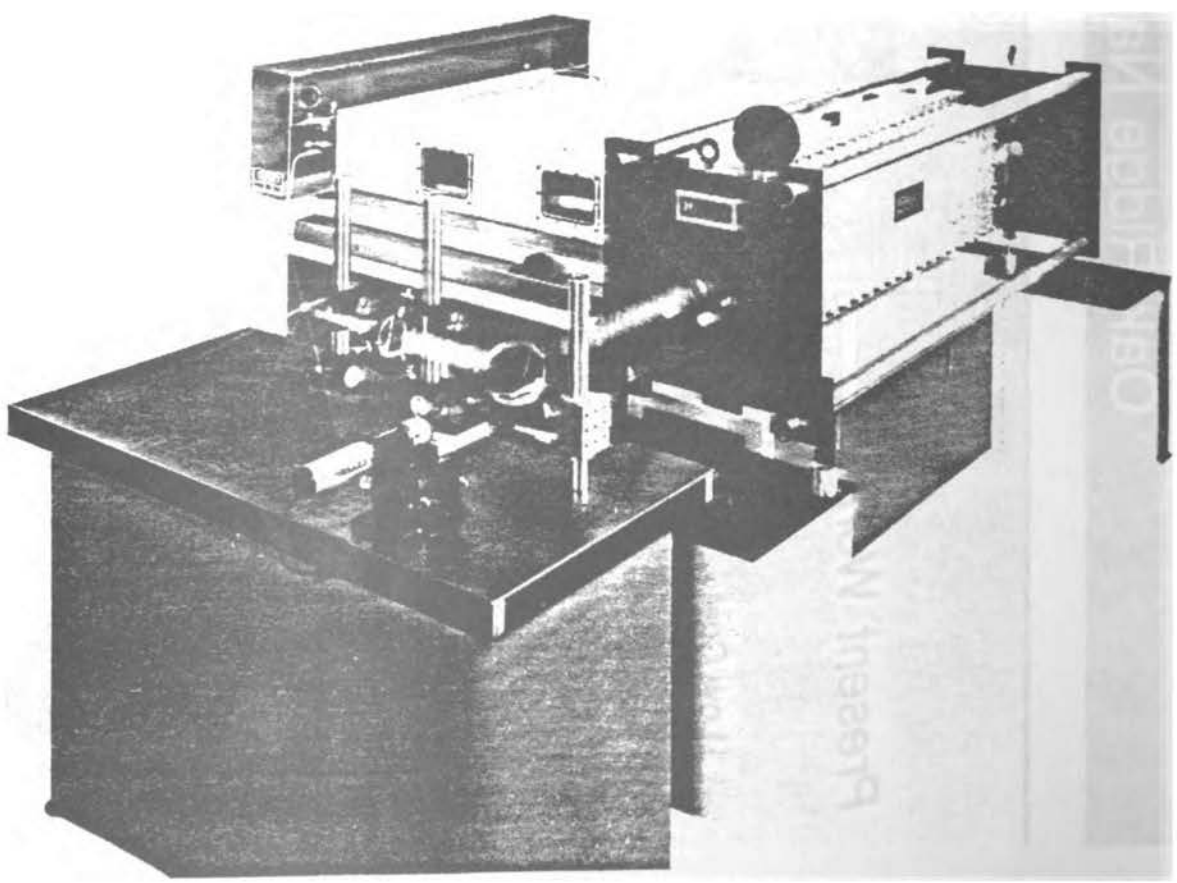


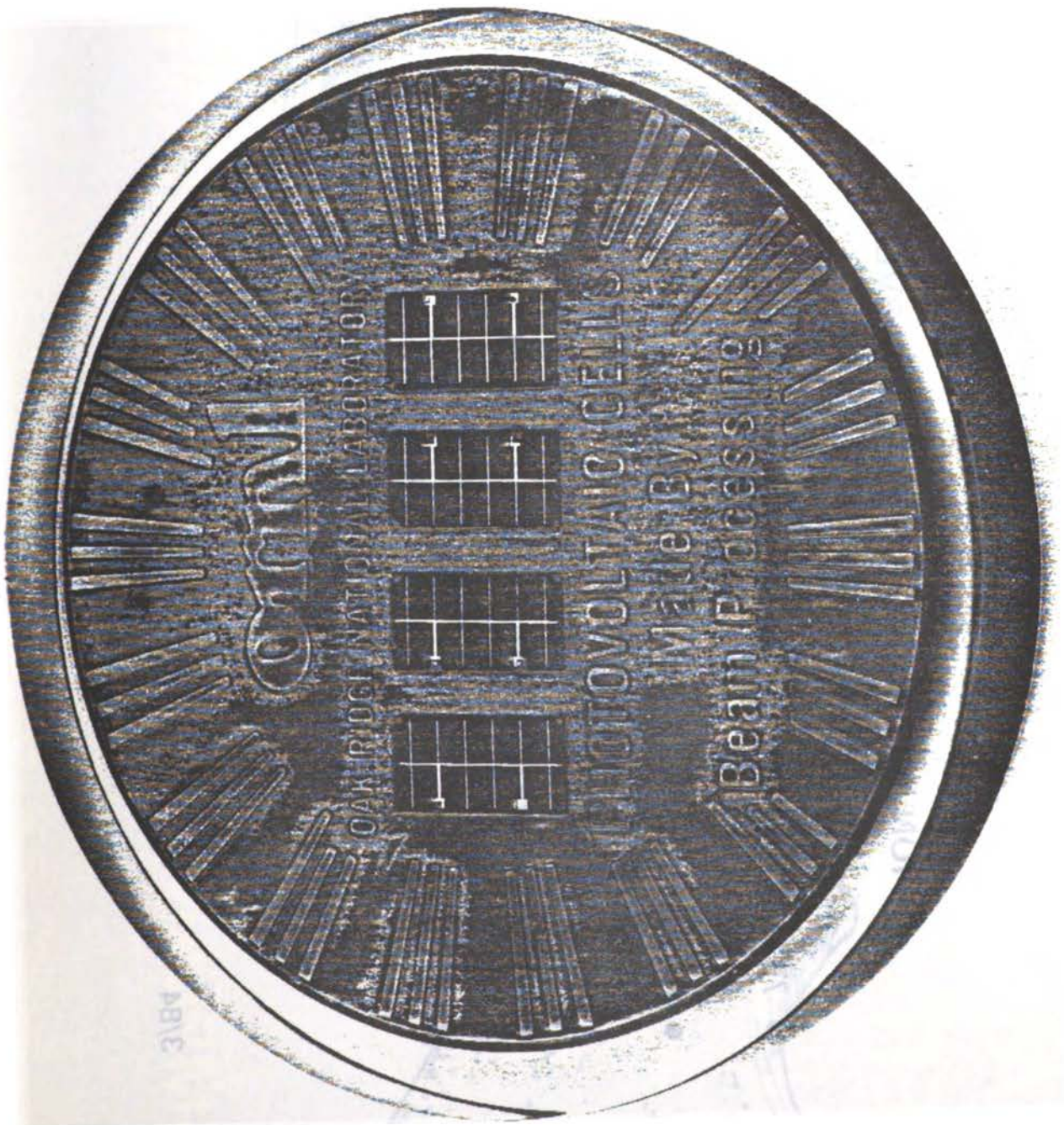
- Pulsed XeCl (308 nm) Excimer Laser Annealing
  - No substrate heater
  - No beam homogenizer
  - Achievable annealing throughput 50 cm²/sec



- Laser energy is used in the material exactly where it is needed
- Laser annealing can be carried out in air
- Localized processing of very fine device structures



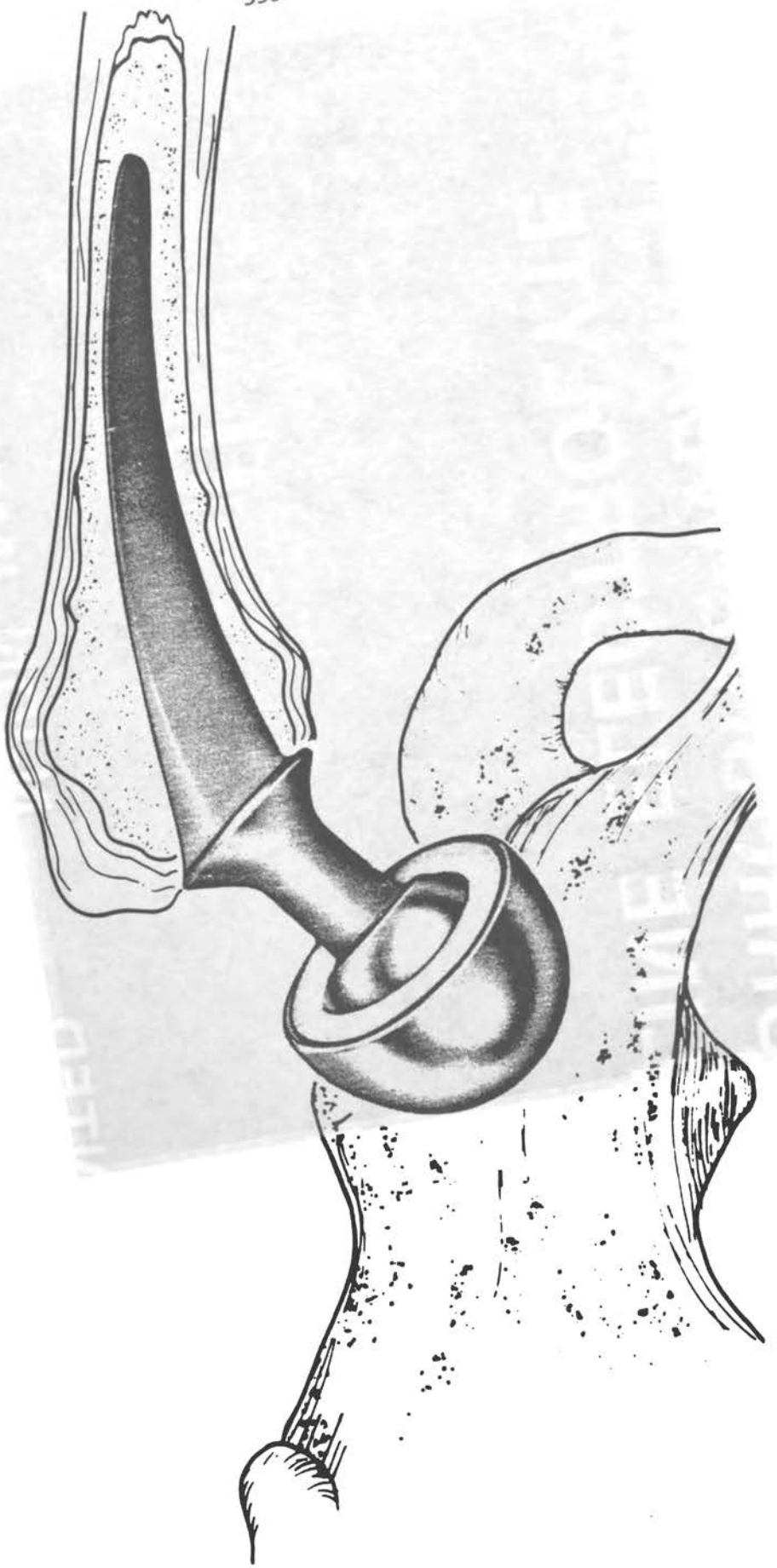


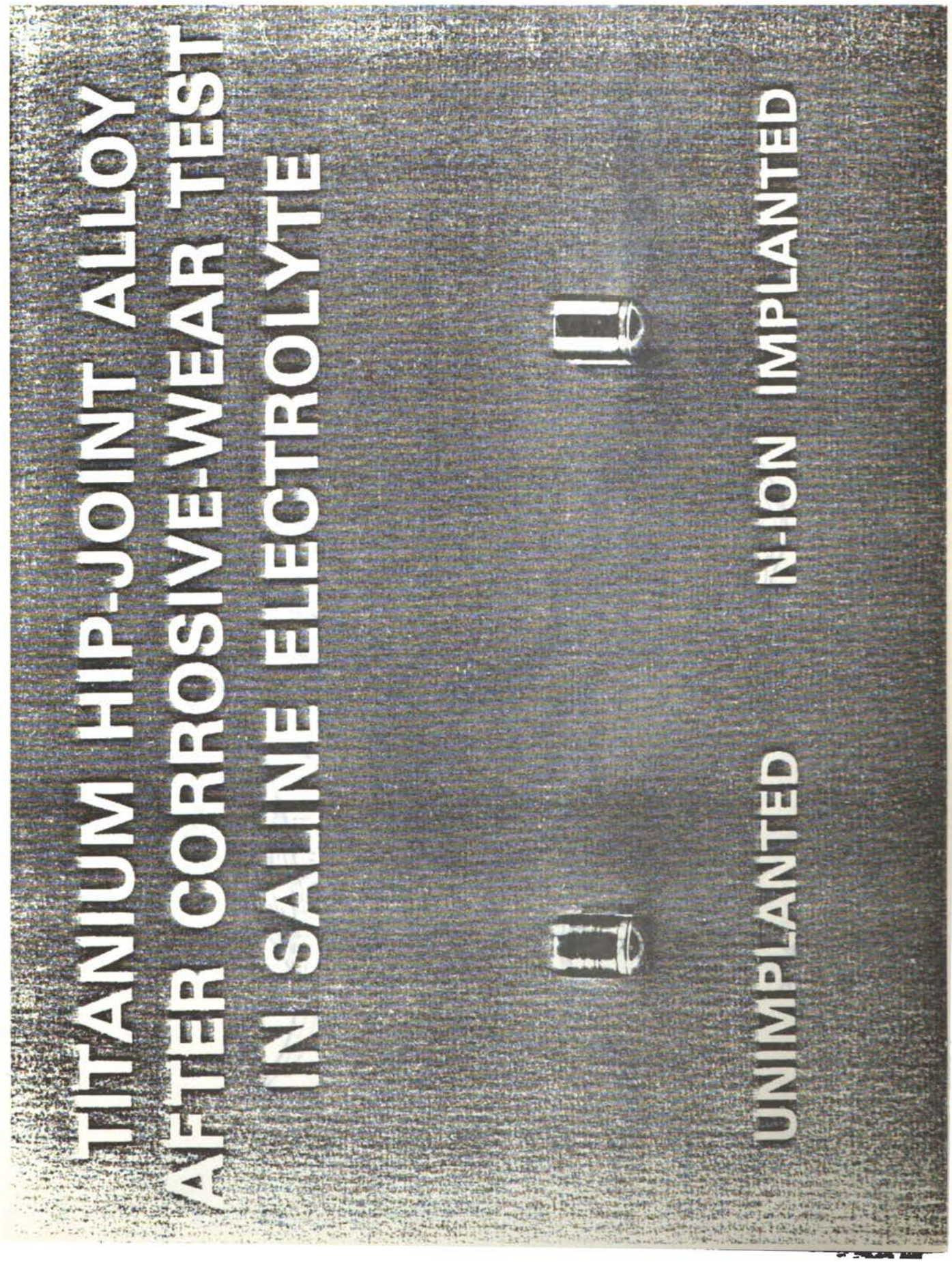

OAK RIDGE NATIONAL LABORATORY
PHOTOVOLTAIC CELLS
Beam Processing

ION IMPLANTATION FOR IMPROVED ARTIFICIAL HIP JOINTS

- 75,000 ARTIFICIAL HIP JOINT SURGERIES ANNUALLY IN THE U. S.
- RUBBING WEAR OF BALL AND SOCKET IN CORROSIVE BODY FLUIDS LEADS TO POOR FIT AND EVENTUAL FAILURE
- METALLIC FLOTSAM RELEASED CAN CAUSE INFLAMMATION
- ION BEAM IMPLANTATION OF NITROGEN INTO SURGICAL ALLOYS REDUCES THESE PROBLEMS BY ORDERS OF MAGNITUDE

3/84





ORNL SURFACE MODIFICATION AND CHARACTERIZATION FACILITY

TECHNOLOGY TRANSFER THROUGH COLLABORATIVE INTERACTIONS
USE OF ION BEAM AND LASER PROCESSING FOR NEAR SURFACE MODIFICATION OF MATERIALS

INDUSTRIES	COLLABORATIVE PROJECT
EXXON	FRICTION, WEAR AND LUBRICATION; CATALYSIS
MOTOROLA	SEMICONDUCTOR DEVICES
WESTINGHOUSE R&D	HIGH T_c SUPERCONDUCTING COMPOUNDS; SEMICONDUCTOR DEVICES
ENERGY CONVERSION DEVICES	SEMICONDUCTOR DEVICES; AMORPHOUS SILICON ALLOYS; SOLAR ABSORBERS
BELL LABORATORIES	H PROFILING OF Au CONTACTS; SUPERCONDUCTIVITY; DEFECTS AND DIFFUSION IN III-V COMPOUNDS; SURFACE STUDIES
IBM	SURFACE PROPERTIES, LASER ANNEALED SEMICONDUCTORS; III-V COMPOUND SUPERLATTICES; ION BEAM MIXING OF CERAMICS
BATTELLE	ION IMPLANTATION-CORROSION; ION INDUCED ADHESION OF POLYMER FILMS
CORNING GLASS	H PROFILING OF GLASSES
UNITED TECHNOLOGIES	GaAs SOLAR CELLS
HUGHES RESEARCH LABORATORIES	CW LASER CRYSTALLIZATION OF Si
UNION CARBIDE CORPORATION	CATALYSIS
MOBILE TYCO	HIGH EFFICIENCY RIBBON SOLAR CELLS
UNIVERSAL ENERGY SYSTEMS	ION IMPLANTATION AND LASER ANNEALING OF GaAs; SURFACE SMOOTHING OF LASER MIRRORS
TEXAS INSTRUMENTS	OHMIC CONTACT FORMATION BY LASER PROCESSING
MINNESOTA MINING AND MANUFACTURING	ION BEAM PROCESSING OF METAL CATALYSTS ON INSULATORS
ZIMMER	SURFACE MODIFICATION OF SURGICAL ALLOYS

COLLABORATIVE RESEARCH CENTERS SPONSORED BY THE MATERIALS SCIENCES DIVISION, BASIC ENERGY SCIENCES, DOE

- NATIONAL SYNCHROTRON LIGHT SOURCE (BROOKHAVEN NATIONAL LABORATORY)
- HIGH FLUX BEAM REACTOR (BROOKHAVEN NATIONAL LABORATORY)
- NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR (OAK RIDGE NATIONAL LABORATORY)
- INTENSE PULSED NEUTRON SOURCE (ARGONNE NATIONAL LABORATORY)
- WNR/PSR SPALLATION NEUTRON SOURCE (LOS ALAMOS NATIONAL LABORATORY)
- NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH (OAK RIDGE NATIONAL LABORATORY)
- NATIONAL CENTER FOR ELECTRON MICROSCOPY (LAWRENCE BERKELEY LABORATORY)
- HIGH VOLTAGE ELECTRON MICROSCOPE – TANDEM FACILITY (ARGONNE NATIONAL LABORATORY)
- SHARED RESEARCH EQUIPMENT PROGRAM (OAK RIDGE NATIONAL LABORATORY)
- CENTER FOR MICROANALYSIS OF MATERIALS (UNIVERSITY OF ILLINOIS)
- SURFACE MODIFICATION AND CHARACTERIZATION LABORATORY (OAK RIDGE NATIONAL LABORATORY)
- COMBUSTION RESEARCH FACILITY – MATERIALS PROGRAM (SANDIA NATIONAL LABORATORIES)
- MATERIALS PREPARATION CENTER (AMES LABORATORY)

3/84

USAGE PROFILES OF SEVERAL NATIONAL MATERIALS RESEARCH FACILITIES

	PERCENT OF USE				
	HFIR	HFBR	IPNS	NSLS*	WNR/PSR*
UNIVERSITIES	40	45	31	42	24
INDUSTRY	12	6	5	31	6
DOE LABORATORIES (SAME SITE)	26	18	39	11	27
DOE LABORATORIES (OTHER SITES)	12	5	6	9	12
OTHER GOVERNMENT LABORATORIES	2	2	2	7	6
FOREIGN	8	24	17	—	24

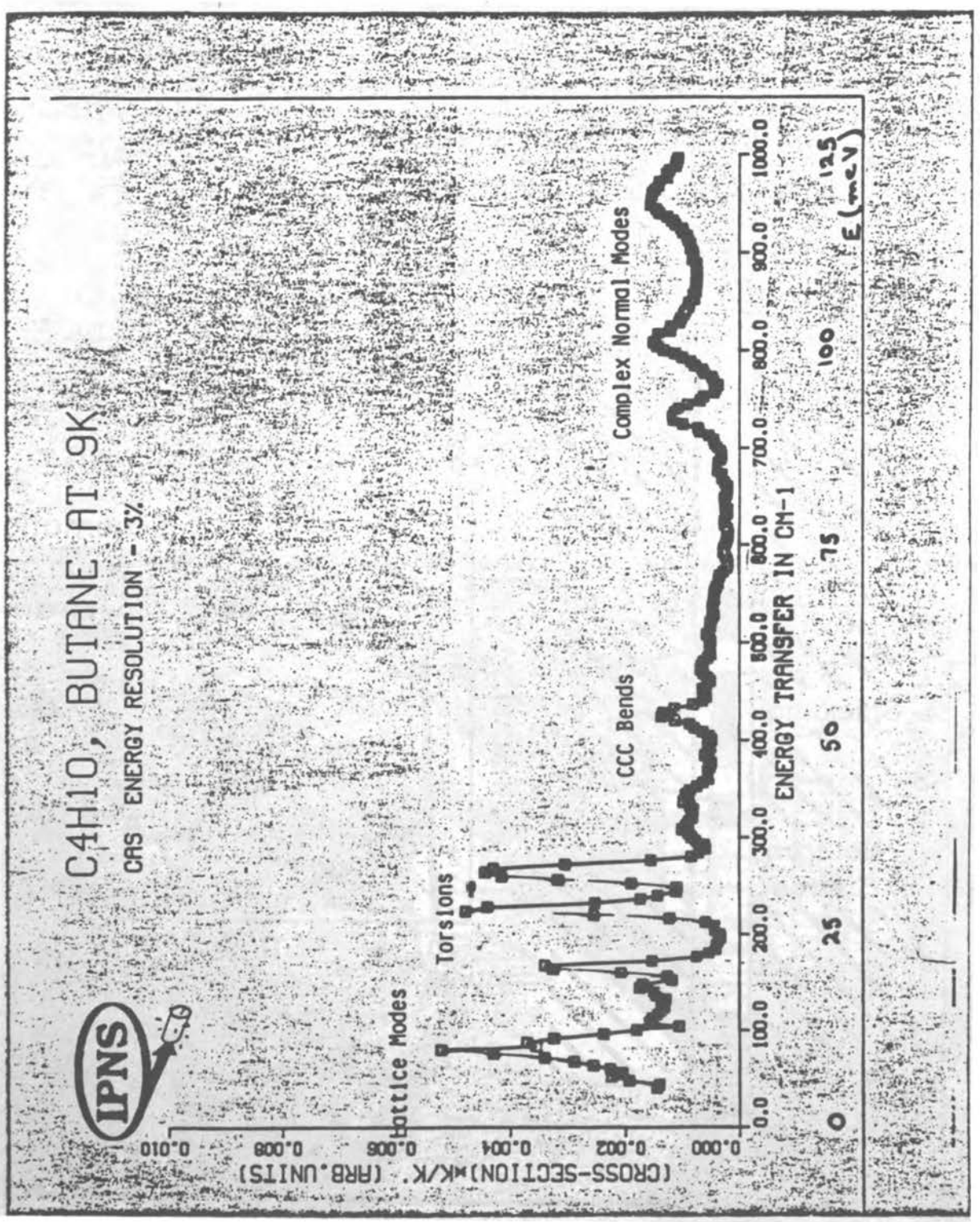
*NSLS FRACTIONS BASED ON TOTAL EQUIVALENT BEAM LINES. WNR/PSR FRACTIONS ESTIMATED FROM FY 1985 REQUEST.

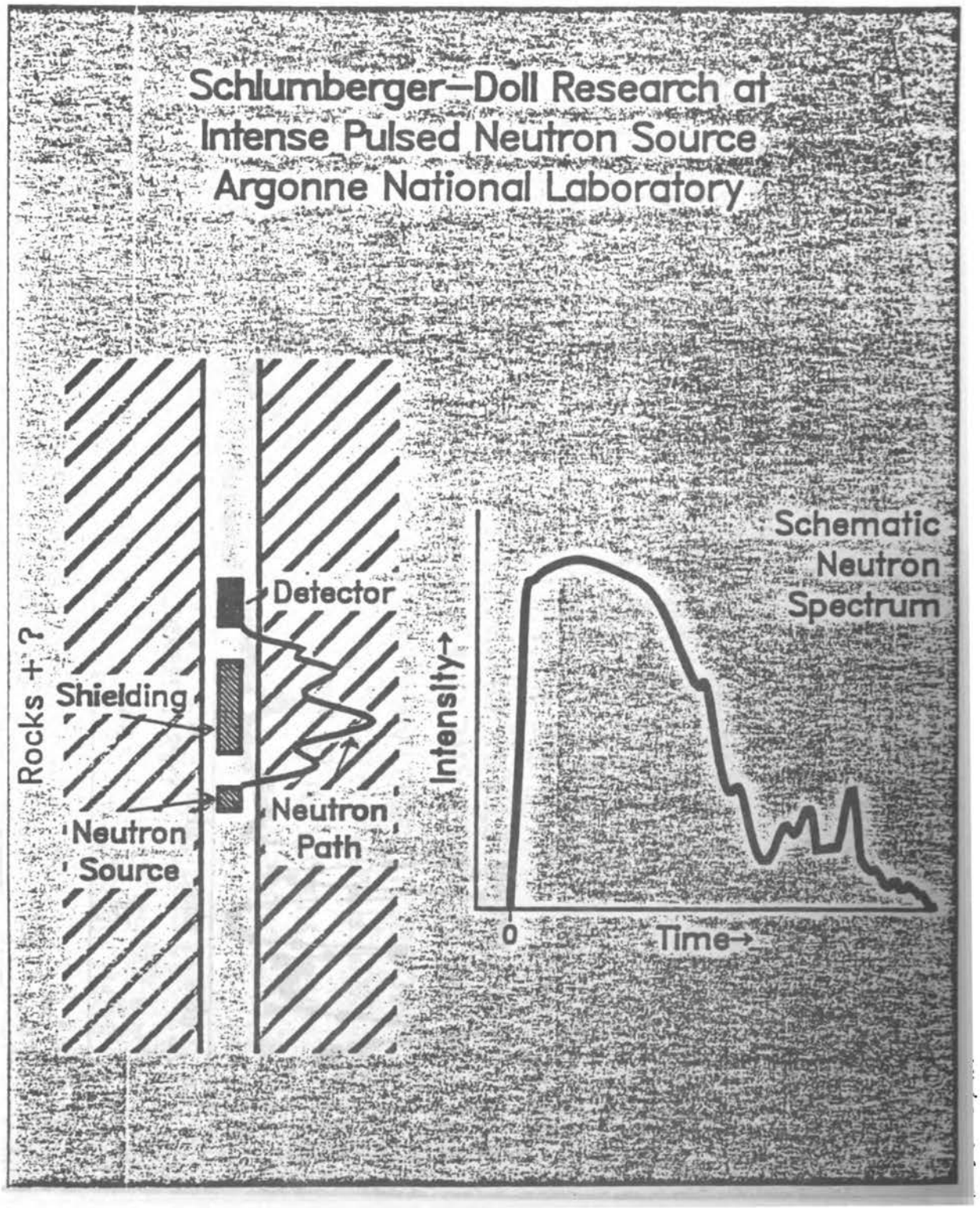
3/84

SCHLUMBERGER-DOLL AND ARGONNE NATIONAL LABORATORY DO COLLABORATIVE NEUTRON SCATTERING RESEARCH AT THE ARGONNE IPNS

- FUNDAMENTAL STUDIES OF VIBRATIONAL MODES OF HYDROCARBONS
- EXPERIMENTS GUIDE DEVELOPMENT OF MOLECULAR DYNAMICS MODELS
- THE MODELS ARE USED BY SCHLUMBERGER-DOLL IN PROPRIETARY OIL-WELL LOGGING WORK

3/84


C4H10, BUTANE AT 9K
CAS ENERGY RESOLUTION - 3%
IPNS
(CROSS-SECTION)*K'/K' (ARB.UNITS)
0.000
0.002
0.004
0.006
0.008
0.010
Lattice Modes
Torsions
CCC Bends
Complex Normal Modes
0.0
100.0
200.0
300.0
400.0
500.0
600.0
700.0
800.0
900.0
1000.0
ENERGY TRANSFER IN CM-1
0
25
50
75
100
125
E(meV)


Schlumberger–Doll Research at
Intense Pulsed Neutron Source
Argonne National Laboratory
Rocks + ?
Shielding
Detector
Neutron
Source
Neutron
Path
Intensity→
Schematic
Neutron
Spectrum
0
Time→

How business is using government laboratories

Facility — **Users**

Argonne National Laboratory

Intense Pulsed Neutron Source — **Du Pont, Exxon, 3M**

Very short, intense pulses of high-energy neutrons are being used to explore the structure and properties of materials, including catalysts and biological systems

National Battery Test Laboratory — **General Motors, General Electric, Electric Power Research Institute**

Tests are determining the cycle life, power, and capacity of batteries, as well as analyzing failures. Advanced sodium-sulfur and lithium batteries are being developed

Brookhaven National Laboratory

National Synchrotron Light Source — **Bell Labs, Exxon, Gulf, IBM, Xerox, Allied**

Intense beams of X-rays and ultraviolet light are being used to study the arrangement of atoms on surfaces, to understand catalysts, and to etch circuits on semiconductor chips

Scanning Transmission Electron Microscope — **Exxon, Merck Institute, Roche Institute**

An electron microscope, coupled with high-resolution imaging systems, is allowing scientists to weigh single molecules, to study the way that DNA binds to proteins, and to examine biological structures

Lawrence Berkeley Laboratory

National Center for Electron Microscopy — **Phillips Research Lab, Rockwell, Hewlett-Packard**

Electron microscopes are enabling researchers to observe chemical reactions as they happen and to analyze the structure of solar cells and semiconductors

2.5 million-electron-volt Van de Graaff Facility — **Fairchild Camera, National Semiconductor, Perkin-Elmer, Signetics**

Beams of protons and ions are aiding scientists in the study of semiconductor materials and the behavior of solid state materials

Oak Ridge National Laboratory

National Center for Small-Angle Scattering Research — **Allied Chemical, Eastman Kodak, Exxon, Firestone, Ford Motor, IBM**

Neutron and X-ray beams combined with sensitive cameras and detectors are enabling researchers to study the structure and properties of polymers and other materials

Sandia National Laboratories

Combustion Research Facility — **Weyerhaeuser, Babcock & Wilcox, Exxon, Westinghouse Electric, GM**

An array of advanced lasers and computers is helping in the study of coal combustion and combustion in advanced engines

Central Receiver Test Facility — **McDonnell Douglas, Northrop, Solar Kinetics, Boeing, Martin Marietta,**

The intense heat generated by a huge solar collecting tower and solar furnace is making it possible to probe the behavior of materials at high temperatures and to simulate the effects of heat on space vehicles during reentry

How neutron scattering is helping Exxon create entirely new polymer materials.

Exxon Chemical's David Lohse can observe the structure and behavior of polymer molecules.

From easy care fabrics to the nose cones of space vehicles, the long chain molecular structures called polymers have become, both literally and figuratively, woven into the fabric of 20th century life. Now, Exxon's David Lohse is exploring the characteristics of polymers to extend the potential of these remarkable materials.

Polymer Blends

Combinations of polymer molecules can produce materials with better properties than those of the individual components. Exxon Chemical developed and is currently marketing, for example, a blend of plastic and synthetic rubber polymer material which has the formability of plastic and the elasticity of rubber. Used in automobile bumpers, this material helps reduce damage from minor fender benders by absorbing impact and then returning to its original shape.

In order to develop more sophisticated blends, David Lohse and others in Exxon Chemicals' Long Range Polymer Research Group are developing the use of Small Angle Neutron Scattering (SANS), a technique that subjects these molecules to controlled scrutiny.

Small Angle Neutron Scattering

Conventional electron microscopy techniques allow scientists to study the structure of a polymer blend at room temperature. But the technique used by Exxon at the National Center for Small Angle Scattering Research (Oak Ridge National Laboratory) and at the National Bureau of Standards in Maryland permits scientists to study polymer molecules at temperatures of 180 C or higher. This technical advance requires high temperatures for the polymer to melt and be processed. In the melt state, the molecules are more mobile and the structure of the blends is known.

Seeing Polymer Structure by SANS

Small Angle Neutron Scattering operates on the same basic physics as other types of scattering such as light or X-ray. A well collimated beam of neutrons is directed into the sample. Some of the neutrons are scattered due to interactions with the atoms in the sample. The angle of the scatter is determined by the size of the molecular structures. Different structures can be labeled by substituting deuterium for hydrogen atoms, which allows a single polymer chain to be "seen" in its environment.

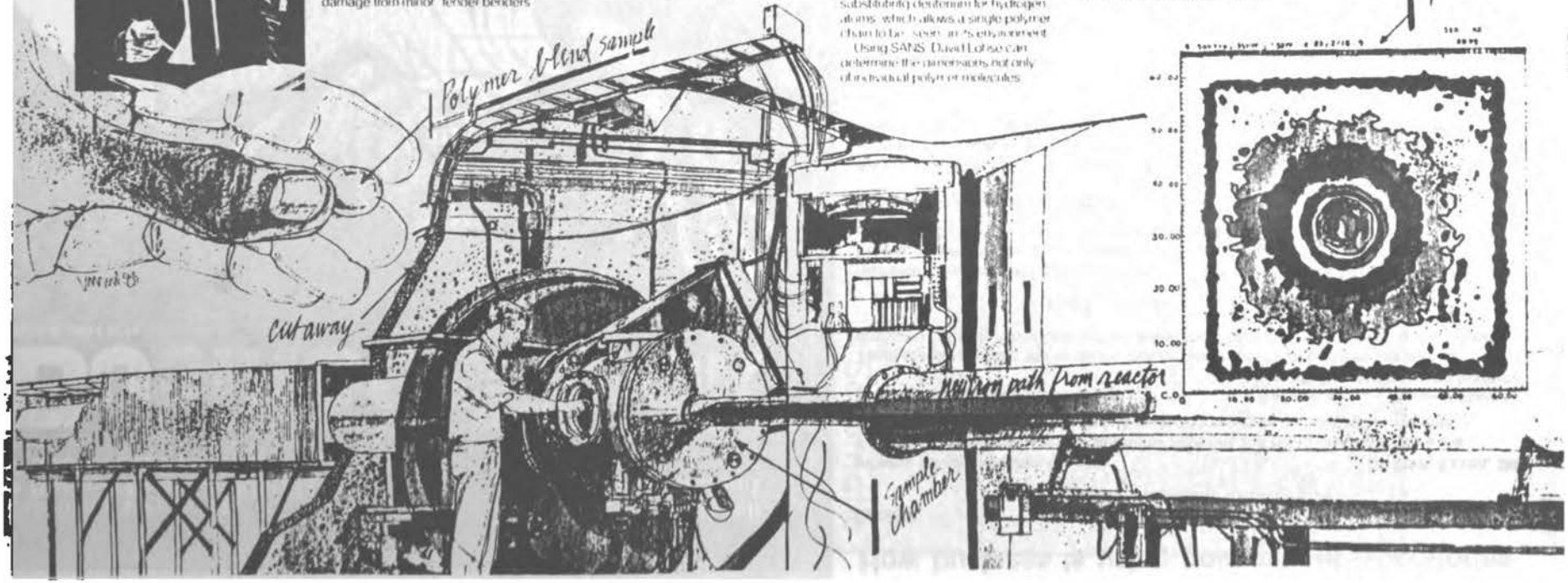
Using SANS, David Lohse can determine the conformations not only of individual polymer molecules (10-100 angstroms) but also the dimensions of the phase domains of the blends (greater than 1000 angstroms). More importantly, while the blends are being heated, he can measure changes in the sizes of the individual molecules and the domains. It's these changes which determine the physical properties of the materials.

The information obtained using SANS will be used to develop new polymer blends that may find important commercial applications in the home, in medicine, medicine, science and space.

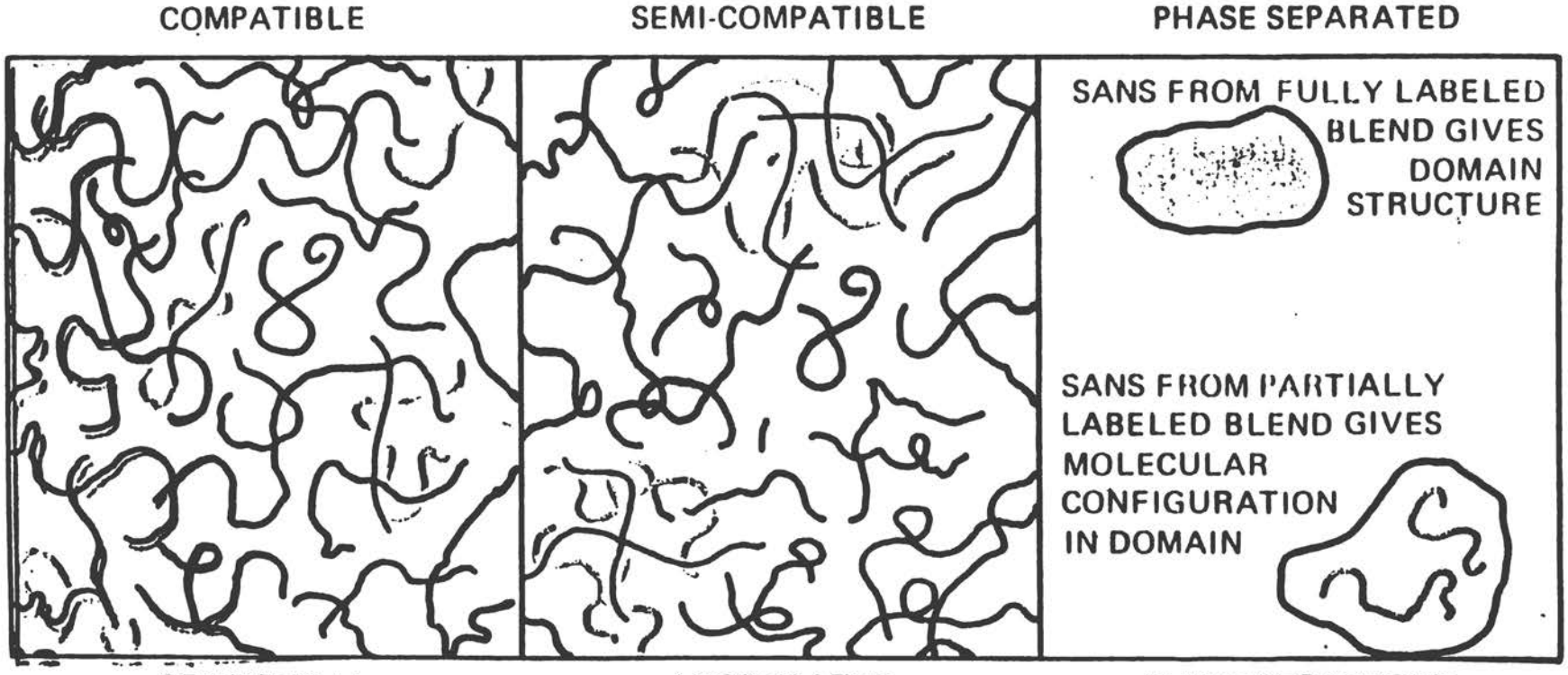
Exxon Chemical Company

Long Range Polymer Research is just one of many programs of Exxon Chemical Company's Technology Department. A division of Exxon Corporation, Exxon Chemical [illegible] its headquarters in Houston, Texas. [illegible] 2,000 scientists, engineers and technicians, [illegible] and advanced technology [illegible] polymers, [illegible] chemicals. For more information [illegible] Exxon Chemical Company, [illegible]

EXXON



AGGREGATION POSSIBILITIES FOR LABELED POLYMER BLENDS



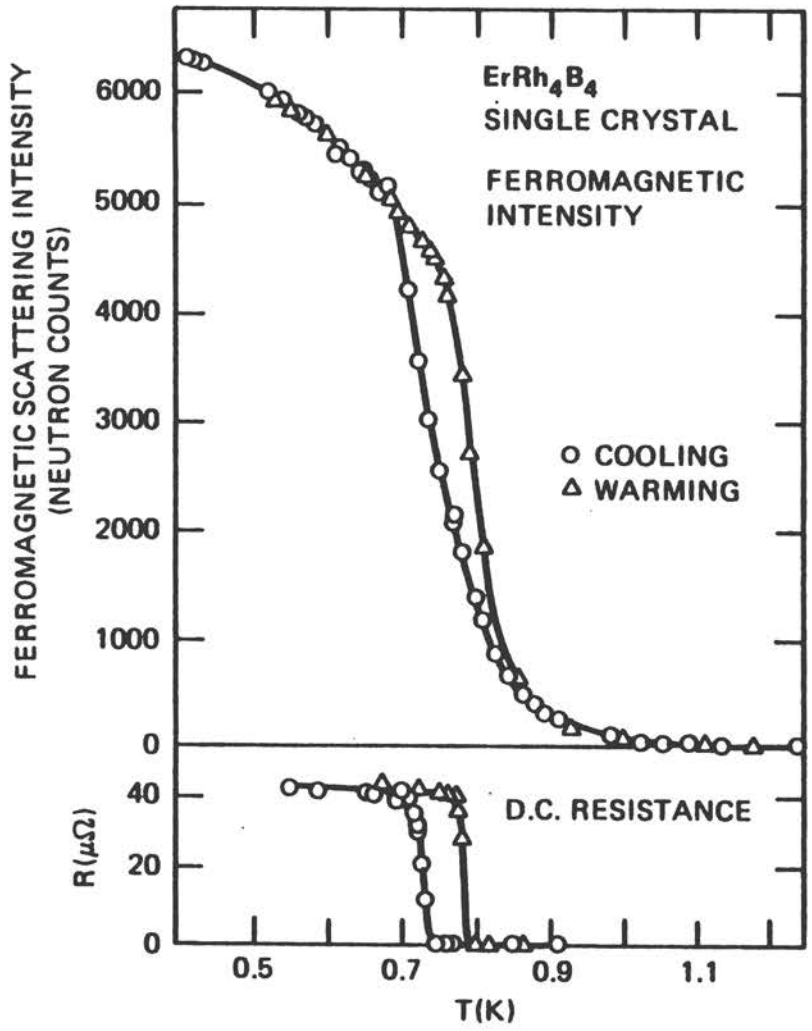
SANS RESULTS ON POLYMER BLENDS STUDIED AT NCSASR

BLEND SYSTEM	INSTITUTION	INITIAL CONCLUSIONS
PS–PVME	XEROX CORP./ U. MASS	COMPATIBLE FOR ALL COMPOSITIONS
ATACTIC/ISOTACTIC PS	U. MASS	COMPATIBLE FOR ALL COMPOSITIONS
PMMA–PVF_2	U. MASS	COMPATIBLE FOR 25–50% PVF_2
PS-POLYORTHOCHLORO-STYRENE	U. MASS	COMPATIBLE FOR HIGH (> 70%) AND LOW (< 30%) CONCENTRATIONS OF POCS
LD/LLP POLYETHYLENE	EXXON	VIRTUALLY COMPATIBLE IN MELT; AGGREGATED IN SOLID STATE
HD/LD POLYETHYLENE	EXXON	PHASE SEPARATED IN SOLID STATE; AGGREGATED IN MELT
PP–EP COPOLYMER (72% ETHYLENE)	EXXON	PHASE SEPARATED IN MELT AND SOLID
PS/POLYPHENYLENE OXIDE	ORNL/GE	COMPATIBLE FOR ALL COMPOSITIONS

IN ADDITION, CONTRACTS FOR THE PERFORMANCE OF PROPRIETARY RESEARCH AT NCSASR HAVE BEEN NEGOTIATED WITH DUPONT, FIRESTONE, AND KODAK.

3/84

NEUTRON SCATTERING MEASUREMENT OF THE COEXISTENCE OF FERROMAGNETISM AND SUPERCONDUCTIVITY IN $ErRh_4B_4$ NEAR 1°K



3/84

DESIGN AND CONSTRUCTION IS ONLY THE FIRST STEP IN OPERATING A SUCCESSFUL NATIONAL USERS FACILITY

- SCIENTIFIC REQUIREMENTS CONTINUALLY EVOLVE, AND FACILITY CAPABILITIES AND INSTRUMENTATION MUST EVOLVE ACCORDINGLY
- USERS LOOK TO FACILITY SCIENTISTS TO CONCEIVE, DESIGN, AND BUILD NEW INSTRUMENTATION
- USERS LOOK TO FACILITY MANAGEMENT TO PROVIDE FOR EFFICIENT AND RELIABLE FACILITY OPERATION, TO ASSURE CONTINUING FUNDING, AND TO DEAL WITH THE NON-SCIENTIFIC UNIVERSE IN GENERAL
- FACILITY MANAGEMENT LOOKS TO USERS FOR EXPRESSION OF NEEDS FOR INITIAL FACILITY, AND FOR SPECIFIC INSTRUMENTATION AND SUPPORT FACILITIES
- EXTENSIVE ANCILLARY FACILITIES MUST BE PROVIDED TO SUPPORT INTERDISCIPLINARY USERS

3/84

ANCILLARY FACILITIES REQUIRED FOR SUCCESSFUL OPERATION OF NATIONAL USERS FACILITIES

1. COMPUTERS
2. ENGINEERING AND MAINTENANCE
3. MACHINE SHOPS
4. ELECTRONIC SHOPS
5. RESEARCH MATERIALS PREPARATION AND CHARACTERIZATION
6. RADIOLOGICAL SERVICES
7. HEALTH, SAFETY, FIRE, etc., PROTECTION
8. VISITOR SUPPORT SERVICES

MAJOR FACILITY FUNDING LESSONS FROM PAST EXPERIENCE

- ADEQUATE FUNDING IS CRUCIAL. PROJECTS BUILT AND OPERATED WITH MARGINAL FUNDING RARELY REALIZE THEIR POTENTIAL
- ADEQUATE CONSTRUCTION-RELATED R&D IS REQUIRED
- INCLUDE STATE-OF-THE-ART INSTRUMENTATION IN CONSTRUCTION BUDGET
- SECURE FUNDING FOR NEW INSTRUMENT DEVELOPMENT

THE MYTH OF THE $\Sigma = 0$ HYPOTHESIS

- LARGE NEW FACILITIES RARELY IMPACT SMALL RESEARCH PROJECTS. THEY DO TEND TO SHUT DOWN LARGE OBSOLETE FACILITIES
- DISCOVERIES MADE AT LARGE FACILITIES ENRICH THE ENTIRE SCIENCE. NEW FIELDS APPEAR WHERE NOTHING EXISTED BEFORE. ESTABLISHED FIELDS ARE OFTEN REVITALIZED
- ESTABLISHMENT OF LARGE SUCCESSFUL MATERIALS RESEARCH FACILITIES WILL CREATE OVERALL GROWTH IN MATERIALS SCIENCE

QUALITY OF BASIC ENERGY SCIENCES (BES) MATERIALS RESEARCH – I

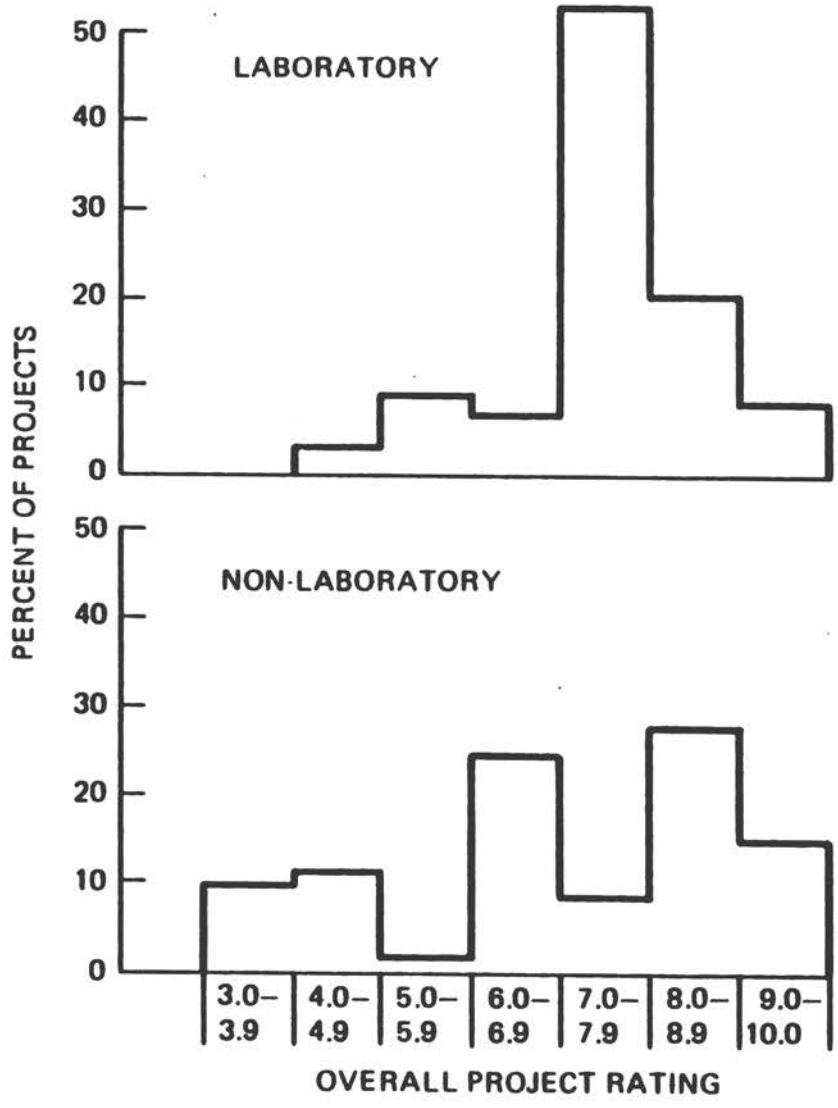
- AN EXTENSIVE PEER REVIEW OF THE BES PROGRAM WAS RECENTLY UNDERTAKEN*
- THE BES PROGRAM INCLUDES A SUBSTANTIAL FUNCTION (~ 30%) OF DOE MATERIALS FUNDING
- THE OVERALL RESULTS INDICATE:
  - BES MATERIALS SCIENCES PROGRAMS ARE WELL-MANAGED AND PROVIDE BOTH HIGH QUALITY SCIENCE AND LONG-RANGE MISSION SUPPORT

**AN ASSESSMENT OF THE BASIC ENERGY SCIENCES PROGRAM,* DOE/ER-0123, MARCH 1982.

QUALITY OF BASIC ENERGY SCIENCES (BES) MATERIALS RESEARCH – II

- BES MATERIALS SCIENCES PROGRAMS HAVE REMAINED STRONG IN SPITE OF FAST-CHANGING DEMANDS
- REVIEWERS FROM UNIVERSITIES AND INDUSTRY CONSISTENTLY RATED LABORATORY MATERIALS PROGRAMS COMPARABLE TO NON-LABORATORY PROGRAMS IN OVERALL QUALITY
- LARGE-DOLLAR PROJECTS (> $500 K/yr) WERE RATED HIGHER THAN NON-LARGE-DOLLAR PROJECTS
- 90% OF BES MATERIALS PROJECTS WERE RATED GOOD OR ABOVE (NO IMPORTANT DEFICIENCIES) WITH 67% STRONG OR OUTSTANDING (DESERVING OF PRIORITY SUPPORT)

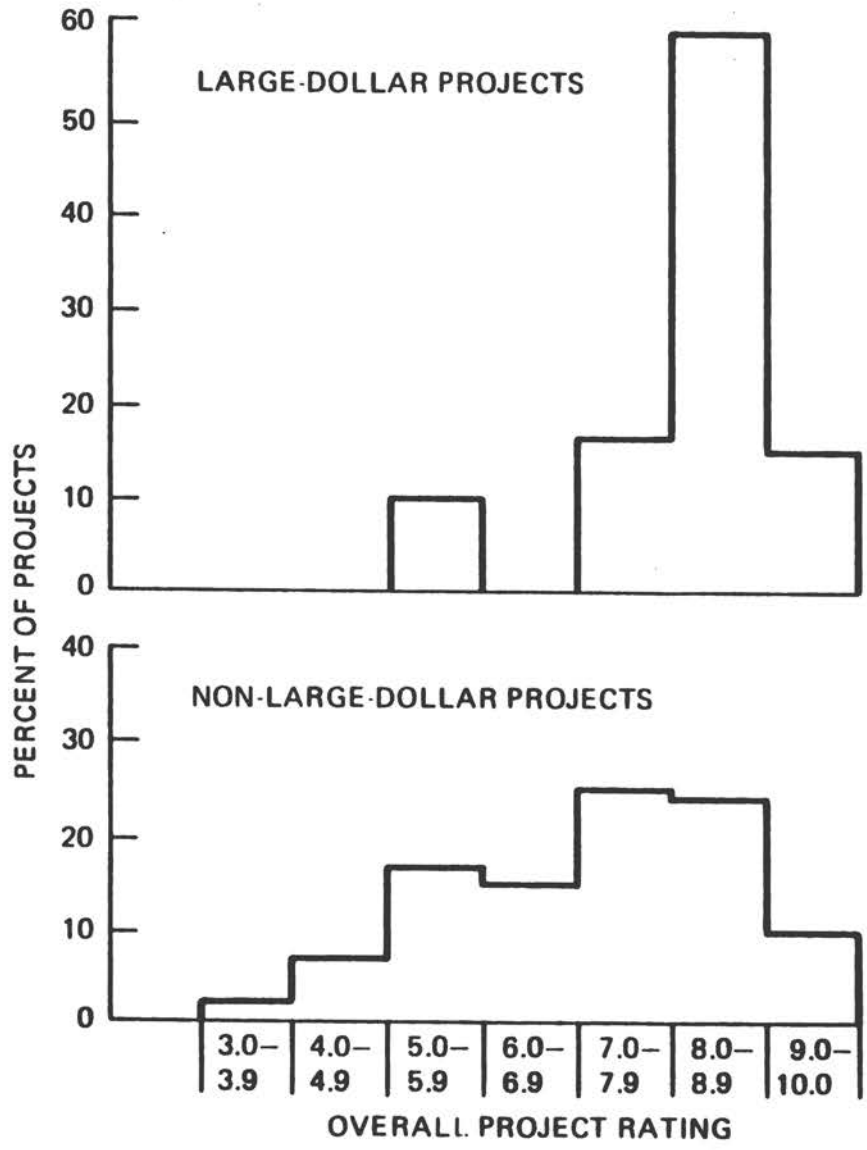
OVERALL RESEARCH QUALITY FOR BASIC ENERGY SCIENCES (BES) PROGRAM
(PROJECTS BETWEEN $100 K AND $350 K/yr)



RATINGS FROM: *AN ASSESSMENT OF THE BASIC ENERGY SCIENCES PROGRAM,* DOE/ER-0123, MARCH 1982

3/84

OVERALL RESEARCH QUALITY RATINGS FOR LARGE-DOLLAR (> $500 K/yr) AND NON-LARGE-DOLLAR (< $500 K/yr) BES PROJECTS



RATINGS FROM: *AN ASSESSMENT OF THE BASIC ENERGY SCIENCES PROGRAM,* DOE/ER-0123, MARCH 1982.

3/84

SYNCHROTRON R&D AT THE DEFENSE PROGRAMS LABORATORIES

Presented to Major Materials Facilities Committee Workshop
of the National Academy of Sciences

Presentation of P. E. Coyle
March 19, 1984

DR. COYLE: Good morning. I appreciate being invited here this morning to speak about some of our materials research. In particular, I am going to emphasize the work of the Department of Energy Defense Programs Laboratories with synchrotrons. I think the neutron work has been covered by John Browne and others in previous sessions.

In appearing here, I am trying to represent the interests of three different laboratories: Lawrence Livermore National Laboratory, where I work; Sandia National Laboratories; and Los Alamos National Laboratory. I have had some help from people at all three labs, but in particular I want to recognize help from Walt Trella at Los Alamos and from Danny Hartley and John Vitko at Sandia.

The Defense Programs Laboratories, as they are sometimes called, are multi-program laboratories like the other national labs, and conduct research in many different areas. Although they are associated mainly with the Defense Programs part of DOE, a good deal of their work is not directly defense related as can be seen in Fig. 1. At Livermore, for example, some 55 percent of our work is in defense programs including nuclear weapons research, the rest is in a variety of programs that are primarily energy related or in fundamental research.

All in all, the three labs represent a staff of about 23,000 people, of whom about 3,400 are PhD scientists and engineers, and a good fraction of those are involved in materials work of one kind or another. Fig. 2 shows the materials science budget for Livermore. I do not have similar numbers for Los Alamos and Sandia, but I suspect that the proportions are comparable. In some areas you will see the fraction of research that is materials related is higher than others but, all in all, it represents a considerable effort. We have a continuing commitment to materials research and put substantial resources into it.

A particular area where we have a number of challenging materials and materials-related problems is in x-ray measurements. We are interested generally in making very high resolution x-ray measurements, whether in space or energy or in time. By that, I mean spatial resolution of about a micron, energy resolution of about a tenth of an electron volt, and time resolution of a tenth of a nanosecond or better.

So there is a lot of work going on in a variety of areas to achieve those kinds of goals. To give you a feeling for why synchrotron x-ray sources are attractive to us, we put together this chart (Fig. 3). It compares first, on the left, the brightness of the synchrotron source at SSRL and the proposed ALS, with the brightness of a nuclear explosion. Then, in the middle, the peak fluxes that one would measure with a

detector at 10 meters from those same x-ray sources are plotted, and on the right you see the flux thresholds where our conventional detectors go nonlinear.

We operate close to these detector thresholds, and yet we do not have any monochromatic sources that even come close to what we need for some development and calibration purposes. A major point of this chart is at the very bottom. The sources we have at Livermore, for example, are something like 10^{12} times weaker than synchrotrons.

Now we are comparing here vastly different kinds of sources, so perhaps the comparison is not fair, but nevertheless we do not have any machines which can get us into desired flux regions. Generally the machines that we do have produce very small currents in our detectors, on the order of 10^{-12} amps. We are also looking for sources that would raise significantly the counting rates for laboratory experiments that would allow us to verify our computational models.

In working with our existing laboratory sources, nevertheless, we have exposed thousands of items every year; here an item may be a detector, crystal, a mirror, foil or some other element of a measurement system. We operate some of those machines for 3,000 or 4,000 hours of beam time each year.

Advanced research requirements at the Defense Programs Laboratories span a wide range of areas and I have listed these in Fig. 4. Our requirements, as can be seen, span the entire synchrotron spectrum. Some of these are research topics in their own right; others are in support of some other work, but whether it is more traditional materials science or other research, we believe synchrotron radiation will be an important tool (Fig. 5).

A first example has to do with the first-wall problem in fusion reactors (Fig. 6). Most DOE laboratories have work in this general area, perhaps not this particular example, but all are trying to understand the damage mechanisms that occur from fusion neutron reactions in a fusion reactor first wall. The high intensity of synchrontron sources would permit experiments involving a wider range of variables than would be practical with conventional x-ray methods.

Another example has to do with understanding the structure and the phases of various kinds of alloys (Fig. 7). We would like to be able to better understand the properties of unusual alloys and the role of displacive and diffusional effects in phase transformation. This next chart (Fig. 8) was prepared by Los Alamos. From it you can see that the phase structures are very complicated for the heavy elements in which we would have the most interest.

Another example is in the area of high-power solid-state lasers (Fig. 9), where we have considerable effort. To understand how metal-doped crystals behave, what makes them work the way they do, we see applications for synchrotron experiments to normalize mathematical models.

There is a lot of work going on at the three labs in optics and here (Fig. 10) is an example of where we at Livermore would like to better understand laser-damage mechanisms and what happens when the laser glass itself is being heated by lasing action. Synchrotron radiation can be used to map time dependent electronic structure in such materials to high resolution. As another example in optics, (Fig. 1) we are working on nonlinear optical materials for harmonic converters. Detailed optical chemical and structural data are needed for families of related materials.

We would like to be able to measure the crystal structure of the actinides, in particular, the high specific-activity transuranics (Fig. 12). To measure the crystal structure of Einsteinium, for example, in order to infer other properties as well as just to understand that structure, we have a problem in that conventional x-ray sources take so long to produce the data that the film would get fogged and, over very long exposure times, the crystal would become amorphous from alpha particle damage. High intensity sources of monochromatic photons would permit good quality measurements with short exposure times.

We have an interest in understanding the oxidation and hydriding of the actinides and here (Fig. 13) is an example where we would want to be able to examine defect clusters in an oxide of uranium. We would want to do similar work with hydrides.

There is a lot of work going on at the laboratories in equation of state and we believe there are opportunities for equation of state experiments on synchrotrons. Right now we are using relatively weak laboratory sources and simply cannot get all the information we would like. We are interested in how materials behave under static high pressures (Figure 14), and during shock loading (Fig. 15). With high x-ray energies and some kind of a pressure or shock source, one can examine how materials change under loading, how their crystal structure changes, and how lattice parameters change. This would be greatly simplified with a bright synchrotron source.

There are applications where the surfaces of materials are exposed to very high energy fluxes and we need to be able to understand what happens to those surfaces under those conditons. On Saturday, Joe Stohr gave an example of photon-stimulated desorption of hydrogen from surfaces with ammonia. Perhaps you could think of this example as analogous, although here (Fig. 16) we are talking about desorption of hydrogen from materials like gold or aluminum. We want to do these experiments at a range of energies up to 30 kilovolts.

Gas solid interactions on actinide metals and compounds are complex and difficult to study with conventional techniques (Figure 17). While ultraviolet sources have helped reveal electron density and structure, synchrotron radiation at various incident energies will permit enhanced sensitivity.

A more specific example in this area has to do with our studies of the use of actinides as catalysts. In this particular case (Fig. 18), thorium compounds are being used to catalyze high-octane hydrocarbons. We would like to understand the role that the thorium plays and be able to measure, for example, valence-band structure in catalysis intermediates.

We also are doing work on laboratory x-ray lasers. Fig. 19 shows an example of an experiment that we plan to do soon. We have already tried this sort of experiment with a smaller laser and we will be trying it again on the NOVA laser. One of needs here is to be able to develop diagnostic instruments that can measure very intense x-ray sources.

To give you an example of that kind of diagnostic intrument, Fig. 20 is a schematic of a microchannel-plate grazing-incidence spectrometer. You can see that there are a number of components in such an instrument which we would need to understand and be able to calibrate. I should also point out that this kind of high resolution instrumentation would have wide application in other research areas that use synchrotron x-rays.

Those are just a handful of examples and in the next two charts (Fig. 22 and 23) we simply tabulate all of the research proposals [for SSRL and NSLS] that are covered in the PRT's composed of ourselves, Los Alamos, Sandia, and the University of California campuses. I have already discussed some of these proposals. Here they are listed according to categories, bioscience, chemical and surface science, materials science, and so forth, and which site, whether it is NSLS or SSRL is shown, what energy of x-rays would be required and whether or not short time structure is important, and it goes on to a second page.

Here are examples in atomic physics, x-ray instrumentation, lithography, and so forth. If you simply take those proposals and count them up according to which energy bins they fall in, you get the histogram shown on the next chart (Fig. 23).

There are 56 different topics there, but there are more than 56 marks because, in some cases, the experiment requires more than one x-ray energy, so they have been counted for each energy range needed. Overall you see the general shape of the needs for x-ray energies in the proposals that we have made to Stanford and Brookhaven so far. These are not all of the proposals we ever expect to make; as the beamlines at SSRL and NSLS become closer to being operational, new ideas will develop and that picture will change.

So far I've described the problems, the kinds of problems we see we want to work on. We will begin to address such problems on two different beamline projects: one which is being led by Los Alamos at Brookhaven, which consists of two stations on the VUV ring and a station on the x-ray ring, and then at Stanford we are leading the group with another beamline project, two stations on a regular line and one off the bending magnet. The difference in the cost between the two is because at Stanford we have to pay for building construction, a wiggler and more alcove transport equipment than at Brookhaven.

Together, these two projects are a fiscal '84 line-item construction project and the money was released in January. We are completing design work and getting ready to start construction, we hope, this summer.

Fig. 25 just describes the Los Alamos stations, the energy ranges in which they expect to operate, and the dates when they could be completed. Similarly, for Stanford (Fig. 26), here are the three stations that we would expect to build first, the energy ranges and, again, the dates when they would be completed.

Eventually we expect to be able to build a more extensive facility at Stanford. We are thinking in terms of five or six stations on the two beamlines, but only three of those are funded in the line-item construction project. (Fig. 27)

I showed the histogram for our PRT. Separately, Sandia has been doing some work for which they have estimated requirements for synchrotron-radiation experiments in a number of areas, materials science, chemistry, detector research and development, atomic physics, and so forth, and what percentage of the total would fall in various energy ranges. This is shown in the next chart (Fig. 28).

Los Alamos has plotted for us the number of diagnostic instruments that they have deployed on their major field experiments over the last five years as a way of illustrating the rapid growth in x-ray instrumentation (Fig. 29). We have been seeing a similar trend at Livermore, and the demand that this creates on our existing laboratory x-ray facilities, even allowing for their limitations, is quite staggering.

To go a little bit farther into the future, there has been a lot of discussion about the importance of brightness that can be achieved from these machines, but this has been in terms of time averaged brightness. We plotted peak spectral brilliance, that is, single-pulse brilliance -- as you can imagine, we tend to think in terms of single pulses -- so we have plotted the peak brightness of two undulator envelopes to compare with intense thermal sources (Fig. 30).

Alongside are plotted black-body spectra at one, two, four, and eight kiloelectronvolts and the point we wish to make here is that on a single-pulse basis, these sychrotron sources would give us the ability to do plasma physics work at levels which just simply cannot be achieved today. There are no laboratory sources that have reached these ranges. We have also shown for comparison the estimated output from the 54-pole wiggler at SSRL.

What all that comes down to is that the requirements for synchrotron radiation, as we see them at the three Defense Program Laboratories, strongly suggest photon energies around one kiloelectronvolt. You saw examples that went from 60 eV up to 30 kiloelectronvolts and there is certainly interest over all these energies, but the centroid tends to be near one kiloelectronvolt.

We want high flux and high brilliance, both average and peak brilliance, of course, and short pulse for some experiments (Figure 32).

I might also say that there are a couple of other requirements that are not listed here. We would like these machines to be reliable. In many of the experiments we conduct, we only get only one chance. In some instances, it may be necessary to do classified research, although at the moment we have not proposed any such experiments, nor are we being kept from doing any at this time.

If these machines turn out to be as good as has been discussed, we can expect that the pace of our activity on these machines could be accelerated.

In summary, then, (Fig. 33) the Defense Programs Laboratories have what we see as a growing need for synchrotron radiation sources. We believe that these needs are best met by participating in state-of-the-art synchrotron facilities with the national scientific community. We are already working with regional facilities at Stanford and at Brookhaven, and we do not have any reason to approach the need any differently in the future.

Synchrotron R&D at the Defense Programs Laboratories

Presented to

Major Materials Facilities Committee Workshop
of the
National Academy of Sciences

Philip E. Coyle
March 19, 1984

University of California
Lawrence Livermore
National Laboratory

Defense programs laboratories

Missions and Programs

- Nuclear weapons research & development
- Nuclear weapons effects
- Nuclear weapons test detection and verification
- Inertial and magnetic confinement fusion
- Advanced isotope separation
- Research
  - — Materials science
  - — Solid state physics — surface science
  - — Chemistry — photochemistry
  - — Atomic physics — plasma physics
  - — Biomedical research — environmental studies
  - — Engineering studies
  - — Geoscience — astrophysics
  - — Nuclear physics

Figure 1

Over 10% of our programmatic effort is materials related

	FY84 operating ($M)	Materials R&D ($M)
Weapons	250.9	20
Inertial confinement fusion	58.7	15
Isotope separation	89.3	17
Magnetic fusion	72.4	5
Energy	16.1	4
Biomed/environmental	11.0	1
Other DOE programs	40.0	5
Reimbursable/work for others	79.5	21
	617.9	88

581

Figure 2

Scale of x-ray sources and detectors

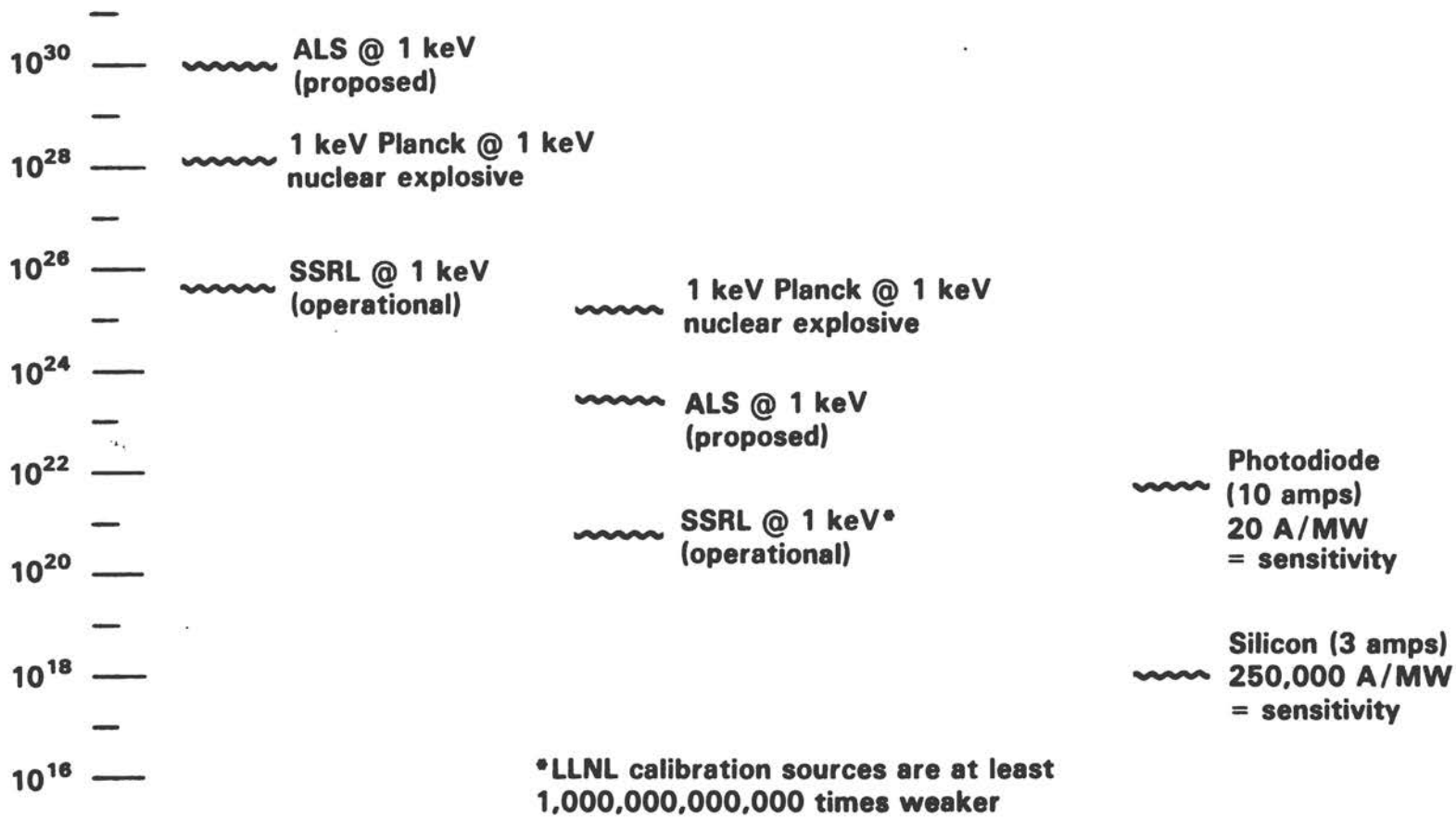


Figure 3

Advanced research requirements

- Materials science
  - — Crystallography, EXAFS, microprobe, microscopy
- Solid state physics
  - — Photoemission, anomalous dispersion, optical properties
- Surface science
  - — Photon stimulated desorption, SEXAFS
- Chemistry/photochemistry
  - — Photodissociation, photoabsorption, photoionization, relaxation
- Atomic and plasma physics
  - — Photoionization, photoemission, inner shell measurements, ionized state absorption, transmission spectroscopy, excited state processes
- Biosciences/environmental sciences
  - — Scattering, microscopy, microanalysis, holography
- Engineering studies
  - — Radiography, microscopy, exotic welding

Figure 4

The synchrotron could benefit our materials projects in many ways

1. High spatial resolution for imaging
2. Detailed electronic structure data
3. Accurate structure and chemistry data for a variety of materials, especially actinides
4. Real-time analysis of materials subjected to high loading rates
5. Real-time reaction histories for
   - Surface interactions
   - Catalysis
6. Tool for enhancing development of advanced diagnostics for soft x-ray lasers

Figure 5

Imaging — High-resolution 3-D images would enhance our understanding of material behavior

1 The degree of radiation-induced degradation of material ductility is related to the number and size of defect clusters in the irradiated solid

2 Tomography coupled with a synchrotron beam could provide 3-D images of the clusters and more detailed atomistic data

Beamline: 60 eV-5 keV

Tungsten defect cluster

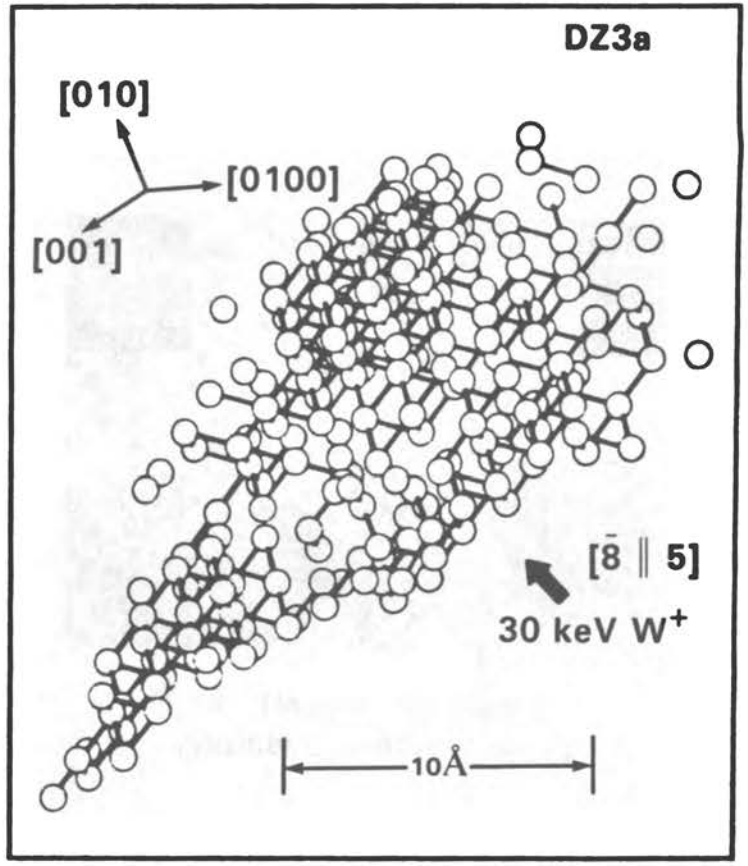


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Figure 6

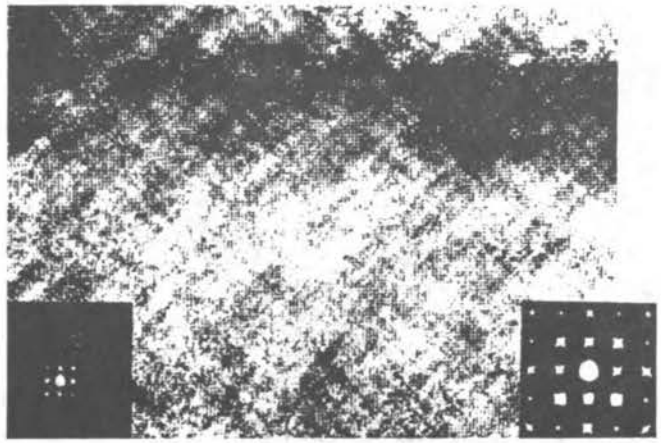
EXAFS data will complement experimental data on martensitic transformation mechanisms

Imaging

1 High-resolution electron and field ion microscopy can determine variations in strain and composition

2 Further data is required on the identity of atoms and their spatial position before and after transformation to unambiguously identify mechanisms

Optical diffractogram of a "tweed" structure



Beamline: 60 eV-1.5 keV

These are the actinide phases

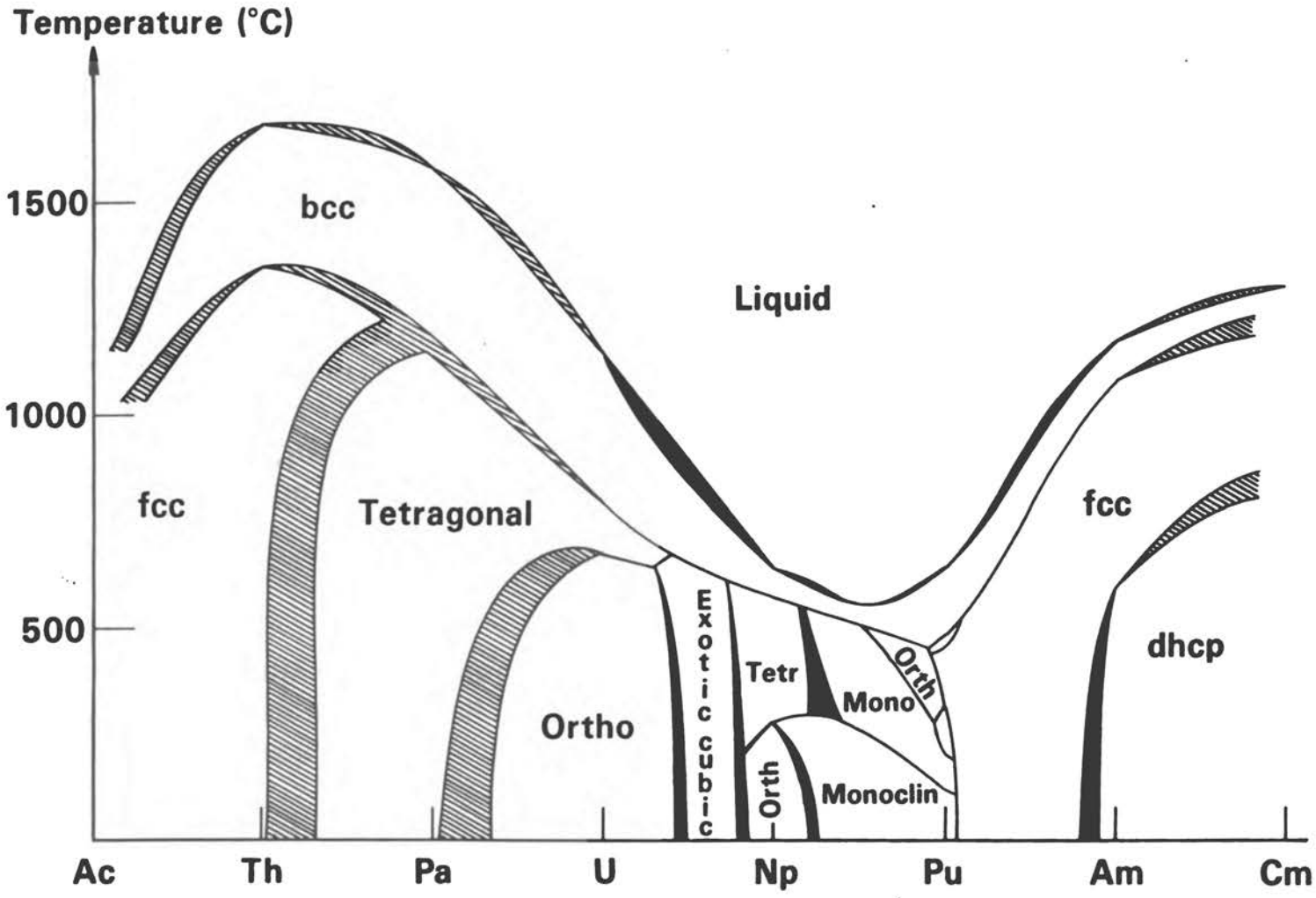


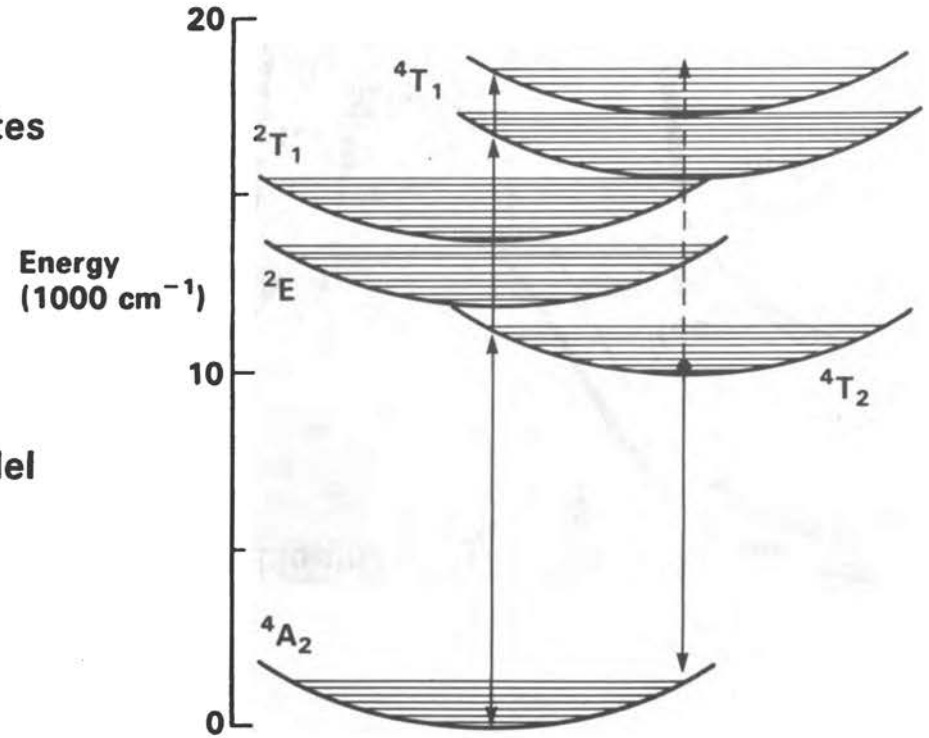
Figure 8

High-powered solid state lasers require materials with a unique electronic structure

Electronic structure

1 The current search for materials involves a modeling approach that only approximates host effects

2 Detailed electronic spectra of lasing ions in the host is required to
- Calibrate the current model
- Broaden the spectrum of materials under study



Beamline: 1 eV-1 keV

More detailed electronic structure data is needed to improve our understanding of laser damage

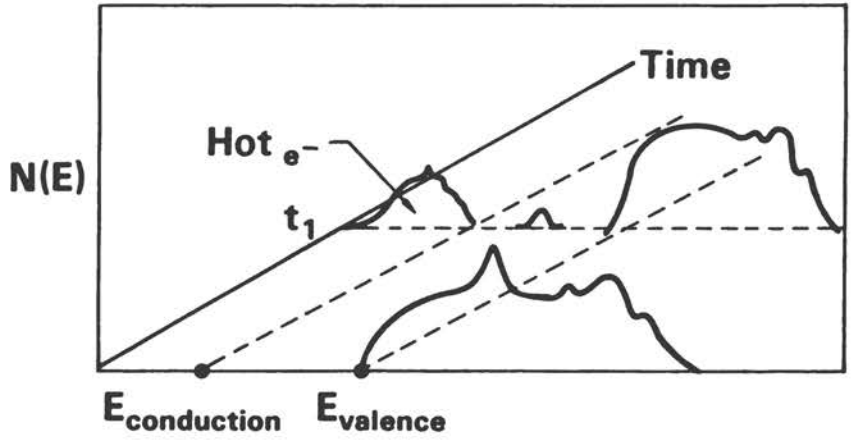
Electronic structure

Measurements of the time-dependent electron concentration in a material during laser exposure yield vital information:

- **Lifetimes of very hot electrons in a solid (1-10 eV)**
- **Cross-sections of multiphoton transitions**
- **Cross-sections of electron-laser photon interactions**

Beamline: 0.1-1 keV

Possible band-structure changes during laser heating



589

Figure 10

Electronic/ crystal structure

Precise determinations of structure would advance the development of nonlinear optical materials

1 Short wavelength lasers can be produced by harmonic conversion

2 The strength of the harmonic radiation is a function of electronic anharmonicity, i.e., crystal structure

3 Development of advanced nonlinear optic material compounds requires
- Precise lattice parameter data
- Electronic structure data over a range of fundamental wavelengths

Nova conversion array

Beamline: 8-10 keV

590

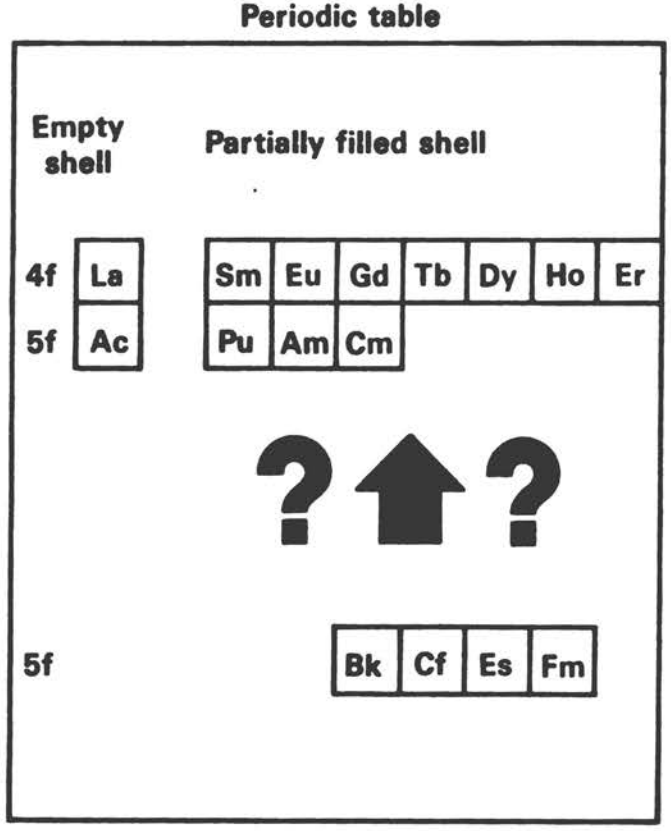
Figure 11

Precise determination of the crystal structure will help characterize actinide elements

Chemical properties

1 The chemical properties of the newer actinide elements could be inferred from other elements, if their crystal structure were known

2 Short exposure times to high intensity diffraction sources are required to determine the room-temperature crystalline phases



Beamline: 8-10 keV

Figure 12

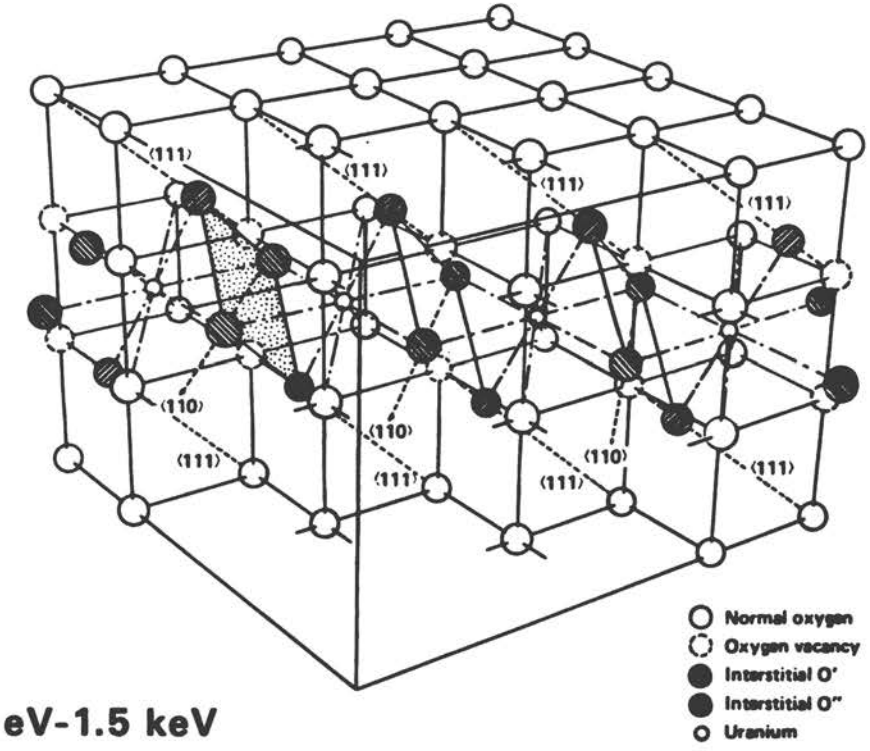
More accurate structure data is needed to characterize defect complexes in actinide compounds

Structure

1 Oxidation and hydriding of actinide elements promotes the formation of detrimental defect clusters

2 Control of the reaction requires data on their crystallographic structures, specifically metal-oxygen and metal-hydrogen bond distances in anion sublattices

Defect clusters in U_4O_9



Beamline: 60 eV-1.5 keV

592

Figure 13

Precise static and dynamic property measurements will advance work on equations of state

Structure

Synchrotron powder x-ray diffraction will provide data on

- **Phase transformations and compressibilities of actinide materials under static high pressures**

- **The crystal structure of phases in actinides and other materials under various loading conditions**

Beamline: 8-20 keV

Figure 14

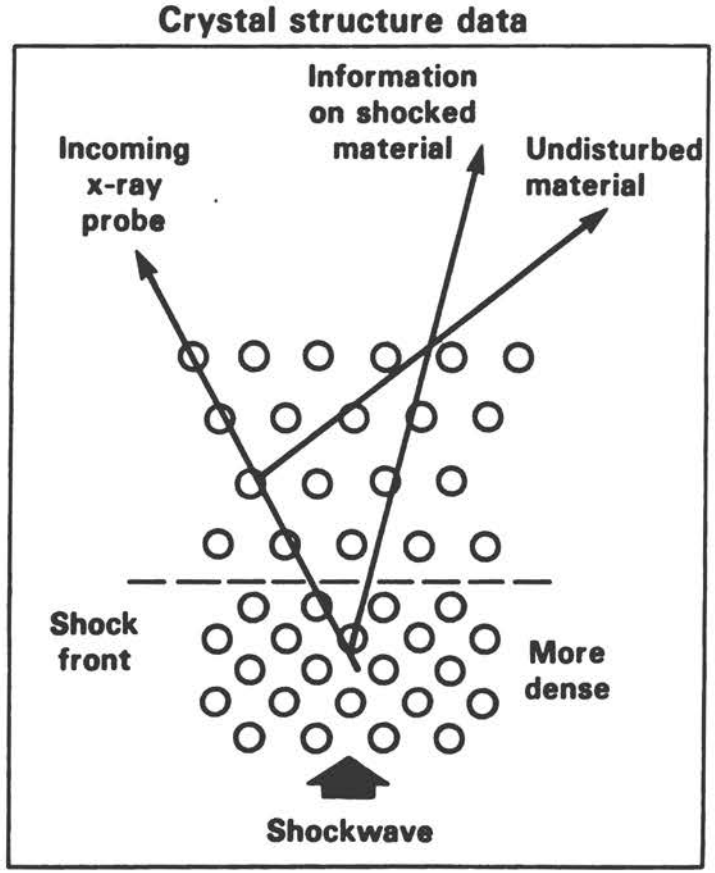
Real-time analysis will identify lattice changes occurring during shock loading

High loading rates

1 Shock loading of a material appears to maintain crystal symmetry, while changing lattice parameters

2 Flash x-ray studies of yielding in materials require knowledge of what the shocked lattice structure looks like

3 Synchrotron powder diffraction could provide real-time data on undetermined lattice changes



Beamline: 8 keV

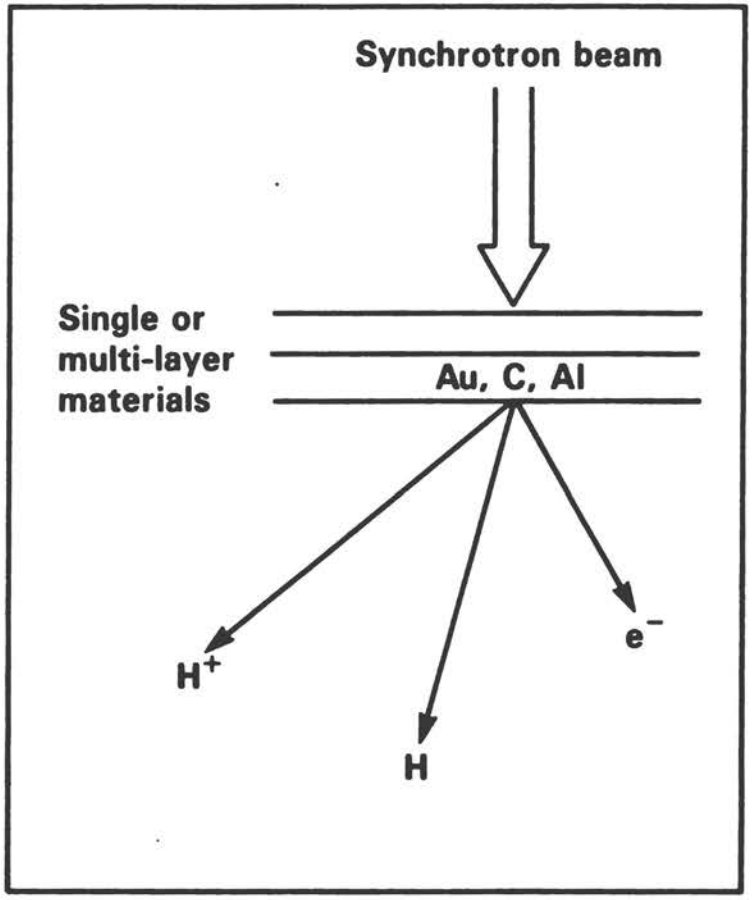
Figure 15

Material surfaces changes under high-energy fluxes are not well characterized

Surface interactions

1 **Photon-stimulated desorption of hydrogen from the surface of a solid cannot be accounted for in current physics calculations**

2 **Precise measurements are required to determine distributions of photoelectrons and hydrogen ions emitted during exposure**



Beamline: 30 keV

Figure 16

Surface interactions

Reaction histories will provide critical data on surface changes in actinides

1 Adsorption and chemisorption studies of gases on actinides and their compounds are complex and difficult to study with conventional techniques

2 New approaches are required to determine

- Orbital character of valence and conduction electrons
- Photoelectron spectra (bulk vs surface)
- 5f electron emission

Beamline: 6-150 eV

596

Figure 17

Reaction histories will enhance development of new catalysts for high-octane hydrocarbons

Catalysis

1 We are studying the use of actinides as catalysts:

$$CO + H_2, O_2 \xrightarrow{ThNi_2,\ ThO_2,\ ThCu_6} C_yH_x$$

2 Understanding the role of thorium requires determination of valence band structure

Catalysis Intermediate

$$ThNi_2 + O_2 \longrightarrow ThO_2 + \underset{\text{clusters}}{\overset{\text{Ni}}{\text{small metal}}}$$

Beamline: 6-150 eV

Figure 18

The development of new x-ray lasers is coupled to the development of diagnostics

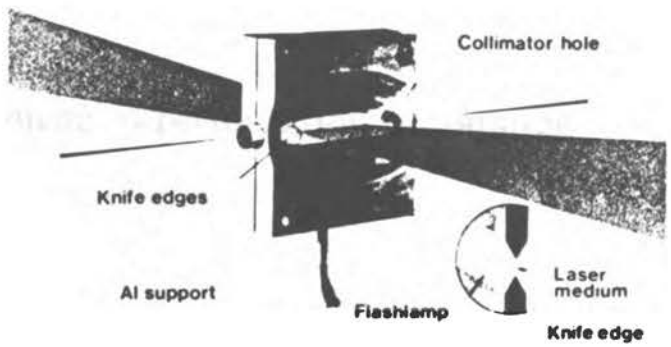
Diagnostics

1 The diagnostic instrumentation needed to test soft x-ray laser concepts has to be precisely aligned with the beam and be able to withstand high photon fluxes

2 Current instrumentation is developed using isotropic x-ray sources, where the photon flux is small and alignment unnecessary

3 Synchrotron sources can be tuned to mimic the x-ray laser

Novette x-ray laser experiment



598

Beamline: 50-500 eV

Figure 19

MCPIGS Micro-Channel Plate Intensified Grazing Incidence Spectrometer

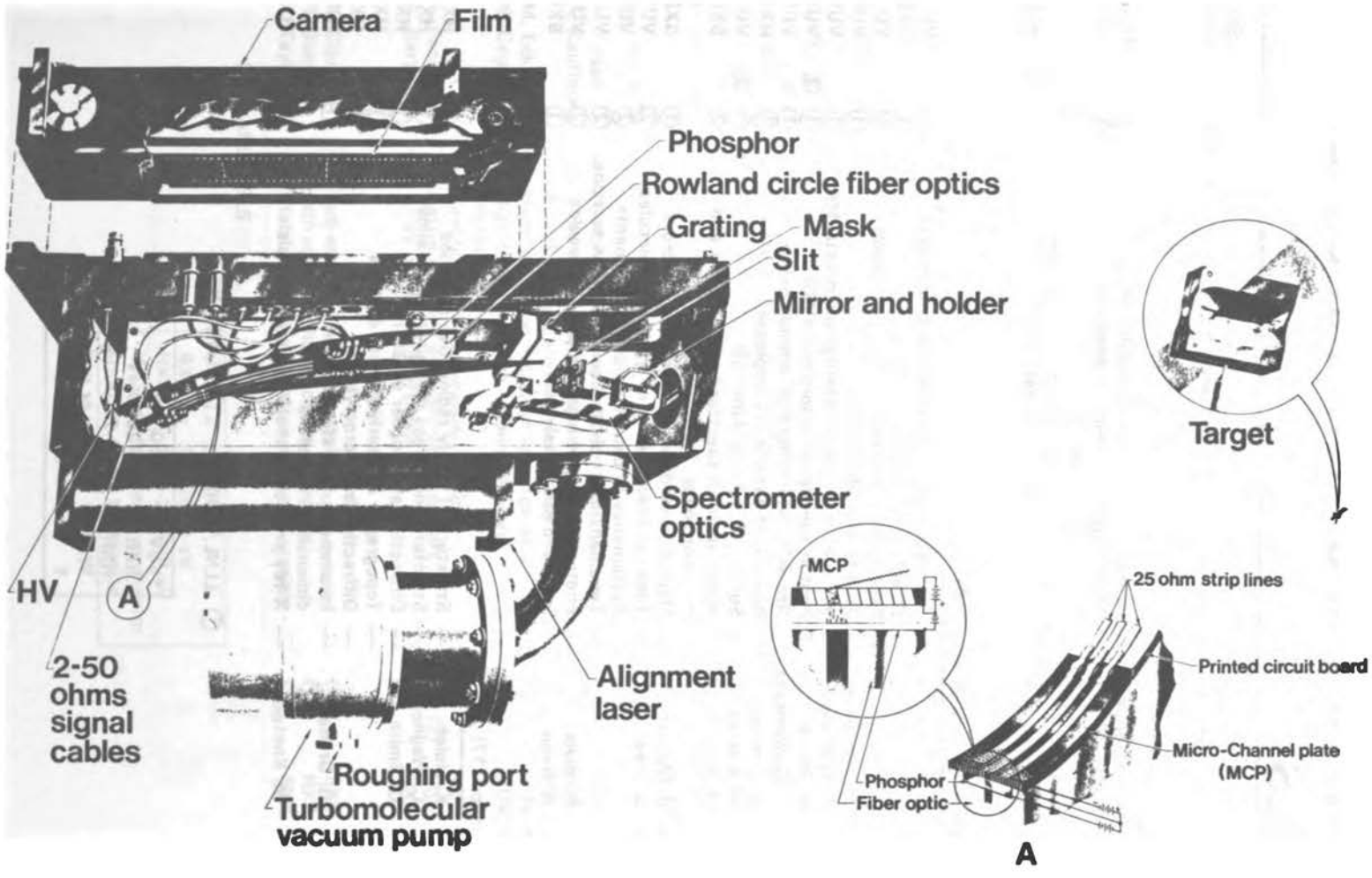


Figure 20

Research proposed by LLNL, LANL, SNL, and University of California at SSRL and NSLS

Laboratory	Investigator	Research	PRT	Source* required
• Bioscience (4)				
UCSF	R. Fletterick	Structures of glycogen phosphorylase	①	HXR-W/U
	R. Stroud	Crystallographic structure analysis of large protein molecules	①	HXR-W/U
		Organization of proteins in the eye's lens	① ②	HXR-W/U
UCLA	D. Eisenberg	Structure of single crystal large enzymes	① ②	HXR-W/U
• Chemical Science/Surface Science (16)				
UCSB	W. Walker	Photodissociation of noble gas compounds	①	VUV
		Structure of organic metals	①	HXR
		Relaxation of excitons in noble-gas solids	①	VUV
UCI	J. Hemminger	Studies of azulene monolayers	①	VUV
UCLA	R. Williams	Surface structure of heterogeneous catalists	①	VUV/SXR
SNL	R. Stulen	Photon stimulated desorption (PSD)	① ②	VUV/SXR
LLNL	C. Colmenares	Gas-solid interactions of actinide oxides	①	VUV/SXR
LANL	G. Cristoph	Bonding of dirhodium complexes	①	HXR-W/U
SNL	M. Knotek	Surface structures with PSD	① ②	VUV/SXR
SNL	M. Knotek	Auger electron spectroscopy in metals and covalent solids	②	SXR
LLNL	J. Mallett	Fluorescence decay in organic scintillators	①	SXR/HXR, t
LANL	J. Tiee	Time resolved studies of transient molecules	②	VUV
		Systematics of photodissociated fragments	②	VUV, t
		Time dependent photoabsorption cross sections	②	VUV, t
LANL	N. Blais	Photochemistry of high explosive molecules	②	VUV
LLNL	R. Ryon	Improved microanalysis	①	SXR/HXR
• Materials Science (17)				
LLNL	K. Hulet	Structure of highly radioactive actinides	①	HXR-W/U
UCLA	C. Wagner	Structure and stress measurement in alloys	①	HXR
LLNL	G. Smith	Diffraction at megabar pressure	①	HXR
		Topography of nearly perfect crystals	①	HXR
		Diffraction by microcrystals	①	HXR-W/U
UCLA	G. Gruner	Incommensurate structures in low dimensional materials	①	HXR
SNL	M. Knotek	X-ray profiles of shock loaded materials	②	HXR, t

① LLNL/SSRL ② LANL/NSLS

*VUV = 5-200 eV
SXR = 200-2000 eV
HXR = 2000-20,000 eV
W/U = wiggler or undulator
t = short time pulse

Figure 21

(Continued)

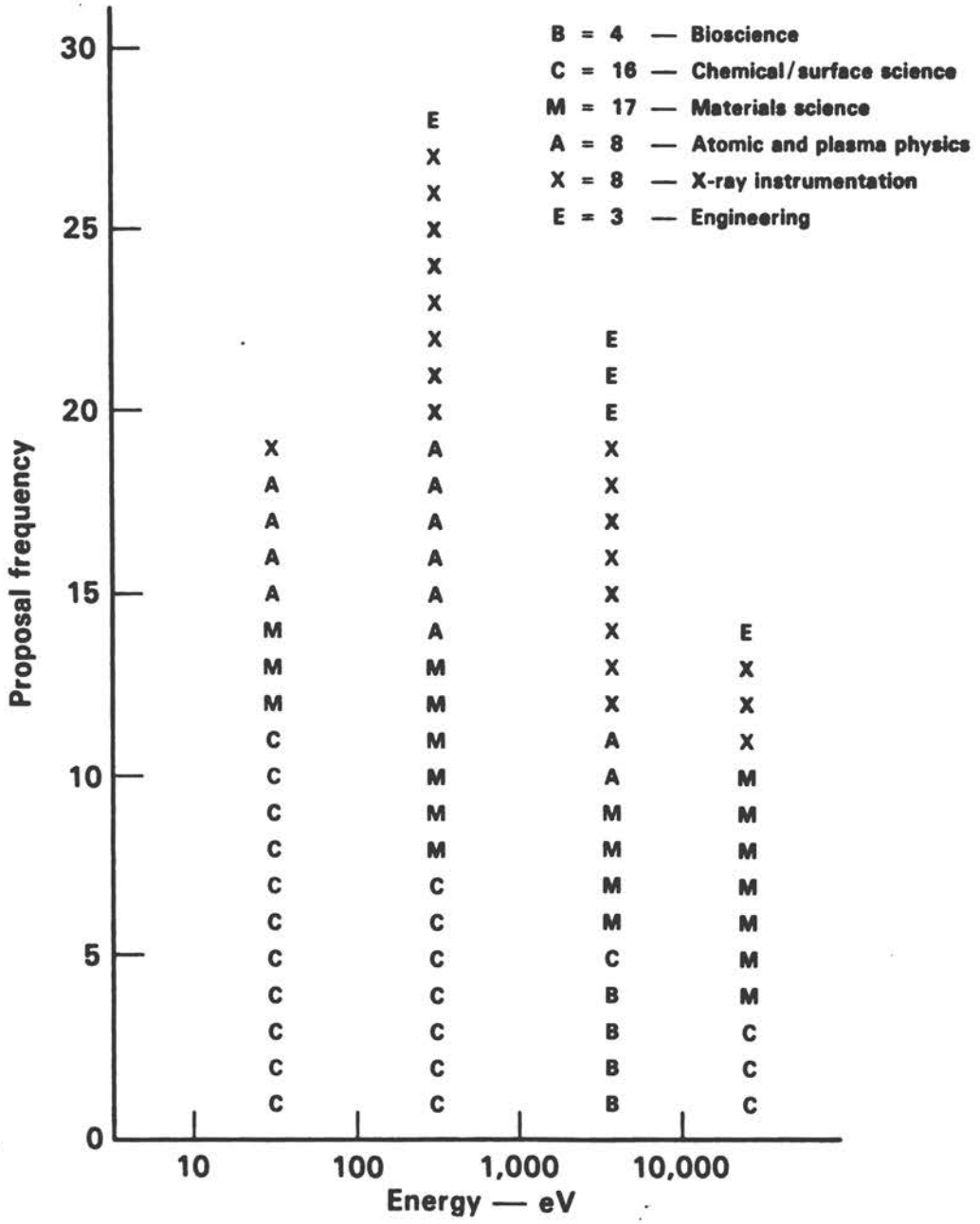
Laboratory	Investigator	Research	PRT	Source* required
• Materials Science (continued)				
UCI	J. Lawrence	Photoemission of anomalous rare-earth compounds	①	VUV-SXR
LLNL	M. Lowrey	Carrier recombination in amorphous semiconductors	①	VUV-SXR, t
LANL	A. Williams	Anomalous dispersion studies of metallic glasses	②	HXR
		EXAFS studies of transition metals	②	SXR
		Small angle scattering studies of amorphous metals	②	HXR
LANL	W. Ellis	Valance band structure of UO_2(111) and UO_2(100)	②	SXR
		Photoemission resonance effects in actinides	②	VUV
		High energy photoelectron diffraction	②	SXR/HXR
LANL	D. Cromer	Structure and electronic studies of actinides	②	HXR
LANL	D. Eller	EXAFS experiments on actinide systems	②	SXR
• Atomic and Plasma Physics (8)				
LLNL	J. Mallett	Coherent and incoherent scattering in low Z elements	① ②	SXR
LLNL	C. Wang	Fluorescence efficiency of low Z elements	① ②	SXR
LLNL	N. Delgrande	Low energy photoabsorption measurements	①	SXR
LLNL	A. Toor	Generation of coherent radiation	①	SXR-W/U, t
LANL	C. Jones	Preionization studies of laser systems	②	VUV
		Cross sections of excimer laser species	②	VUV, t
LANL	D. Kania	Non-linear VUV/x-ray optics	②	VUV/SXR/HXR, t
		Plasma transmission spectroscopy	②	VUV/SXR, W/U, t
• X-ray Instrumentation (8)				
LLNL	K. Tirsell	Photoemission of metals and alkali halides	①	VUV/SXR/HXR, t
LLNL	R. Kauffman	X-ray instrument characterizations	①	VUV/SXR
		Streak camera absolute calibration	①	VUV/SXR/HXR, t
LLNL	M. Eckart	High resolution, ultrafast spectrometry	①	VUV, SXR, t
LLNL	N. Ceglio	High efficiency, high resolution x-ray microscope	①	VUV, SXR
		Calibration of transmission gratings	①	VUV, SXR
LANL	E. Fenimore	Astronomy and astrophysics detectors	① ②	SXR/HXR
LANL	R. Bartlett	X-ray detector calibrations	②	SXR/HXR, t
• Engineering (3)				
LLNL	D. Ciarlo	Sub-micron x-ray lithography	①	SXR
UCLA	R. Bunshah	Diffraction by hard coating materials	①	HXR
UCLA	R. Taylor	Stability of fusion reactor surface materials	①	SXR

① LLNL/SSRL ② LANL/NSLS

*VUV = 5-200 eV
SXR = 200-2000 eV
HXR = 2000-20,000 eV
W/U = wiggler or undulator
t = short time pulse

Figure 22

Spectrum requirements of LANL, LLNL, SNL and UC



Some proposals fall in more than one energy range
56 separate topics

Figure 23

Current synchrotron radiation projects

- **Beam line development project at NSLS***
  - — **Los Alamos: Line on VUV ring (two stations), port on x-ray ring (one station) $3.6 M**

- **Beam line development project at SSRL***
  - — **LLNL/UC: Wiggler line (two stations), bending magnet line (one station) $6.4 M**

***The NSLS and SSRL projects are a collaboration of Lawrence Livermore/Los Alamos/Sandia/University of California**

603

Figure 24

LOS ALAMOS BEAM LINE DEVELOPMENT AT THE NSLS

	TYPE OF LINE	LOCATION	ENERGY RANGE	COMPLETION DATE
1.	SOFT-X-RAY SPECTROSCOPY	VUV RING PORT U3	12 TO 1200 eV	10/84
2.	X-RAY SPECTROSCOPY	X-RAY RING PORT X7	2 TO 22 keV	7/85
3.	RADIOMETRY	VUV RING PORT U3	100 TO 2000 eV	4/86

604

SOURCE: Los Alamos

Figure 25

Livermore beam lines at SSRL

Type of Line	Location	Energy Range	Completion Date
1) Vacuum ultraviolet	B.L. VIII-B	5-180 eV	10/85
2) Soft x-ray	B.L. VIII-W	100-2000 eV	3/86
3) Hard x-ray	B.L. VIII-W	1500-20000 eV	1/86

Figure 26

Planned beam line layout at SSRL

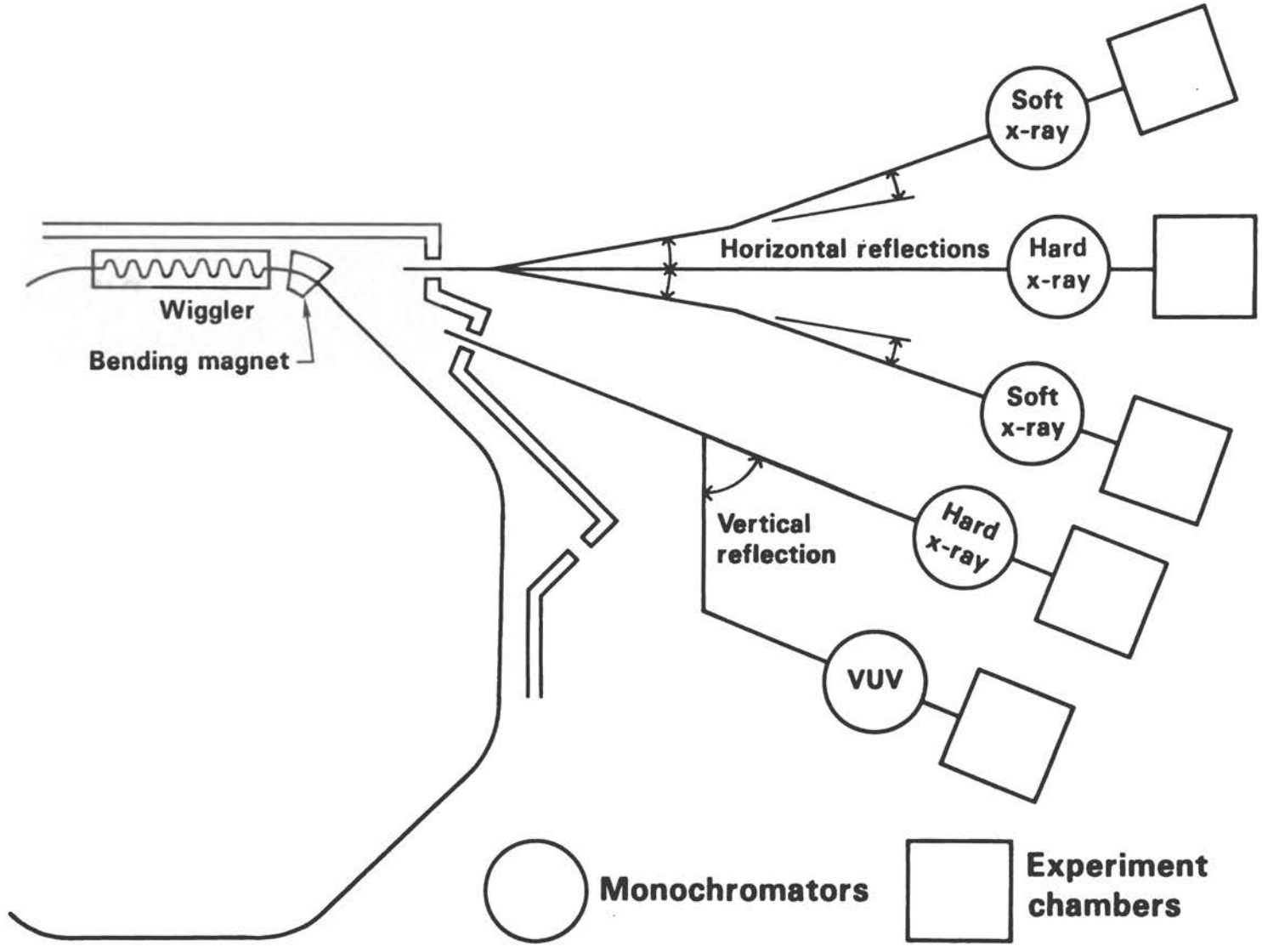
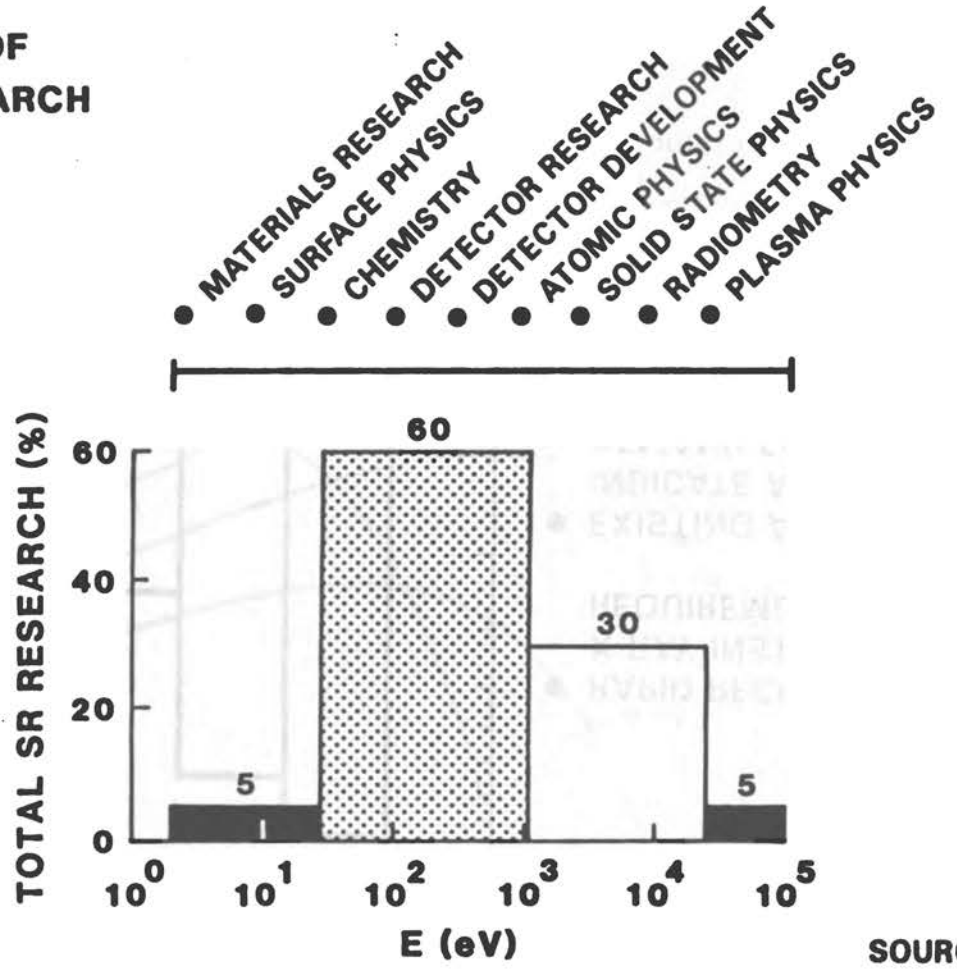


Figure 27

FUTURE REQUIREMENTS FOR SYNCHROTRON RADIATION

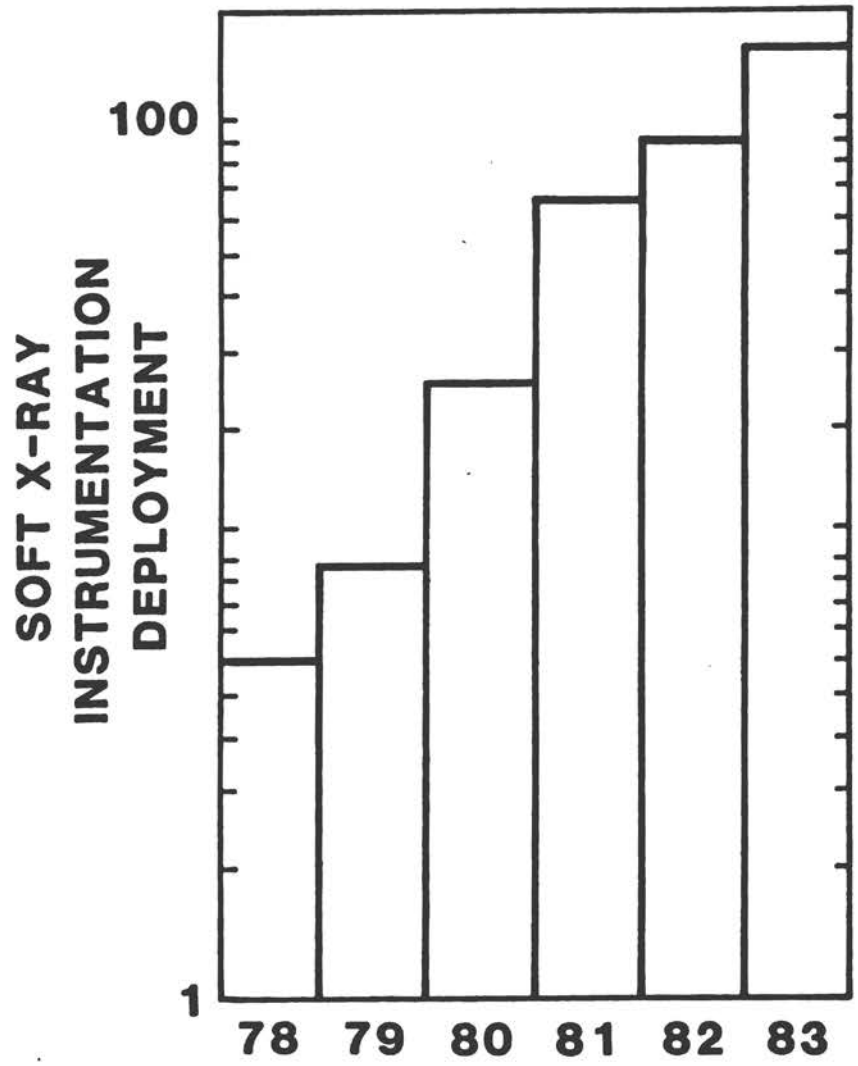
WIDE RANGE OF PROPOSED RESEARCH



SOURCE: Sandia

Figure 28

FUTURE REQUIREMENTS FOR SYNCHROTRON RADIATION



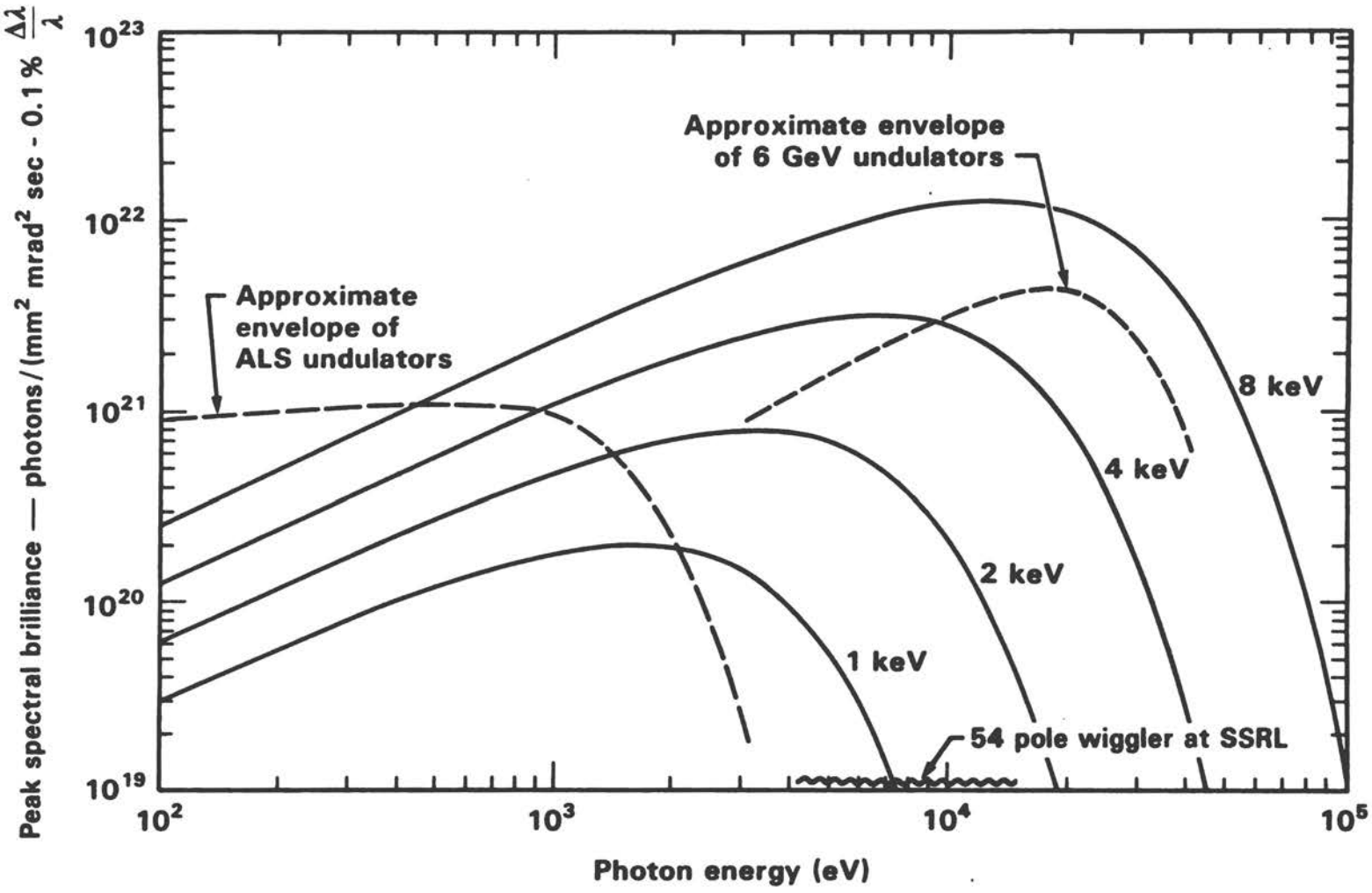
- RAPID RECENT GROWTH IN X-RAY INSTRUMENTATION REQUIREMENTS
- EXISTING AND NEW PROGRAMS INDICATE AN INCREASING DEMAND FOR ADVANCED X-RAY CAPABILITIES

608

SOURCE: Los Alamos

Figure 29

Spectral brilliance of black bodies and undulators



609

Figure 30

Future requirements for synchrotron radiation

Technical Specifications

- Most desirable energy is $\sim$1 keV
- Monochromatic flux at 1 keV $> 10^{18}$ PH/s·cm^2·0.1% BW
- Average brilliance $> 10^{18}$ PH/s·mm^2·mr^2·0.1% BW
- Pulse length $<$50 ps

610

Figure 31

Summary

- Weapons labs have a large and growing need for synchrotron radiation

- Weapons labs believe that these needs are best met by participating in state-of-the-art synchrotron facilities with the national scientific community

- The type of source that satisfies the majority of the weapons lab's needs has low energy (1 keV), high intensity, high brightness, short pulse length

611

Figure 32

Overview of the Recent ERAB Report on
Materials Research and Development

Testimony of Robert Pry to the
Major Materials Facilities Committee,
National Research Council, N.A.S.

DR. PRY: Thanks. I have no passouts, slides or overheads. What I would suggest is that if anybody wants to go over what I say in more detail when I have said it, go down the street to the complement of the Smithsonian Museum, to the Forrestal Building, and they have 5000 copies of this report of the ERAB Panel on Materials Research and Development.[1]

As you know, ERAB is an advisory board of DOE which theoretically reports to the Secretary but has major interaction with Al Trivelpiece. We undertake a number of studies from time to time. We are not a policy-making but simply a recommending body of people who do not serve for a living, but do it because I guess we are, I do not know, masochists or something.

In any event, we were asked by the then-Deputy Secretary, back in the fall of '82, if we would undertake a study of materials research and development. We were asked to answer several questions at that time. I think it is probably worth going through them very quickly.

What DOE was interested in was: first, Are DOE's materials needs translated into R&D materials programs, and are the results used? That is a short wording of what they asked, but fundamentally correct. Second, Are new materials opportunities being overlooked? Everybody always asks that -- looking for goodies. Third, Is coordination between government national laboratories and university and industry effective with respect to resource allocation and the usefulness of the results? There is a mouthful. Fourth and finally, what is the significance of the role of DOE materials science relative to the nation's overall effort with respect to development and support of major facilities, and how can the nation's benefit from DOE materials science programs be improved?

About a dozen people worked on these issues as a Panel, and I was chairman of that group. The other members were people like Arden Bement, former professor of nuclear materials at the MIT who went to DARPA. Many of you know him; he is now Vice President of Technical Resources at TRW. Others were Marty Blume from Brookhaven; Al Clogston, late of Bell Labs now living out around Sandia; Charlie Cook, Vice President of Phillips Petroleum; Professor Dresselhaus, who is, I think, a member of this group. Also, Jim Economy from IBM; John Galt from Sandia; Bill Manley from Cabot; Al Schriesheim, a member of this Panel; Professor Charlie Slichter of the University of Illinois; and Dale Stein, President of Michigan Tech.

---

[1] Materials Research and Development; A Report of The Energy Research Advisory Board to The Department of Energy, November 1983 (DOE/S-0027).

We started by asking ourselves how to attack these questions, which are fairly profound questions to try to address. We came to the conclusion that within the time frame we had and the effort we could spend -- we had about 10 days worth of meetings and about eight days worth of site visits, spanning from January to about October -- we would have to limit the scope of our study.

During that time, it was not possible to study the laundry list of all the programs and attempt to judge if anything was overlooked. Moreover, such a study briefly addressed gets to be a question of one person's opinion over others as to what should be emphasized and what should not. Consequently, we chose to examine instead the process by which those program decisions were made and the process by which the results of the programs were utilized, if any, and the process by which one developed priorities of the kinds of programs to emphasize from the needs that were recognized. We then took a look at the issue of the efficient utilization of results.

Finally, we transformed the original four questions into five others. Let me say what those are and then I will give you the report briefly on what the findings and recommendations were.

The first is: What is the role of DOE in basic materials research, and what should the balance be between the roles and the performers. If you look at DOE Basic Energy Science Materials Programs, the level of spending is of the order of $127 million a year. Total materials R&D in DOE is somewhere in the neighborhood of $380 million a year.

Of that $127 million, if we look at it in some detail, most of it comes in over the transom; that is, unsolicited. You will have to excuse my crude manner of speaking. By and large, the unsolicited proposals are judged on excellence. Another set, which is more like negotiated programs, is funded at the national laboratories. That is a reasonably large amount of basic materials science work. The $380 million total materials R&D of DOE is about a third of what the government does in funding materials science that is recognized as such.

I make that qualification because the numbers are all flaky, and they are flaky by more than the 10 or 20 percent that one usually thinks of as flakiness. In DOD, for example, a large bulk of the materials research is not ever reported as materials research; it is called engine development or rocketry or air-frame developing, and it is buried in those systems programs and never brought out so you can see it. As a consequence, there is no good way of determining the total materials effort, just as it is almost impossible to determine what the materials science applied effort is in industry, for exactly the same reasons.

In any event, of those materials programs that are counted, DOE accounts for about a third of the total. We came to the conclusion that DOE has three fundamental roles in Basic Materials Research. One is to provide basic knowledge for the long-term energy needs of the country. A second is to support university research to educate graduate students for future research in this field. The third role is to operate unique large materials research facilities used by the research community, that is, government, universities and industry for materials science.

The panel had some concerns about the extent to which BES had any real feeling for the balance in emphasis in program awards between these three roles, and we felt that a great deal could be gained by looking explicitly in the funding patterns as to what was being spent where for what purpose. We recommended that that, in fact, be done for existing contracts. But over and above that, specifically, BES should provide explicit funds for research surrounding large materials facilities. There is never a problem in putting a line item in the budget in the national laboratories for plumbers, electricians, and latrine cleaners, floor-sweepers and whatnot, that are needed to maintain large facilities in an operating physical condition.

However, there are no funds explicitly assigned to keeping large materials research facilities in a proper scientific condition with respect to instrumentation development, to improving and expanding upon the utility of those machines, so that when people come in to use them they can get expert advice. We recommended that such funds be put specifically into the budget for the operation of such facilities for people who fundamentally do research on the facilities and do research around the facilities in some core way to provide that basis of expert advice, counsel, and recommendations for upgrading. I see this need as no different from the plumbers and electricians that are hired to make the facility work efficiently.

A second is to provide some base funding for the laboratories with explicit applied missions. I think you heard a couple of cases here where devious means must be found like taking money from an overhead account, which all of us do in industrial or government laboratories to provide seed money for new starts, but it would be much more effective if the labs could explicitly have a fund of 2 percent up to, say, 10 percent, for those kinds of research surrounding the applied mission to make that connection between the applied effort and the basic research more clear.

Then, lastly, it was our feeling that all other basic materials research should undergo peer review and be judged on the basis of those three roles; that is to say, how they provide basic knowledge for long-term energy needs, how they support university graduate students, and the operation of unique large facilities, already covered in the above recommendation.

The Panel believed there should be no pre-decision as to what should be done at national laboratories versus universities in that regard. It should be judged on excellence in those two categories.

The second question that we asked ourselves was how much should we spend on major materials facilities -- that is a subject near and dear to the heart of this group. That, as you well know, is a tough issue. It is difficult enough to determine among the kinds of new facilities that are coming along, what is the priority time order that one ought have for installation for the benefit of materials science; it is quite another matter to say how much should we spend overall on materials-facilities compared to materials research.

I did a quick little calculation on the way down here, as a matter of fact, just to try to bring home the importance of that question. In 1974, about 10 percent of the BES materials budget was for the operation -- I am not talking about construction -- <u>operation</u> of large facilities; BES materials budget, 10 percent.

In 1984, it was 20 percent of the BES materials budget, for the operation of large facilities. If NCAM and the rest of the initiatives of the decade go through, the projection by 1990 is 30 percent of the BES materials budget will be spent on the operation of large materials facilities.

Let me put that in another perspective. If I take a look at the last four years, using an 8 percent deflator, facilities operations expense has gone up by 76 percent. Materials, less facilities operation expense, over that whole four-year period -- not per year but the whole four-year period -- has gone up 4 percent; in other words, stayed constant.

In other words, the materials research that BES has done that is not operation of large facilities has stayed constant over the last four years. If you include facilities, it looks like the expenditure, or effort, has gone up by 10 percent. The applied materials R&D over that same time has gone down about 20 percent.

In this perspective, the question of how much one spends on the operation of large facilities is not a whimsical question; it is a very serious question and it has to be viewed in the light of all of the other kinds of materials research and development that needs to be accomplished in the country.

Now that is completely separate from Herman's appeal that we ought to join a "union," like the high energy physicists, and get at the trough like everybody else. I think that we perhaps need to do a little of that as a materials community. We have too many different directions in which we are going for our own benefit, but I am not sure materials facilities is the single issue on which one ought to put a spear in the ground.

In any event, quite frankly, the Panel had no panacea for solving the facilities issue, and I am very happy to see this group getting together to at least take a stab at it. Again, when one goes into a capitalization question, we took a look at several facilities, it turns out that the operating expense after three or four years, in things like a high-voltage microscope, is roughly equivalent per year to the original cost. About $10 million could build such a machine and, after a few years, it takes $10 million per year to operate, so one does have an operating budget problem with some of these very large facilities, and I am talking about the very large ones.

DR. ENGELEMAN: Are you talking about constant dollars?

DR. PRY: No, I am not talking about constant dollars, in that sense, so you can discount it by, say, 30 percent. It is still very material, and particularly material if you throw in the extra, which I would like to see thrown in, which is the scientific maintenance of the facility along with the physical maintenance.

DR. FISHER: You are including instrumentation update in that figure or not?

DR. PRY: I am not including any capital -- only operating expense in the normal government accounting practice.

Somehow or other we have got to get around to doing our facilities additions planning by reviewing it against all the other uses of the funds involved, particularly in the operating areas. I am not sure that is really done. I must admit that we seem to have entered, I would not say a new era because the legislature has always had a hand in capital funds of this magnitude, but close to a new era. If I look back at some of the facilities that were put in place in the sixties and seventies, it was not unusual for something of the order of three or four years to pass, with a lot of peer review and an awful lot of grinding around in the scientific and technical community before a decision was really made to take the facility to the Hill.

In other words, the technical aspects of the problem were first solved before the political aspects were broached. Somehow, the roles have gotten reversed, in my view -- that is a personal opinion. Many of these facilities are coming to the Administration by way of the legislature. At least recently there have been a couple cases of that sort where either the technical merits were argued first in the Congress or, in one case, the concept itself.

Herman makes a plea that outmoded facilities are always promptly shut down, and I guess I take that with a grain of salt, Herman -- sorry about that. I know they do at Oak Ridge.

(Laughter)

But I do believe that in DOE we should somehow have new facilities proposals reviewed by the materials science community, not just the people who understand that particular method of measurement, but the people who will be using that method and other methods for measurements and analysis and applying it to materials needs in order to get some concept, really, of facilities priorities.

The Panel then went on to take a look at a couple of other things. One of these is something that has been a whipping boy for several years: "are the responsibilities assigned to the non-defense labs adequate to allow effective development of relevant materials programs?"

This gets into the question, of the assignment of responsibility and authority, which has been a real problem in DOE laboratories ever since the onset of ERDA around 1974 and 1975. As long as the AEC had relatively a single mission, the development of nuclear energy, it was not a tremendous problem, and the recognition of the national laboratories, in fact, had the responsibility for that development and the recognized if not statutory authority to go along with it.

As soon as we got away from that concept and pulled some of that authority and responsibility back to Washington, we found, in particular with respect to materials science, that, first, the laboratories then had some responsibility but no authority any more. Then one had to create a matrix of both management and reporting relationships which, as everybody knows, makes the reporting assignments go up roughly by the square of the number of people involved and, indeed, it did.

Second, which I think is far more important to the materials science community, is that, except at the bench level, there occurred a separation between the people who were attempting to do the systems design and development and the people who were doing the basic materials science.

Applied materials, the co-called applied materials science, is now under the systems group and that is not really applied science; it is really materials engineering support. That always occurs when applied materials gets placed under a systems design group. They do the materials engineering work to fit the specifications they had already decided on with respect to off-the-shelf materials. They do not look forward to what materials might do to change the specification -- if you can do something like develop nickel aluminum alloys, for example.

We therefore felt that there was a real gap. But the problem of management and program development in materials science is that it is a second-order effect, if you like, in terms of developing applications to real systems. The program is not created in a vacuum. If the systems development responsibility is diffuse, the materials responsibility for filling those systems needs is diffuse squared.

It makes it very, very difficult to put together a coherent program for coal gassification or fluid-bed combustion or for almost anything you can think of, particularly for the breeder technology. Nobody wants to admit that they really have responsibility for the breeder. It is very tough to get really meaningful programs going in those areas.

This subject of diffuse responsibility and authority and the micromanagement that results is something that we in ERAB have complained about on many occasions; it was also complained about in the Packard Report; it was complained about in a number of other communications to the Administration.

Are there gaps in the materials programs? I alluded to the specific gap that I think honestly exists in the materials programs of DOE, and that is what I call a need for generic materials development, that part of applied materials development that, in fact, looks ahead.

Again, I have to go back to Herman's Oak Ridge nickel aluminide development and say that is really only the start of the development program. I would guess that you will not see that material used in anything commercially useful for roughly 10 years, because of all the other than strength boundary conditions that have to be met and all the performance evaluation required in order to make it a useful material product.

The intervening period, for about the next five years, is what I would call generic-materials development program, looking into what happens in high-temperatures, what happens with corrosion resistance under varying conditions at high temperature, what happens if you cycle the temperature, what enhancements are available by alloying heat treatment, etc., all those things you have to do in order to see whether that material is useful, and to tailor around the difficulties that you inevitably find.

That is not completely missing but largely missing in the DOE materials program. And we think that is a significant step and the reason why, out of the $380 million a year, one finds only a few odds and bodds, heres and theres, that, in point of fact, one can point to as being actual applications. Now that is a little unfair, and it is unfair because the national labs really only expanded their charter in the last 10 years, and I just said it takes 10 years to do anything, so they only now should be getting measured. Certainly if measured against nuclear energy goals, they have done not a perfect but a commendable job.

But I do think a great deal more can be done if one had that linkage between the basic sciences and industry in application of materials.

Lastly, how can the results of the materials R&D program be more effectively incorporated into energy development? I am very happy to report, although we made some recommendations there which I am not going to go through now because it is a little tangential, I think, to this Committee's charge, but a lot of the kinds of recommendations that were made are, in fact, being undertaken and, I must say, with very encouraging results.

The patent policy has been completely changed, it is possible to do proprietary work in the national laboratories, so we get people other than the Japanese and Germans who do not care what they sign to come in and work, and we have a possibility of the laboratory people themselves starting centers to work with industry on specific kinds of problems. That is already being started. A lot of interaction that did not occur as little as two years ago is now occurring in much larger abundance in at least all the laboratories I looked at.

Many of the remarks that I have made really refer to what I term the "defenseless" laboratories as opposed to those laboratories like Sandia and Los Alamos, where they have a good targeted mission; they have the responsibility and authority; they have, in the case of Los Alamos, an IRAD program or an amount of research that they can themselves decide to put into basic sciences.

But in the other national laboratories such as Argonne, Brookhaven, Oak Ridge, Ames, and so on, this does not occur. Going back just one more time on the facilities issue, I think there are two things that one has to keep in mind. One is the growing amount of facilities required in universities doing materials research. The second is that capital expenditures for large facilities is only the tip of an iceberg, named downstream operating costs. This part of large facilities is now getting so large that it must be considered, upfront, as encroaching on R&D program expense. Therefore, I think a better job must be done than we have done in the recent past in getting inputs across the materials science community as to the actual need for new large facilities and instrumentation. Thank you.

DR. SEITZ: Comments or questions?

DR. FISHER: Can I pick you up on one of the recommendations, just to be a little more specific. You have stated that each assistant secretary should provide a needs-oriented technology development program. The sort of question I have in mind is the following:

Let's take the question of materials substitution for strategic materials. Would you have in mind here that contracts should go out to find ways of substituting, let's say, turbine blades, with new materials, and this would go out? In other words, I am just asking for a few more specifics of how you --

DR. PRY: We ran into a buzz saw on that one and that is why this is worded in a somewhat vague way. We played around with various and sundry ways that one might organize the generic materials effort so that it would not come totally out of the hide of the basic-energy sciences.

If you give the budget and responsibility to Al Trivelpiece, you know that it is going to be a line item in his budget and his budget will not grow much but it will come out of the rest of the BES stuff. We did not want to do that. We thought a lot of the effort should be borne by the system programs.

At the same time, we could not put it under the system's project management, because it would likely turn into materials engineering. So we did the only thing we could do, which was to look around to other kinds of organizations and, in particular, to industries, how that problem is solved in, for example, the manufacture and development of jet engines.

What I think you find both at Pratt or G.E. is a materials engineering group under the engine management, but they have a separate materials laboratory that is looking for such things as substitutes, upgrades, changes in materials, irrespective of this next engine development.

They have really two functions. One is to do research generically, knowing what the requirements are, and to work at new materials outside of the jurisdiction of the systems management and, secondly, of course, they provide the expertise to provide a materials specification sign off on anything that is put in an engine, so that they feel responsibility to make developments work.

That separation of function industry has found generally is required in management if you do not want, on the one hand, generic materials work to become materials engineering and specification refinement on the one hand or have it slip over to a branch of solid-state physics, on the other.

We really felt a new entity had to be formed, but we wanted it close enough to the system so that they understood it; however, we did not want it under the system's program office.

DR. FISHER: So you think it is a feasible problem to have an interface group that can --

DR. PRY: I do. Every time I bring this up, people say, "Oh, we tried that but it doesn't work." But it does work in some organizations and it certainly worked way back in the AEC.

DR. POSTMA: I could answer that partially. The last time -- I guess the materials science is part of DOE -- put together such a needs analysis, what they wanted in the technology, was 1977, across the board, and those reports exist. I did not get them, of course. That was at the height, say, of the growth of the Department of Energy.

Since the recession and the oil glut and the present Administration policy, a lot of those kinds of things changed, because the technologies that were being pushed and the needs that were being expressed in the late seventies are, of course, changed now.

DR. PRY: No, the notion of the needs has changed.

(Laughter)

DR. POSTMA: With those conditions. I agree with you, the needs are still there, except they are not being supported now. Perhaps to re-do that in the light of current constraints on the system, which are quite different from what they were six years ago, along the line Bob is talking about, is a realistic expectation.

But we do not need another whole set of reviews. I mean, if what is called for is yet another set of reviews --

DR. SEITZ: What we might do, since lunch is ready, is have people go out and grab a sandwich and come back, and we will continue the discussion.

(A brief recess was taken.)

High Magnetic Field Research in the U.S. - Status of the National Facility and Future Opportunities

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Francis Bitter National Magnet Laboratory, MIT

1. Background Concerning Francis Bitter National Magnet Laboratory

A. Facilities

The Francis Bitter National Magnet Laboratory (NML) is the primary high field research facility in the U.S. It serves users throughout the country and from abroad. Core support is provided by a NSF contract which, in BY84, was $5.3M. These funds are used to (1) operate and maintain the high field facility (2) advance the state of the art of magnet technology and develop new high field magnets in response to needs of the research programs, and (3) support a program of basic and applied research using high magnetic fields. The Laboratory is organized into divisions according to these tasks. Operations and Administration account for the lion's share (60%) of the core contract; Magnet Technology and Research each receive 20%. The largest in-house research program is that concerned with the properties of high field superconductors (about 45% of core research support). Other research projects, in semiconductors, magnetism, solid state chemistry, liquid crystals, and NMR, have modest funding via the core contract. Besides the core contract, NML also has a

number of other grants and contracts. Total support for the Laboratory is ~$10M/year.

NML's key facilities are four large dc generators (producing 10 MW total) and 25 high field magnets. At least two generators are needed to reach peak field in these magnets; thus, the Laboratory is limited in the number of experiments it can perform by its power plant. This resource is used optimally by providing many magnet stations, setting experiments up in parallel, and transferring power from one to the other as needed. The system works well because the staff is efficient and dedicated. Replacement cost of the facility is estimated to be $20M, including the building.

Until recently, all NML magnets were Bitter solenoids - a reliable design that has served users well. The peak field achieved in 3 cm. bore in a Bitter solenoid is 23 tesla (230 kG). About five years ago the Laboratory deployed a new class of high field magnet, the hybrid, which boosts the field of a Bitter solenoid by surrounding it with a large superconducting solenoid. Hybrids are complicated, and exceedingly expensive to build (about $1M as compared to $25K for a standard Bitter solenoid) and operate. At present, however, they provide the only avenue to higher dc fields. NML currently holds the dc world record of 30.4T. This mark will eventually be surpassed by hybrids to be built in Grenoble, Japan, and at NML. The next NML hybrid will probably use a novel Nb_3Sn conductor (as opposed to NbTi in the present one) and generate 33T in a 3 cm bore. Some funds for NML hybrid II are budgeted in the current NSF contract.

Regular user scheduling of the NML hybrid began about 2½ years ago.

Several outstanding experiments have since been performed in it. Among them are:

1.) Low temperature studies of the anomalous quantized Hall effect at GaAs/(Ga,Al)As interfaces by Stormer and Tsui. These experiments were an outgrowth of earlier work, also performed at NML, for which Stormer, Tsui, and Gossard were awarded the Buckley Prize.

2.) Discovery of a field-induced, charge-density-wave transition in graphite at 25 T (Iye, Timp, Dresselhaus). The transition causes an abrupt anomaly in the basal plane magnetoresistance.

3.) Studies of H_{c2} vs. T in $EuMo_6S_8$. The experiments required the hybrid and pressures to 18 kbar. The phase diagram, strongly distorted by exchange interactions with Eu^{2+} moments, is in excellent agreement with theory. Work done by M. Decroux (Geneva), M.B. Maple (UCSD), and R.P. Guertin (Tufts).

The hybrid has not been trouble free. There have been several stack failures (each costing $20K); the cryogenic system is finicky and expensive. Overall, the magnet system has been less than 50% reliable. Reliability will improve with experience and modified stack designs.

Despite its problems, the hybrid has paid for itself in terms of scientific achievement. At the Detroit APS meeting, for example, there were four invited papers - all concerned with 2D electron dynamics - based in part on experiments performed in the hybrid. Furthermore, recent work at the Laboratory suggests that there is much more physics of 2D electron systems to be explored in the 20-50T field range. 2D

electron dynamics is now an especially active topic at NML; about ten user groups are studying them in such varied systems as GaAs/(Ga,Al)As; InAs/GaSb; Si MOSFETS; HgTe/CdTe; $TaSe_2$; graphite; and ultra-thin metal layers.

B. Operations

A skilled and dedicated support staff is required to operate a facility in a "user friendly" mode. Much of the NML's success results from the quality of its Operations Division; its work is praised by users and visiting committees alike. One report states that: "It is hard to imagine that one could find a better person to manage a user facility [than L. Rubin, Head Ops. Div.], or that the operation could be carried out more efficiently"; such comments are typical. Services provided to users by the Operations Division include:

i) Maintenance and operation of the magnets.

ii) Scheduling of magnet runs, with special emphasis on providing easy access for first time users.

iii) Assistance in performing experiments.

iv) Development and maintenance of specialized, dedicated instrumentation such as on-line data processing, variable temperature sample holders, magnetometers, ^3He refrigerators, high field de Haas - van Alphen apparatus, etc. The sophistication of the dedicated instrumentation is gradually increasing; in particular, the Laboratory recently began offering low temperature/high field (50 mK at 19 T) facilities to users. The development of such auxiliary facilities is an important part of the Laboratory's obligation to its users.

NML operations are costly in terms of materials, power, and staff. Operations and administration now account for 60% of the core budget, as compared to 35% five years ago. That trend cannot continue; otherwise the Magnet Technology and Research Divisions will be squeezed out of existence. Unfortunately, there seems little chance of reducing operating costs, whose main components are electrical power, magnet and plant parts, and salaries. The situation is exacerbated by the fact that the hybrid magnet is exceedingly expensive to operate.

II. Higher Fields - Technical Limitations and Research Opportunities

Barring a major breakthrough in superconducting materials, the ultimate limit for dc hybrid magnets appears to be 35-40T. Higher fields can only be achieved with pulsed systems. Rugged coils driven by large condenser banks may generate fields approaching 100 T in 5mm bore. Higher fields require implosive techniques that often destroy the sample, dewar, etc.

Much of the pulsed magnet technology was developed by Foner of NML over a decade ago. However, the Laboratory has only recently begun offering pulsed field facilities (45T) to users; in this area it is well behind the Japanese. The high field facility at the Univ. of Tokyo has provided 45T fields for several years (in a system like Foner's), and recently has developed a 250T, electrical implosion system. A fast high voltage condenser bank is required for the latter. In addition, Osaka Univ. is gradually developing an 80-90T, non-destructive, pulsed field facility. The system now operates at 60T.

The Tokyo and NML 45T pulsed field systems use simple, inexpensive, copper-wound coils, and can be driven by modest, low voltage condenser banks. Copper is a favorable material because of its high conductivity; however, its low yield stress sets an upper limit of 45T on the field attainable in a coil of reasonable bore (2 cm.). Copper-coil, pulsed-field systems are inexpensive (NML's could be duplicated for $200K). However, dedicated instrumentation drives up the cost of such a facility. The Tokyo laboratory already has extensive instrumentation; NML will eventually spend $200-400K for such purposes.

To attain fields exceeding 45T in a non-destructive mode, the Osaka group has developed high strength steel coils. Such a system can potentially achieve 80-100T (there is some disagreement regarding the ultimate limit). However, the gain in coil strength is achieved at the cost of a much more complicated and expensive electrical system. The high resistivity of steel necessitates a large, fast, high voltage condenser bank; the Osaka bank stores 1.25 MJ at 26.6 kV, and would cost $750-1,250K in the U.S. Typical pulse lengths are 10-100μsec, as compared to 10 msec. in copper-coil systems.

In assessing the scientific opportunities in the 40-100T range, it is interesting to consider the Japanese experience. The two Japanese pulsed field laboratories have completed about 25 projects in various areas of solid state physics (magnetism, semiconductors, metals, superconductivity). The resulting papers are of good (Phys. Rev.) quality, but none would be termed outstanding. Likewise, extensive discussions with American

physicists have revealed no potential "show-stopper" experiments in the 40-100T region. Based on these observations, the NML Visiting Committee has recommended a cautious approach to the construction of a pulsed, high field facility at the Laboratory. In particular, neither the Visiting Committee nor NML management believes it is appropriate at this time to request the sort of funding ($3-5M) required to build the ultimate (~100T) in non-destructive, pulsed field facilities. NML opinion is based on extensive studies, by its Magnet Technology group, of steel coil systems similar to those used at Osaka. These studies indicate that it may not be possible to achieve 100T in coils of reasonable bore that can survive many shots. Moreover, even if it could be built, the system would be exceedingly expensive - about 5 times the cost of a 75T system.

III. NML Plans for New Facilities

Though the Laboratory has deferred a decision regarding the 100T project, it is aggressively developing pulsed field facilities in the 45-75T range, new dc magnets, and specialized, dedicated instrumentation. Projects now underway include:

1.) Further development and full instrumentation of the 45T facility. Four-channel data acquisition and a tunable, IR diode laser spectrometer are now available. A dedicated IR/FIR laser system will be purchased soon. Coil designs are being improved. Three NML staff spend part-time assisting users and improving instrumentation. The facility is beginning to evolve a user community.

In the future, the condenser bank will be enlarged to permit operation of larger volume coils. More dedicated instrumentation, especially visible optics and an OMA, are also needed.

2.) Development of strong copper wire. Preliminary experiments have shown that the Bevk Cu:Nb process can be scaled-up to produce high conductivity (60% pure Cu), 3/16" diameter wire samples with yield strength of 210 ksi. The wire program will expand, but funds are needed for coil development. Stronger wire could extend the range of the 10 msec. pulsed field system. Better materials might also serve the Bitter magnet program.

3.) 75T project. NML has ordered a 250 kJ, 20 kV, fast condenser bank to energize steel coils similar to those used in Osaka. This equipment will produce 50T in a 3.5 cm. bore, and will initially be used for engineering studies of coil designs. Later the system will be upgraded with a larger condenser bank to 70-75T in 1.5 cm. bore. With adequate funding, this facility could be operational in 1986. Magnet fabrication and the condenser bank will cost $1000K. There are no funds in the core contract for such purposes, or to acquire dedicated instrumentation for a 75T facility.

4.) High B/Low T Facility. NML, with great assistance from Prof. J. Brooks of B.U., now provides a 19T/50mK capability to users. The facility is popular; several outstanding experiments have been performed in it during the past year. However, with the present dilution refrigerator, sample change is slow and cumbersome. The Laboratory hopes to acquire a top-loading refrigerator and dedicated computer for the facility; total equipment cost is $312K. $200K/yr for operations is also needed.

NML is making long range plans, with assistance from Prof. J. Reppy of Cornell Univ., for a 15T/1 mK facility. This is an expensive project that will require $900K for capital equipment and $600K for site preparation (largely for vibration isolation). The potential payoff is also large. Topics that could be studied with such a system include: spin polarized hydrogen, A-1 phases of superfluid ^3He, spin polarized ^3He, spin waves in solutions of ^3He in ^4He, electron localization, 2D electron dynamics, heavy fermion superconductors, and p-wave superconductivity. Facilities for working in this field/temperature region have been or are being constructed in France, Japan, and Germany.

Projects planned for the near future include:

5.) Hybrid II. The Magnet Technology group is now completing a 30T, pumped helium, Nb-Ti hybrid for the Univ. of Nijmegen. Experience gained in its construction will be invaluable for building NML Hybrid II. Design of Hybrid II will begin in 1984; construction should be completed in early 1987. The magnet will be wound with Nb_3Sn, and probably achieve 33T. Routine operations will require a larger and better engineered cryostat than that of Hybrid I. Some funds for Hybrid II are budgeted in the current NSF contract; however, about $700K additional is required to complete the job within two years. Support for development of higher field superconducting wire is also needed. Both NML and NIH Visiting Committees have urged the Laboratory to take the lead in such development.

6.) Helium systems. Helium for Hybrid I is now provided by a liquefier belonging to the Plasma Fusion Center. The Laboratory needs its own, high capacity liquefier. Cost is about $500K. The availability

of a high capacity liquefier could save the Laboratory about 50K/yr., now used for purchase of liquid helium.

7.) Facility for high field, optical studies of large molecules. The Laboratory has recently dedicated a magnet to optical studies of microemulsions and similar systems. Some equipment funding is being provided by an IBM grant awarded to Profs. Benedek, Chen, Litster, and Tanaka; operations will begin in the Fall. The facility will be available to qualified users. Initially the system will perform precise birefringence measurements. Later we hope to add an auto-correlator for light scattering and a circular dichroism capability. Prof. Orme-Johnson of the MIT Chemistry Department has expressed special interest in the latter. Total cost: $150K.

8.) High field optical studies of semiconductors. Three cells at NML are instrumented for optical studies of crystals: two for Raman scattering; the third for magneto-reflection measurements. All three are now fully utilized; the lack of additional optical equipment has discouraged users. The Laboratory badly needs another standard optical laboratory, and picosecond optical capabilities.

9.) Refractory metal MBE. NML has a sizable ($\simeq$\$1M/yr) research and materials development program in high field superconductivity. It aims to become a national leader in this area; that goal has been enthusiastically endorsed by NSF, NIH, and the NML Visiting Committee. The program is interdisciplinary, involving three NML research staff and faculty members from EE&CS, and Materials Science.

Materials preparation is crucial to understanding and application of

superconductors. NML projects will ultimately require refractory metal MBE for preparing tunneling junctions and other structures of A15 superconductors. Such a facility - to be shared by all - would be almost unique. The Laboratory has (unsuccessfully) sought funds from the DOD instrumentation program for such a laboratory. Total equipment cost is $1,140K; $300-400K/yr will be needed to upgrade and operate the facility. These figures do not include the cost of a clean room.

10.) All-purpose Laboratory Computer. Considerable economies (~$30K/yr) could be achieved with a shared system for computation and office management. At present, the Laboratory owns no computer larger than a DEC 1120.

In assessing the future of high field research, it is important to realize that the technology is mature; qualitative improvements are unlikely. The outlook is different from that for synchrotron radiation where 10-100 fold increases in brilliance are anticipated; no such revolution in magnet technology seems imminent. Nevertheless, recent experience at NML suggests that even modest increases (~40%) in field capability can break open important new problems in condensed matter science, and significantly increase the demand for NML facilities. These problems could not have been anticipated 3-5 years ago. One cannot be sure, but it seems probable that a similar set of interesting and important scientific questions will be revealed in the 30-75T region. NML plans to develop both pulsed and dc field facilities in that range and, equally important, develop the techniques and instrumentation required to make optimal use of them. Some education of the scientific community will

also be required. Potential users of a facility are often reluctant to travel long distances to use unfamiliar equipment that may not accomplish the task they hope to perform. This psychological barrier will be especially high for a pulsed magnetic field facility that, at best, can produce a few pulses per hour, of 10-100μsec duration, at 60-70T. NML staff must demonstrate, through successful research projects, that a pulsed, high field facility can truly serve the scientific community.

IV. Funds Required to Implement NML Facility Plans

1.)	45T Facility.	
	a.) Capacitor bank (0.5MJ) with switching to permit multiple magnet station operation.	$ 600K
	b.) Cryogenic instrumentation.	175K
	c.) Optical instrumentation.	260K
2.)	Development of coils of high strength/high conductivity wire.	300K
3.)	75T Facility.	
	a.) Coil fabrication.	300K
	b.) High voltage condenser bank.	700K
	c.) Dedicated instrumentation.	550K
4.)	High B/Low T Facility.	
	a.) Improved 19T/50mK capability.	312K
	b.) 15T/1mK facility.	1,500K
5.)	Hybrid II - additional funds required to complete by 1986.	700K
6.)	He liquefier.	500K
7.)	Instrumentation for microemulsion facility	150K
8.)	General purpose optical instrumentation and picosecond optics.	250K
9.)	Refractory metal MBE.	
	a.) MBE and diagnostics.	1,140K
	b.) Clean room.	200K
10.)	General purposes laboratory computer system.	361K
	TOTAL	$7,998K

ilf/ 5/84

TOWARD AN ADVANCED MATERIALS PROCESSING AND ANALYSIS CENTER (AMPAC)

A Memorandum to the

National Academy of Sciences Committee
on
Major National Facilities for Materials Research

By

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June 1984

(Revision of 28 March 1984 Memorandum)

Toward an Advanced Materials Processing and Analysis Center (AMPAC)

Executive Summary

The future of U.S. basic and advanced industries is linked to new and improved materials technologies; of particular importance in this connection is the field of materials processing. To facilitate the generation of new knowledge and innovative processes, to educate a needed talent base, and to reeducate practicing engineers and scientists, it is proposed that one or more appropriate centers be established.

In particular, an Advanced Materials Processing and Analysis Center is described here, including goals, research programs, and the organization of cross-cutting, generic research groups involving industrial participation. Such a Center would have about 200 associates and would cost approximately $30 M to initiate. It would have a user-operating budget of $3 M/yr, and separately funded research projects of approximately $10 M/yr.

Statement of the Problem

U.S. leadership and competitiveness in modern systems depend directly on advanced materials science and technology. New materials and the capability to manufacture materials and components reproducibly and reliably constitute a most pervasive problem, and should be addressed on a national scale. We have found that advanced materials technology is a core theme in Japan's new government/industry thrust; indeed, that nation's continued economic growth of basic industries as well as high-tech industries is closely linked to superior materials development.

In the United States during the past 20 years, substantial attention has been focussed on the field of materials science; however, much of the emphasis has been on studying the structure and properties of existing materials. Many scientists and engineers (especially those at universities and national laboratories) abstained from research on the fundamentals of materials processing. Only recently have industrial, governmental, and academic leaders realized that the nation's productivity and ability to fabricate advanced systems are vitally coupled to advanced materials processing and manufacturing technology.

The development of new materials to fulfill present and future needs depends on finding new ways to generate and control structure at all levels from the submicroscopic to the macroscopic. It also requires being able to analyze the resulting structures and the processing/structure interactions. From an engineering point of view, materials processing is the field that seeks to control structure, shape, and properties of materials, and to do so in a cost-effective way with acceptable social costs. The science-base of materials processing and analysis seeks to evolve a deep understanding of the complex processes which control the structure. Only recently have the elegant tools for analysis and characterization become available. These allow for a quantitative description of the structure both physically and chemically from the angstrom- to the macro-levels. Materials processing and

analysis lie at the heart of the broad field of materials science and engineering, as illustrated in Figure 1, and link together three cornerstones of the field: materials structure, properties, and performance.

There are numerous examples of the impact that materials processing research can have on the advanced systems which are so important to our modern world. The development of optical waveguides (silica glass) is a sterling example of how structure and property relationships (notably extremely low transmission loss and total internal reflection of light and very high tensile strength) were obtained by radically new processing technology. The result is the substitution of materials (glass for copper) and of the system (telecommunication). This new optoelectronic system required equally as revolutionary processing developments of the compound semiconductor laser light sources, repeaters, and detectors. The important lessons to be learned from the processing science necessary for optoeletronics, or for numerous other cases such as silicon-based microelectronics, single crystal, superalloy turbine blades, rapid solidification processing, and sol-gel processing of structural and electronic ceramics is that processing and manufacturing is required at the atomic level as well as at the macroscopic level. Construction of advanced engineering systems of the future will be limited by the availability of process sensitive materials rather than from bulk materials which are bent, stamped, glued, welded, or machined as in conventional manufacturing.

A comprehensive generic-base in materials processing offers a broader platform for leveraging technology into useful systems than does the study

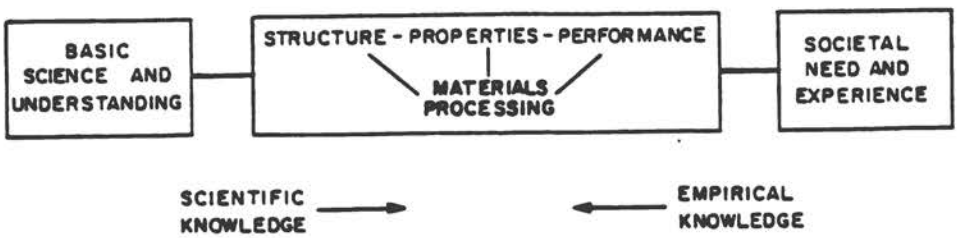

Figure 1: Materials Processing as part of Materials Science and Engineering

The rapid incorporation of new ideas for components, machines, and systems requires this broad materials processing foundation. Involvement of universities in these efforts also offers an effective rallying point for closer interactions with industry. Many of the systems that the nation will need in the next 30 years will require materials processing advances which have not been applied or even discovered to date. This new knowledge will include the synergism of concepts from many diverse disciplines: research, education, and modes of knowledge-transfer. Because the competetiveness among companies of the future will require unique levels of processing and of properties alone (Fig.2). Processing science which permits control of structure can be used as a springboard to produce advanced materials for many applications; thus, there is a much greater opportunity for technological advantage and international competitiveness.

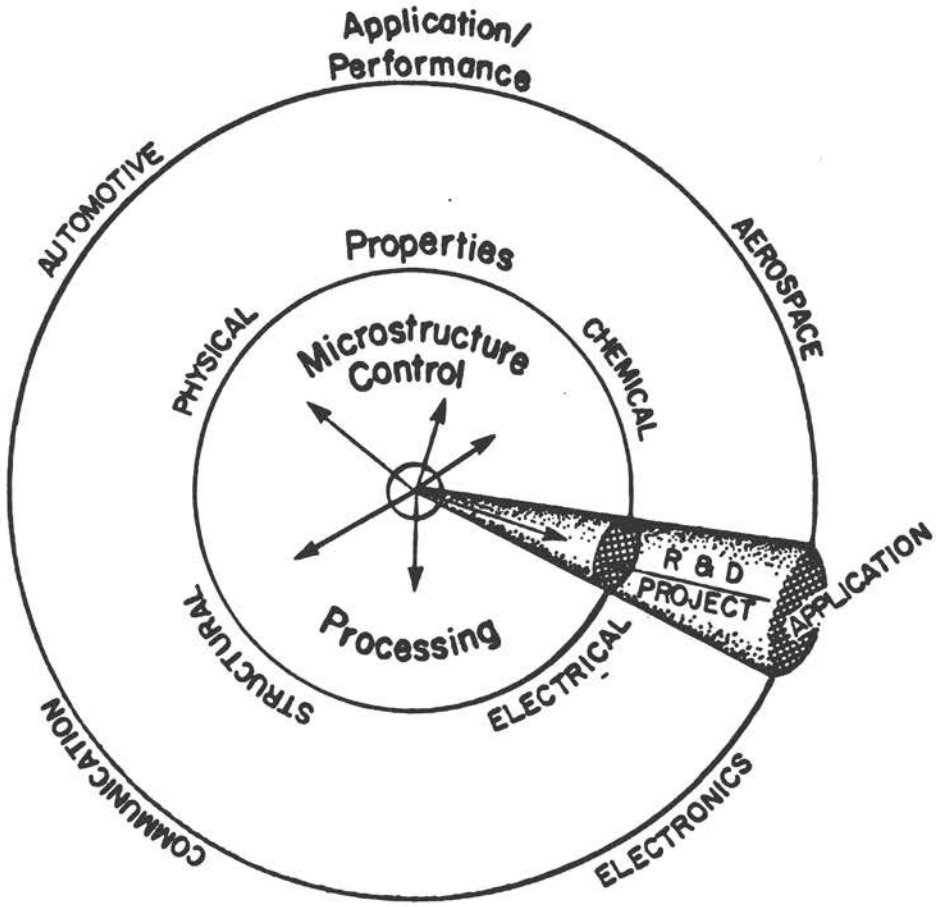

Figure 2. Schematic representation of how Generic Processing Research can be leveraged into many different applications while Performance/ Property-Initiated Research leads to a narrow processing technology base which may not be applicable to the manufacture of materials for other applications.

manufacturing science and engineering, the U.S. must have interdisciplinary materials processing centers in addition to the more familiar approaches to materials research.

This Nation has been slow, however, to respond to the materials processing/manufacturing challenge from abroad. The price that the country will pay if proper initiatives are not taken promptly will be non-competitive domestic industries left in the wake of our international trading partners.

Industry/University Collaboration

For about 40 years, the U.S. science and engineering community has carried out the world's best research in the field of materials. However, much of this research has not been transferred from the university, governmental, or industrial laboratory to the factory as expeditiously as it should have been (e.g., as in modern-day Japan). In many areas of technology, Japan was able to view both U.S. technology and science, and incorporate the best into their evolving industrial base. Japan's implementation of new technology and science in a more timely fashion is illustrated schematically in Figure 3. Examples of more rapid implementation of materials processing technologies in Japan are numerous; one recent advance is the use by Sony Corporation of magnetic fields to improve silicon single crystal growth, a process invented in 1972 at M.I.T. but not practiced in U.S. industry. Other examples are related to the processing of steel, ceramics, and semiconductor chips.

In the light of this experience, appropriate modes of interaction, relationships, and collaboration must become one of the key features of an Advanced Materials Processing and Analysis Center of Excellence; outstanding research is not enough, industry must be involved and people, the change-

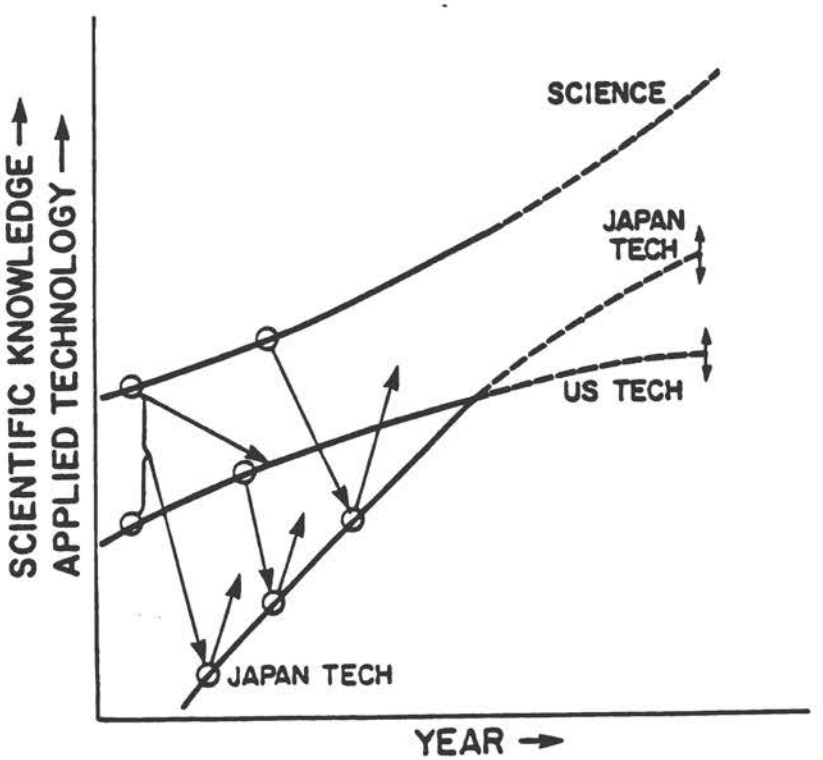

Figure 3. Schematic representation of how Japan has been able to look to better U.S. technology and to scientific knowledge and incorporate it into their own technology. The arrows imply a more timely incorporation of science and U.S. technology into Japan's more rapidly improving industrial base.

agents, must move from the Center to companies with innovative concepts and models for understanding, inventing, and improving materials processing and manufacturing. The Center must have unique research teams and facilities to be successful in attracting industrial scientists and engineers to participate in the generic research.

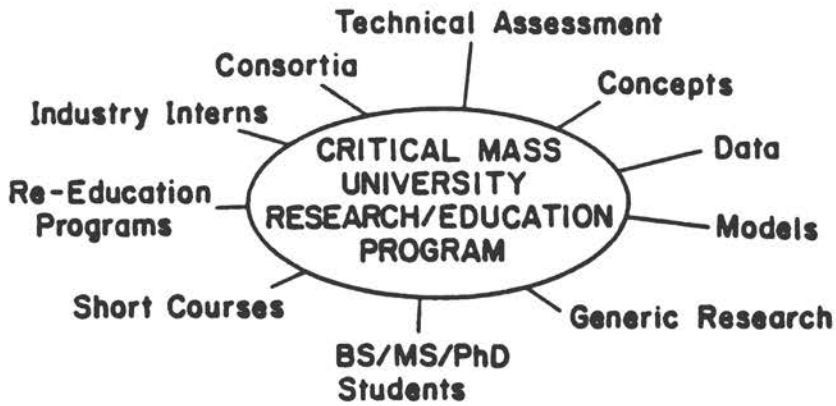

Figure 4. Contributions that AMPAC might make to improving the knowledge-base and talent-base for competitive materials process industries.

Ideally, the Center would carry out materials processing research in about 10 topical areas each of which would cut across more than one discipline and would be generic in nature--scientists and engineers working on common materials, equipment and processes. These technology-driven programs, which are also fundamentally founded in the engineering and science disciplines can be broadly used by U.S. industry and need not be specific to a particular company's problems or to a specific material or component. The best method for generating broad industry participation at such a Center is to encourage companies to sponsor research consortia and to send scientist/engineers for periods of residence. This will be the surest form of expedient transfer of processing concepts, models, and experimental results from the Center to U.S. industry.

The major goals of an Advanced Materials Processing and Analysis Center would be to:

1. Improve the relevant scientific base for materials processing technology by focussing major resources and efforts on both currently practiced and new processes. This will include research on:

   1.1 Mathematical- and physical-chemical models, concepts, and theories;

   1.2 Critical experiments to test models using prototype materials systems;

1.3 Sensing and measuring techniques which will allow access to the detailed knowledge needed to confirm the models and thus lead to the control of processes in industrial operations; and

1.4 Development of analytical tools to verify the structure and establish the ties between process variables and the reproducibility of chemical-physical structures.

2. Contribute usefully to the complex issues involved in the establishment and improvement of materials processing operations and in the production, management, and conservation of national resources by:

2.1 Innovating new materials processing techniques;

2.2 Disseminating modern technology and fundamental knowledge; and

2.3 Seeking rational solutions to societal and systems problems related to the processing and analysis of materials.

3. Develop an expanded talent-base in materials processing and analysis by:

3.1 Providing research programs for undergraduate and graduate education;

3.2 Establishing fellowships to attract the best students to the field;

3.3 Developing postdoctoral programs and junior faculty appointments in processing and analysis, especially by attracting talent from outside the traditional materials fields;

3.4 Developing a Master's degree program in materials processing and manufacturing systems engineering to provide more professionals for the manufacturing-processing industries; and

3.5 Educating and motivating post-graduate professionals and managers in the field of materials processing through the development of curricula and educational programs in close liaison with industrial personnel; and

3.6 Involving visiting interns from U.S. industry and other universities in 6-12 month research programs.

4. Strengthen institutional relationships among universities, industries, and govenment by providing a focal point for dealing with issues in materials processing, manufacturing, productivity, and technology assessment through:

4.1 Organizing public forums such as industrial collegia, consortia, and advisory boards;

4.2 Cooperating with NAS/NAE/NRC committees such as the National Materials Advisory Board and the Solid State Sciences Committee; and

4.3 Programming of conferences and special sessions with technical societies.

Establishing AMPAC

In order to meet the objectives of AMPAC, and thus to advance U.S. materials processing technology, one or more major national facilities need to be established. For the "user facility" concept to be workable and have substance, visiting scientists/engineers who are AMPAC interns must participate in meaningful ways in ongoing research programs at the Center.

An example of a format for such a Center of Excellence follows. The major costs are related to construction (or renovation) of a building consisting of approximately 60,000 ft of laboratories, offices, and classrooms. About 10 cross-cutting, multidiscipline research facilities would be outfitted, each requiring more than $500,000 in processing and diagnostic equipment. There would also be a general materials analytical facility which would service the 10 programs. An operating budget is required for the staff which runs the processing and analytical facilities and for support of 40 interns from U.S. industry and other universities.

The operating budget for the faculty, staff, and students of the host university should be generated through separate individual research grants and contracts, and should emphasize the use of industrially sponsored consortia. For the size of the proposed Center, this separately sponsored research would be at the level of approximately $10 M/year and involve 20 faculty members who will spend essentially all of their research effort within the Center plus 20 faculty who are part-time affiliates. These sponsored research programs would employ approximately 100 graduate students, 50 undergraduates, and 20 professional staff members.

The research facilities would be established for processing of ceramics, composites, metals, polymers, and semiconductors, but generally will be interdisciplinary. Each individual program is to be built around a processing concept rather than a material class or particular component. For example, the facilities for processing metal organics are important to new processes and innovations related to thin film metals, to ceramics and ceramics fibers, to active polymers, to compound semiconductors, and to composites, and will require chemists, physicists, ceramists, metallurgists, etc., working on joint projects.

Facilities for Materials Processing

The research groups and the facilities should be formed around generic processing concepts, rather than individual classes of materials. The purpose is to bring together the diverse talents that have hitherto focussed on one kind of processing problem or on one category of materials. Examples of the suggested groupings are:

1. Alloy Processing (Polymer Blends, Super Steels)
2. Rapid Solidification (Metals, Ceramics, Polymers, Electronic Materials)
3. Plasma Spraying (Metals, Ceramics)
4. Joining Dissimilar Materials (Welding, Bonding, Adhesion)
5. Plasma Deposition and Etching (Electronic Materials, Metals, Ceramics, Polymers)
6. Powder Processing (Ceramics and Metals)
7. Energy-Directed Processing (Lasers, Electron Beams, Ion Beams)
8. Processing Metal Organics to Form Fibers, Films, Powders, and Crystals
9. Processing Composite Structures (Matrix and Fibers)
10. Electrochemical Processing (Ionplating, Particulate Processing)
11. Sensors, Detectors, and Computers for Process Control and Systems Integration

Facilities for Analysis of Materials

The analysis and characterization of materials must be accomplished with a degree of sophistication sufficient to elucidate the details of microstructure as it evolves during processing and evaluate the performance of materials in service conditions. Fortunately we are now at a point where significant advances in microanalytical techniques are at hand. Much of the analysis equipment is for the purpose of measurement and detection ability connected with each of the process research thrust areas. Here we describe the facilities likely to be used by all research groups.

Of relevant importance is the ability to analyze compositional variations on the scale of $\sim$ 1.0 nm. To this end, four instruments must be given special consideration: (a) A new generation of scanning transmission electron microscopes (STEMs) operating in the 300-400 eV range is about to become commercially available. These instruments will have a spatial resolution for compositional analysis in the regime of 1.0 nm as well as

detection limits for heavy and light elements far superior to present-day microscopes. (b) In addition, field-ion microscope/atom probes (FIMAPs) are now being produced commercially and, for many metallic materials and possibly semiconductors and ceramics, will yield compositional information on a near-atomic level. (c) Moreover, a new generation of high spatial-resolution Auger units, built upon a STEM framework, is now being produced. These instruments exhibit a spatial resolution for surface analysis on a < 10 nm level. (d) Finally, impressive image resolution is becoming available in compact (i.e., housed in a regular one-bay laboratory) medium-high-voltage transmission electron microscopes. In particular, the 400 kV JEOL 4000 EX has a spatial resolution that allows atom imaging and will complement the microanalytical instruments discussed above.

Of course, analysis must also be undertaken with less-than-the-highest resolution. Instruments such as the secondary-ion mass spectrometer (SIMS), nuclear magnetic resonance (NMR), Fourier-transform infrared spectroscopy (FTIR) are important for the determination of internal and surface structure and composition. A Center of the suggested scope must likewise have the more conventional analytical techniques of light microscopy, X-ray diffraction, scanning electron microscopy, ESCA, mass spectroscopy, electron microprobe analyzer, etc.

AMPAC Personnel

A typical faculty/student/staff distribution for the subject Center might be the following:

- 20 Full-time associated faculty members distributed among analysis, metals, ceramics, polymers, electronic materials, and composites from Departments of Materials Science and Engineering, Electrical Engineering, Computer Science, Mechanical Engineering, Chemical Engineering, Physics, and Chemistry.
- 20 Part-time associated faculty members (~ 50% of research time associated with the Center).
- 40 Professional research staff members, such as senior research scientists, postdoctoral researchers, technicians, equipment designers and operators.
- 100 Graduate students (M.S./Ph.D. candidates).
- 50 Undergraduate students (B. S. candidates).
- 30 Research interns from U.S. industries (internships varying from 3 months to 2 years).
- 10 Research interns from other U.S. universities.

Tentative Cost Estimates

1. Facilities and Equipment

1.1	Building: 60,000 ft^2 x \$200/ft^2 = \$12 x 10^6 (containing for example, clean rooms, chemical hoods, some high bays, and office and labs for 190 personnel)		\$12.0 M
1.2	Processing Facilities (see alternate listing)		
	Ceramics (powder, vapor, melt)	2.3 M	
	Composites (metal, polymer, carbon, ceramic matrix)	1.9 M	
	Metals (powder, melt, thin film, rapid solidification)	2.7 M	
	Polymers (blends, films, plasma, melt)	1.9 M	
	Semiconductors (melt, vapor, etch, plasma)	2.1 M	10.9 M
1.3.	Analysis (see alternate listing)		5.4 M
	TOTAL		\$28.3 M

2. Annual Operating Budget (Annual Basis)*

2.1	Facilities Staff 40 x \$27,000 = \$1,280,000	0.896 M	
	Facilities Use Reimbursement -384,000		
	\$ 896,000		
2.2	Support Staff for 40 Interns (3 x \$18,000)	0.054 M	
2.3	Equipment Service Contracts	0.120 M	
2.4	Materials and Services (Interns plus Facilities Staff)	0.800 M	1.870M
	Overhead and Employee Benefits		1.230M
	TOTAL		3.3 M

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* It is assumed that the operating expenses for the research programs (faculty, staff and student salaries and materials/services) will be covered by other separate research grants and contracts from various agencies and industries; this will require that the Center Faculty have additional on-going research programs at a level of \$10 M/yr.

This tentative Operating Budget covers 70% of the salaries and also the materials and services for the technicians/engineers/scientists who will run the processing and analytical equipment. It also covers support of the 40 interns from industry and other universities.

Alternate Classification of Equipment

		Estimated Cost	
A.	Processing Equipment		
	Alloy Processing	$1.0 M	
	Rapid Solidification	1.2	
	Plasma Spraying	0.8	
	Joining Dissimilar Materials	0.7	
	Plasma Deposition and Etching	0.7	
	Powder Processing	1.6	
	Energy-Directed Processing	1.8	
	Metal Organic Processing	1.4	
	Processing Composite Structures	0.7	
	Electrochemical Processing	0.5	
	Sensors and Detectors for Process Control	0.5	$10.9 M
B.	Analytical Equipment		
	High-Voltage (300-400 keV) Scanning Transmission	0.95	
	High-Voltage (50 kV) Field-ion Microscope/ Atom Probe	0.45	
	Secondary-Ion Mass Spectrometer (SIMS)	1.00	
	High-Resolution Auger Microscope	0.75	
	Nuclear Magnetic Resonance (NMR) for Solids	0.45	
	Laser Raman Surface Spectroscopy	0.40	
	High-Resolution High-Voltage (440 kV) Transmission Electron Microscope	0.90	
	Electron Spectroscopy for Chemical Analysis (ESCA)	0.50	5.4 M
	TOTAL EQUIPMENT		16.3 M

Closure

This memorandum is being submitted to the Committee on Major National Facilities for Materials Research as an urgent suggestion to establish at least one Advanced Materials Processing and Analysis Center in the United States. The purpose, nature, and scope of such a Center are briefly described. It is emphasized that new facilities are not enough in terms of the challenge to the U.S. from our international trade competitors. A mechanism for implementing and integrating major facilities into a national program for materials processing is crucial to the basic and high technology industries in the U.S.

H. Kent Bowen

Ronald M. Latanision

John B. Vander Sande

APPENDIXES

APPENDIX A

List of Relevant Reports

1. NRC Solid State Sciences Committee, An Assessment of the National Need for Facilities Dedicated to the Production of Synchrotron Radiation, National Academy of Sciences, Washington, D.C., 1976.

2. NRC Solid State Sciences Committee, Neutron Research on Condensed Matter: A Study of the Facilities and Scientific Opportunities in the United States, National Academy of Sciences, Washington, D.C., 1977.

3. NRC Solid State Sciences Committee, High-Magnetic-Field Research and Facilities, National Academy of Sciences, Washington, D.C., 1979.

4. NRC Solid State Sciences Committee, Subcommittee on Free Electron Laser, The Free Electron Laser, National Academy Press, Washington, D.C., 1982.

5. NRC Solid State Sciences Committee, Subcommittee on Synchrotron Radiation Facilities, Current Status of Facilities Dedicated to the Production of Synchrotron Radiation, D. W. Lynch, ed., National Academy Press, Washington, D.C., 1983.

6. Ames Laboratory, Report of the Review Panel on Neutron Scattering, IS-4761, Ames, Iowa, October 1980.

7. NRC Solid State Sciences Committee, Panel on Neutron Scattering, Current Status of Neutron-Scattering Research and Facilities in the United States, National Academy Press, Washington, D.C., 1984.

8. National Synchrotron-Radiation Planning Committee, Planning Study for Advanced National Synchrotron-Radiation Facilities, Sandia National Laboratories, Albuquerque, NM, 14 March 1984.

9. D. Allan Bromley, "Neutrons in Science and Technology," Physics Today, Vol. 36, No. 12, 30-39, December 1983.

10. Remarks by Dr. George A. Keyworth, "Materials Research: A Model for Improved University/Industry Cooperation," Address to Materials Research Society, Boston, MA, Office of Science and Technology Policy, Washington, D.C., 14 November 1983.

11. National Science Foundation, "Workshop on a National Facility for the Study of Heterogeneous Catalysis," Division of Chemical and Process Engineering, National Science Foundation, Washington, D.C., 8-9 May 1981.

12. U.S. Department of Energy, Report of the 1983 HEPAP Subpanel on New Facilities for the U.S. High Energy Physics Program, DOE/ER-0169, Washington, D.C., July 1983.

13. NRC Astronomy Survey Committee, Astronomy and Astrophysics for the 1980's: Vol.1: Report of the Astronomy Survey Committee, Chapter 2, National Academy Press, Washington, D.C., 1982.

14. Energy Research Advisory Board, Materials R&D Panel, Materials Research and Development, DOE/S-0027, Energy Research Advisory Board, Washington, D.C., November 1983.

15. DOE/NSF Nuclear Science Advisory Committee, A Long Range Plan for Nuclear Science, U.S. Department of Energy, Washington, D.C., December 1983.

16. NRC Solid State Sciences Committee, Panel on Support of Small Research Projects in Materials Sciences at Universities, Support of Small Research Projects in Materials Sciences at Universities, National Academy of Sciences, Washington, D.C., 1979.

17. H. Winick, G. Brown, K. Halbach, and J. Harris, "Wiggler and Undulator Magnets," Physics Today, Vol. 34, No. 5, 50-63, May 1981.

18. J. Spencer and H. Winick, in Synchrotron Radiation Research, H. Winick and S. Doniach, eds., Plenum Press, NY, 1980, p. 663.

19. A. Hoffman, "Synchrotron Radiation From The Large Electron-Positron Storage Ring," Physics Reports, Vol. 64, 253-281, 1980.

20. E. E. Koch, ed., Handbook of Synchrotron Radiation, Vol. I, parts A and B, North-Holland, Amsterdam, 1983.

21. NRC Solid State Sciences Committee, Subcommittee on Muon Sources for Solid State Research, Muon Sources for Solid-State Research, National Academy Press, Washington, D.C., 1984.

22. George H. Vineyard and L. M. Falicov, "National Facilities for Research in the Physics of Condensed Matter," Review of Scientific Instruments, Vol. 55, No. 4, 620-630, April 1984.

23. An Assessment of the Needs for Equipment, Instrumentation, and Facilities for University Research in Science and Engineering, National Academy of Sciences, Washington, D.C., 1971.

24. Division of Science Resources Studies, Science Resources Studies Highlights, One-fourth of Academic Research Equipment Classified Obsolete, National Science Foundation, Washington, D.C., 1984.

25. D. M. Mills, A. Louis, A. Harootunian, J. Huang, and B. Smith, "Time-Resolved X-ray Absorption Spectroscopy of Carbon Monoxide Myoglobin Recombination After Laser Photolysis," Science, Vol. 223, No. 4638, 811-813, 24 February 1984.

26. D. M. Mills, "Time-Resolution Experiments Using X-ray Synchrotron Radiation," Physics Today, Vol. 37, No. 4, 22-30, April 1984.

27. K. J. Kim, K. Halbach, and D. Attwood. Proceedings of the Second Topical Meeting on Laser Techniques in the Extreme Ultraviolet, Boulder, 3-7 March 1984 (to be published).

APPENDIX B

Participants at the Workshop, Committee, and Panel Meetings

Meeting of the Committee of Major Facilities in Materials Sciences, January 20-21, 1984, National Academy of Sciences

Committee Members

Dean E. Eastman, IBM (Co-Chairman)
Frederick Seitz, Rockefeller University (Co-Chairman)
Richard B. Bernstein, University of California, Los Angeles
Robert J. Birgeneau, Massachusetts Institute of Technology
Jerome B. Cohen, Northwestern University
Mildred S. Dresselhaus, Massachusetts Institute of Technology
Peter Eisenberger, Exxon Research and Engineering Co.
Donald M. Engelman, Yale University
Walter Kohn, Institute of Theoretical Physics, Santa Barbara
David W. Lynch, Iowa State University and Ames Laboratory
Albert Narath, AT&T Bell Laboratories
William D. Nix, Stanford University
Edward Rubenstein, Stanford University Medical Center
John J. Rush, National Bureau of Standards
Albert I. Schindler, Naval Research Laboratory
Arthur W. Sleight, E.I. du Pont de Nemours & Company, Inc.
William P. Slichter, AT&T Bell Laboratories
Joseph V. Smith, University of Chicago
Richard S. Stein, University of Massachusetts
H. Guyford Stever, Universities Research Association
John M. White, University of Texas at Austin

Guests

Louis C. Ianniello, Department of Energy
George J. Keyworth, III, Office of Scicence and Technology Policy
Lewis H. Nosanow, National Science Foundation
Donald K. Stevens, Department of Energy
Alvin W. Trivelpiece, Department of Energy
Joel A. Snow, Department of Energy
Herman Feshbach, Massachusetts Institute of Technology

NRC Staff

Herbert Friedman
Raphael G. Kasper
Robert L. Park
Donald C. Shapero
Robert M. Simon
William Spindel
Teresa Trotta
Jean E. Yates

Meeting of the Neutron Scattering Panel
February 26-27, 1984, National Academy of Sciences

Panel Members

Robert J. Birgeneau (Chairman)
Mildred S. Dresselhaus
Donald M. Engelman
John J. Rush
Frederick Seitz
Joseph V. Smith
Richard S. Stein
Michael E. Fisher, Cornell University (Consultant)

Guests

John C. Browne, Los Alamos National Laboratory
Victor J. Emery, Brookhaven National Laboratory
Ray G. Kammer, National Bureau of Standards
Robert L. Kustom, Argonne National Laboratory
Gerard H. Lander, Argonne National Laboratory
Herbert A. Mook, Oak Ridge National Laboratory
Ralph M. Moon, Jr., Oak Ridge National Laboratory
Michael M. Rowe, National Bureau of Standards
Benno P. Schoenborn, Brookhaven National Laboratory
Richard N. Silver, Los Alamos National Laboratory

NRC Staff

Donald C. Shapero
Robert M. Simon
William Spindel
Jean E. Yates

Meeting of the Synchrotron Radiation Panel
February 28, 1984, University of California, Los Angeles

Panel Members

David W. Lynch (Chairman)
Richard B. Bernstein
Donald M. Engelman
Edward Rubenstein
Joseph V. Smith

Guests

David T. Attwood, Lawrence Berkeley Laboratory
Boris W. Batterman, Cornell High Energy Synchrotron Source
Arthur I. Bienenstock, Stanford Synchrotron Radiation Laboratory
Martin Blume, Brookhaven National Laboratory
Yanglai Cho, Argonne National Laboratory
Thomas E. Hutchison, University of Virginia
Kenneth L. Kliewer, Argonne National Laboratory
Samuel Krinsky, Brookhaven National Laboratory
Dennis M. Mills, Cornell High Energy Snychrotron Source
David A. Shirley, Lawrence Berkeley Laboratory
Helmut Wiedemann, Stanford Synchrotron Radiation Laboratory

NRC Staff

William Spindel

"Other" Materials Facilities Panel
March 8-9, 1984, National Academy of Sciences

Panel Members

Albert Narath (Chairman)
Richard B. Bernstein
Mildred S. Dresselhaus
Dean E. Eastman
Walter Kohn
David W. Lynch
William D. Nix
Albert I. Schindler
Arthur W. Sleight
William P. Slichter
Frederick Seitz
Richard S. Stein
H. Guyford Stever
John M. White

Guests

Albert M. Clogston, Los Alamos National Laboratory
Robert H. Heffner, Los Alamos National Laboratory
Louis C. Ianniello, Department of Energy
John D. Joannopoulos, Massachusetts Institute of Technology
Dean L. Mitchell, National Sciences Foundation
Marvin K. Moss, Office of Naval Research
Elliot S. Pierce, Department of Energy
Gerd M. Rosenblatt, Los Alamos National Laboratory
Fred E. Saalfeld. Office of Naval Research
Victor J. Tennery, Oak Ridge National Laboratory
Harlan L. Watson, Subcommittee on Energy Development and Applications, U.S. House of Representatives Committee on Science and Technology
Michael K. Wilkinson, Oak Ridge National Laboratory
Peter A. Wolff, Los Alamos National Laboratory

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Robert M. Simon
William Spindel
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Major Materials Facilities Workshop
March 17-20, 1984, National Academy of Sciences

Committee Members

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Frederick Seitz (Co-Chairman)
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Robert J. Birgeneau
Jerome B. Cohen
Mildred S. Dresselhaus
Harry G. Drickamer
Peter Eisenberger
Donald M. Engelman
Walter Kohn
David W. Lynch
Albert Narath
William D. Nix
Edward Rubenstein
John J. Rush
Albert I. Schindler
Arthur W. Sleight
William P. Slichter
Joseph V. Smith
Richard S. Stein
H. Guyford Stever
John M. White
Michael E. Fisher, Cornell University (Consultant)

Guests:

Ernest Ambler, National Bureau of Standards
David T. Attwood, Lawrence Berkeley National Laboratory
John D. Axe, Jr., Brookhaven National Laboratory
Arthur I. Bienenstock, Stanford Synchotron Radiation Laboratory
Martin Blume, Brookhaven National Laboratory
John C. Browne, Los Alamos National Laboratory
Yanglai Cho, Argonne National Laboratory
Philip E. Coyle, Lawrence Livermore National Laboratory
Paul J. Ebert, Lawrence Livermore National Laboratory
Victor J. Emery, Brookhaven National Laboratory
Brian E. F. Fender, Institut Laue Langevin, Grenoble
Herman A. Grunder, Lawrence Berkeley National Laboratry
Keith O. Hodgson, Stanford University
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Thomas E. Hutchison, University of Virginia
Louis C. Ianniello, Department of Energy
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Kenneth L. Kliewer, Argonne National Laboratory
Michael L. Knotek, Sandia National Laboratory
Martha A. Krebs, Lawrence Berkeley National Laboratory
Samuel Krinsky, Brookhaven National Laboratory
Richard H. Kropschot, Department of Energy
Robert L. Kustom, Argonne National Laboratory
Gerard H. Lander, Argonne National Laboratory
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Boyce D. McDaniel,Cornell High Energy Synchrotron Source
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Meeting of the Major Materials Facilities Committee
May 3-4, 1984, National Academy of Sciences

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Meeting of Major Materials Facilities Committee
June 14, 1984, National Academy of Sciences

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