[This PDF is available from The National Academies Press at http://www.nap.edu/catalog.php?record\\_id=19504](http://www.nap.edu/catalog.php?record_id=19504)



Distribution, posting, or copying of this PDF is strictly prohibited without written permission of the National Academies Press. Unless otherwise indicated, all materials in this PDF are copyrighted by the National Academy of Sciences.

To request permission to reprint or otherwise distribute portions of this publication contact our Customer Service Department at 800-624-6242.



Copyright © National Academy of Sciences. All rights reserved.

# REFERENCE COPY

### $\Lambda$  Current Status **PROPERTY OF** of Facilities ΩÌΙ Dedicated to the L PR 1996 Production of Synchrotron Radiation<sup>NRC</sup>

 $\downarrow$  Subcommittee to Assess the Current Status of Facilities Dedicated to the Production of Synchrotron Radiation  $\sim\neq$  Solid State Sciences Committee

')- Commission on Physical Sciences, Mathematics, and Resources .

National Research Council

 $\lambda$ 

NAS-NAE

MAR 2 � 1983

## **LIBRARY**

NATIONAL ACADEMY PRESS Washington, D.C. 1983

Copyright © National Academy of Sciences. All rights reserved.

> NOTICE: The project that is the subject of this report was approved by the Governing Board of the National Research Council, whose members are drawn from the councils of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine. The members of the committee responsible for the report were chosen for their spec ial competences and with regard for appropriate balance.

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.

The National Research Council was established by the National Academy of Sciences in 1916 to associate the broad community of science and technology with the Academy's purposes of furthering knowledge and of advising the federal government. The Council operates in accordance with general policies determined by the Academy under the authority of its congressional charter of 1863, which establishes the Academy as a private, nonprofit, self-governing membership corporation. The Council has become the principal operating agency of both the National Academy of Sciences and the National Academy of Engineer ing in the conduct of their services to the government, the public, and the scientific and engineering communities. It is administered jointly by both Academies and the Institute of Medicine. The Na tional Academy of Engineering and the Institute of Medicine were established in 1964 and 1970, respectively, under the charter of the National Academy of Sciences .

The work reported here has been supported by the U.S. Department of Energy, Office of Basic Sciences under grant No. DE-FG01-81ER10844 and by the National Science Foundation under grant No. DMR 8119500.

Available from

we Solid State Sciences Committee 2101 Constitution Avenue, N.W. Washington, D.C. 20418

#### SUBCOMMITTEE TO ASSESS THE CURRENT STATUS OF FACILITIES DEDICATED TO THE PRODUCTION OF SYNCHROTRON RADIATION

 $\sim$ DAVID W. LYNCH, Iowa State University and Ames Laboratory, Chairman BORIS W. BATTERMAN, Cornell University ARTHUR BIENENSTOCK , Stanford University PETER EISENBERGER, Exxon Research and Engineering Corporation JOHN P. McTAGUE, Brookhaven National Laboratory EDNOR M. ROWE, University of Wisconsin J. MICHAEL ROWE, National Bureau of Standards STEPHEN E. SCHNATTERLY , University of Virginia NEVILLE V. SMITH, Bell Laborator ies

#### Liaison Members

DEAN E. EASTMAN, Solid State Sciences Committee LOUIS IANNIELLO, U.S. Department of Energy WILLIAM T. OOSTERHUIS, National Science Foundation

#### Staff

CHARLES K. REED, National Research council

#### SOLID STATE SCIENCES COMMITTEE

MARTIN BLUME, Brookhaven National Laboratory, Chairman WILLIAM F. BRINKMAN, Bell Laboratories, Chairman-Elect DEAN E. EASTMAN, IBM Corporation, Past-Chairman ROBERT T. BATE, Texas Instruments, Inc. ANTHONY G. EVANS, University of California, Berkeley FRED R. GAMBLE, Jr., Exxon Research and Engineering Company ROY G. GORDON, Harvard University VINCENT JACCARINO, University of California, Santa Barbara WI LLIAM D. NIX, Stanford University RAYMOND L. ORBACH, University of California, Los Angele s S. ELAINE PETRIE, Eastman Kodak Company ALBERT I. SCHINDLER, Naval Research Laboratory WILLIAM A. SIBLEY, Oklahoma State University MICHAEL K. WILKINSON, Oak Ridge National Laboratory

#### S taff Consultant

WESLEY N. MATHEWS Jr., Georgetown University

#### Staff

CHARLES K. REED, National Research Council

i v

#### COMMISSION ON PHYSICAL SCIENCES, MATHEMATICS , AND RESOURCES

HERBERT FRIEDMAN, Nat ional Research Council, Cochairman ROBERT M. WHITE, University Corporation for Atmospheric Research, Cochairman STANLEY I. AUERBACH, Oak Ridge National Laboratory ELKAN R. BLOUT, Harvard Medical School WILLIAM BROWDER, Princeton University BERNARD F. BURKE, Massachusetts Institute of Technology HERMAN CHERNOFF, Massachusetts Institute of Technology WALTER R. ECKELMANN, Exxon Corporation JOSEPH L. FISHER, Office of the Governor, Commonwealth of Virg inia JAMES C. FLETCHER, University of Pittsburgh WILLIAM A. FOWLER, California Institute of Technology GERHART FRIEDLANDER, Brookhaven Nat ional Laboratory EDWARD A. FRIEMAN, Science Applications, Inc. EDWARD D. GOLDBERG, Scr ipps Inst itut ion of Oceanography KONRAD B. KRAUSKOPF, Stanford University CHARLES J. MANKIN, Oklahoma Geological Survey WALTER H. MUNK, University of California, San Diego NORTON NELSON, New York University Medical Center DANIEL A. OKUN, University of North Carolina GEORGE E. PAKE, Xerox Research Center CHARLES K. REED, National Research Council HOWARD E. SIMMONS, JR., E.I. du Pont de Nemours & Co., I nc. HATTEN S. YODER, JR., Carnegie Institution of Washington

RAPHAEL G. KASPER, Executive Director

v

 $\mathcal{L}(\mathcal{A})$  and  $\mathcal{L}(\mathcal{A})$  .

 $\hat{\mathcal{L}}$ 

 $\mathcal{L}^{\text{max}}$ 

 $\hat{\theta}$ 

 $\mathcal{L}^{\text{max}}_{\text{max}}$  , where  $\mathcal{L}^{\text{max}}_{\text{max}}$ 

#### PREFACE

In 1976 an NRC panel was created to assess the national need for facilities dedicated to the production of synchrotron radiation.<sup>1</sup> The principal recommendations of that panel were that a new national facility be constructed and that existing facilities be upgraded . The panel also made projections of the numbers of users and areas of science that would benefit from these facilities. The recommended construction and upgrading have now been carried out, although the new facilities are not yet fully available to the user community.

In the spring of 1982 the Solid State Sciences Committee, in implementing one of a series of studies important to maintaining the health of this discipline, asked a group of experts to assess the present status of f acilities dedicated to the production of synchrotron radiation, to review accomplishments during the past five years, and to make projections for the future. The Solid State Sciences Committee has reviewed the Subcommittee's r eport, unanimously approves its conclusions and recommendations, and recommends it be issued as a report of the Committee .

> Martin Blume, Chairman Solid State Sciences Committee

vii

 $\hat{\mathbf{z}}$ 

 $\Delta\sim 10$ 

Copyright © National Academy of Sciences. All rights reserved.

 $\hat{\mathbf{z}}$ 

#### 1. CONCLUSIONS AND RECOMMENDATIONS

#### CONCLUSIONS

1. The use of synchrotron radiation has undergone a rapid growth in many areas of science during the past five years. Unforeseen fields have emerged, creating new opportunities. In addition, there is a growing impact on many technological areas that will increase further on the emergence of new sources and experimental stations.

2. The growth in the use of synchrotron radiation has been so great that all existing experimental stations will be fully utilized when all current facilities in the United States begin full-time operation for users. Development of the remaining potential experimental stations at existing facilities will satisfy predicted demand until 1985.

3. Insertion devices (wigglers and undulators) provide orders-of-magnitude br ighter sources of radiation than bending magnets and are making possible new experiments not feasible, or even conceived, a few years ago.

#### RECOMMENDATIONS

1. The Subcommittee recommends that an immediate commitment be made to construct new wiggler and undulator insertions on storage rings. This recommendation includes the new beam lines and experimental stations associated with these insertions, which are required to pursue new scientific and technological opportunities.

2. The Subcommittee recommends that a review mechanism involving the scientific community be established to monitor scientific and technological progress and oppor tunities for synchrotron radiation facilities and to provide recommendations for action. Further, we suggest consideration of a broader-based review mechanism for major facilities in condensed-matter science that would include synchrotron radiation facilit ies.

#### 2. CURRENT STATUS OF SYNCHROTRON RADIATION FACILITIES IN THE UNITED STATES

We describe briefly the current status of the five synchrotron radiation (SR) laboratories in the United States, the numbers and characteristics of the users ( along with a compar ison with the projections made in 1976), and a general description of the makeup of the synchrotron radiation user community. A briefer description of overseas facilities is given in Chapter 3. It should be noted that even at a mature facility t here is constant evolution in the nature of research carried out. Moreover, with the development of insertion devices (described in the Appendix), even the spectrum and brightness\* available from a given storage ring may change in only a year or so. In view of ongoing rapid progress with these devices, it is the judgment of the subcommittee that continuous monitoring of insertion device performance be carried out.

\*Spectral brightness is defined as the number of photons, within a differential energy bandpass, emitted per unit area of the source and per unit solid angle. Spectral intensity is the integral of spectral brightness over the source area. For some experiments high intensity is all that is needed. For others, high brightness is mandatory. Also in the following we use the terms ultraviolet (UV), or vacuum ultraviolet (VUV) , to refer to the photon energy range 5-3000 ev, which includes the soft x-ray region, and x ray to refer to the range above 3 keV.

#### FACILITY DESCRIPTIONS

#### Cornell High Energy Synchrotron Source (CHESS)

CHESS is a synchrotron radiation laboratory parasitic to the part icle-phys ics operation at the 4-8 GeV Cornell Electron Storage Ring (CESR) . Both CESR and CHESS are funded by the National Science Foundation (NSF). CHESS has supplied SR to users at full capacity for 1 1/2 years. Because of the large circumference of the storage ring, single-bunch operation of CESR gives a particularly useful time structure. Three primary-beam lines supply hard x rays to six experimental stations for general use, entirely constructed from \$1.3 million of NSF funds. The useful energy range is from 3 to about 90 keV. Three stations scan continuously from 3 to 20, 35, and 50 keV, respectively. Two other lines provide focused x-ray beams of high flux. CHESS has about 75 active proposals, about one third from Cornell faculty and staff and the remainder divided about equally between university and industry, including National Laboratories. A 6-pole wiggler, on the loan from the Stanford Synchrotron Radiation Laboratory, providing a critical energy of 34 keV, was installed in one of the CHESS lines in September 1982.

#### National Synchrotron Light Source (NSLS)

NSLS at Brookhaven National Laboratory is a national user facility consisting of an 800-MeV storage ring for UV and soft x-ray use and a 2.5-GeV ring for x-ray use. Each has been designed for high brightness, and each is dedicated 100 percent to photon production. The UV ring currently is in an early operational stage, while the x-ray r ing stored its f irst beam in September 1982. There are 16 ports on the UV ring and 28 on the x-ray ring, each of which can be divided to support several experimental stations. Thirteen of the 16 UV ports and all the currently accessible x-ray ports have been assigned to user groups. Eight of the x-ray ports cannot yet be utilized owing to space requirements for support groups. There are 19 experimental stations on the UV <sup>r</sup> ing and 34 on the x-ray r ing. Approximately 60 percent of the beam lines are being constructed by participating research teams (PRTs) from a wide variety of university, industrial, and national laboratories, using capital

expenditures of \$6.1 million, \$7.3 million, and \$5.8 million, respectively. The PRTs, many of which are cooperative university/industry efforts, receive up to 75 percent of the beam time in recognition of their investment in equipment and support. The remaining 25 percent of the time, as well as the majority of the time on NSLS lines, is available to the general scientific and technological community on a proposal basis. There are currently 32 PRTs with a total membership of 185 scientists. Several hundred other individuals have inquired about general usership. The first solicitation of proposals from non-PRT scientists for the UV ring was made in late fall 1982. A free electron laser (FEL) for the UV is under development, along with several wigglers and undulator s.

#### Stanford Synchrotron Radiation Laboratory (SSRL)

SSRL at the Stanford Linear Accelerator Center (SLAC) is a national user facility currently utilizing the 4-GeV storage ring, SPEAR. Electrons can be stored at energies up to 4 GeV. With its high electron energy and 14 usable straight sections, it is particularly well suited for wigglers and for  $x$ -ray and soft  $x$ -ray undulators, for the production of ultrahigh fluxes. Fifty percent of its operating time is dedicated to SR production, and parasitic use is possible at other times. At present it has 15 experimental stations on 5 beam lines. Of these, 3 use bending magnets and 2 are illuminated by 8-pole wiggler magnets. Each of these wigglers may be replaced by an existing 30-period undulator. Two new beam lines are being developed in collaboration with outside groups. One will contain a 54-pole wiggler, whereas the other will be illuminated by interchangeable undulators that are optimized for different portions of the spectral r eg ion between 10 and 1000 eV. Of the remaining straight sections, one is committed for development of an i n-vacuum unulator capable of produc ing 8-keV x rays and another for an additional multipole wiggler to be developed in collaboration with outside groups. The rest will be assigned on the basis of proposals that have been solicited. Almost all of the time on the existing 15 experimental stations and at least one third of the time on the stations being built under collaborations with outside groups is available to the general scientific and technolog ical community on a proposal basis. In recent

6

years industry has contributed \$2.5 million of capital equipment funds for beam lines, and university/national laboratory groups contributed \$2.3 million. Future plans call for the utilization parasitically of an existing undulator on PEP (a 16-GeV storage ring) to produce ultra-h igh-br ightness hard x rays.

#### Synchrotron Radiation Center (SRC)

SRC is operated by the Graduate School of the University of Wisconsin-Madison. It is funded entirely by NSF as a National Facility. At present, research at the SRC is carried out using Tantalus I, a 240-MeV electron storage ring that has been in operation since 1968. Concurrently the new 1-GeV machine, Aladdin, is being commissioned. It is designed specifically as a very-high-brightness source for the UV and soft-x-ray range (6-3000 eV). It has 36 primary ports, averaging 50 mr, 35 of which are available for SR research. The thirty-sixth port is dedicated to use as an inverse-Compton-scattered beam of gamma photons at energies  $\geq$ 50 MeV. At present, 20 of the ports are being equipped with beam lines, 7 by PRTs, and 13 by the SRC with either new monochromators designed spec ially for Aladdin or instruments currently installed at Tantalus, suitably upgraded. Four more possible PRTs are awaiting action on proposals. Capital outlays for beam lines by PRTs have been \$1.9 million and \$0.8 million, from universities and National Laboratories, respectively. Besides the normal bending-magnet sources, there are four long straight sections, three of which are available for the future installation of wigglers, undulators, and FELs. Low-current stored beam was first achieved in January 1982. Currently, improvement of reliability and beam current are being pursued apace with the installation of beam lines.

#### Synchrotron Ultraviolet Radiat ion Fac ility (SURF)

SURF II is a 280-MeV storage ring at the National Bureau of Standards, used in a mode dedicated to the production of synchrotron radiation. The small beam cross section results in a high-brightness source for photon energies up to 400 eV. There are 11 experimental stations, and 2 more are planned for installat ion in 1983. All are used regularly. These are used for atomic and molecular

spectroscopy, including the spectroscopy of laser-excited states, photoelectron spectroscopy of atoms and molecules , and surface physics. The users are usually NBS scientists, with collaborators from National Laboratories and unive r sities.

#### THE USER COMMUNITY

As time passes it becomes more difficult to characterize the synchrotron radiation user community. There are three modes of use that may be labeled as "committed," "mixed," and "transient." Committed users are those whose research programs are built almost exclusively around synchrotron radiation. This category includes (a) the scientific staff members of the SR facilities and (b) members of PRTs. Such PRTs usually design and construct their own beam lines, including monochromators, and maintain them. They usually have one or more people in permanent residence at a facility. The teams normally have priority usage of the majority of the beam time on the beam lines they construct. Other committed users are (c) sc ient ists not falling into committed categor ies ( a) an (b) but whose research programs are centered around SR .

These committed scientists are the core of the community, for they are the ones who develop new instrumentation and techniques and who introduce new users to SR utilization. Graduate students associated with them often become committed users when they finish and take employment elsewhere. They also are hosts for a variety of visitors, and many permanent and transient collaborat ions form around them. The number of such scientists has grown significantly as the new synchrotron radiation facilities come on line. These groups are easy to count.

The second mode of use is that employed by people who have an ongoing research program at their home institution but for whom the use of synchrotron radiation adds a new dimension to their programs. Examples are those doing x-ray diffraction or photoemission with fixed wavelength x-ray or UV sources and those whose interest may be in a class of materials, such as catalysts or metalloproteins, and whose main research does not involve photons. Such users may bring a sample chamber to a facility for one run per year, or they may use the apparatus available at the facilities, supplying only samples and ideas. Such individuals often become regular users but not with the frequency of the committed users.

The third mode is that of the transient, who may make a few measurements then leave. Such people may not come from the traditional user community. They frequently obtain interesting results but do not participate regularly in the development of better techniques or i nstrumentation. Examples occur most frequently in the biological, biochemical, medical, and materials-science f ields. There have been many such users at all facilities, and few fail to continue in this mode. Instead, they return periodically to improved sources, instrumentation, and techniques with increasingly sophisticated approaches to their problems. Such users can be counted easily in retrospect, but their future number is difficult to estimate. They may account for fewer hours of beam time than do committed users, but they apply SR to diverse fields and do a great deal of new science with SR.

The original users of synchrotron radiation in the United States often were either atomic and solid-state spectroscopists or surface scientists. The experiments were simpler than those carried out today. The early users often used SR to extend into a new spectral region measurements that they had been doing in the past. These measurements then became the rationale for designing new methods and instrumentation. As a result, the majority of soft x-ray and VUV lines today are used for photoelectron spectroscopy of atoms, molecules, solids, surfaces, and interfaces. These beam lines emphasize high flux at moderately high resolution and a wide range of photon energies. The experiments often involve many measurements in addition to the primary one, in order to produce well-characterized samples. In addition to photoelectrons, emitted ions or photons may also be detected, sometimes in coincidence with the electrons. Other common uses of VUV beam lines include solid-state spectroscopy and modulation spectroscopy, absorption , emission, and circular dichroism spectroscopy of gases.

The x-ray lines are devoted primarily to  $x$ -ray absorption and scattering (including what is often termed diffraction). Since scattering and x-ray absorption, inc luding EXAFS , are generally applicable to a var iety of disciplines, the user community for these lines is most diverse. Samples may be located in living cells, inside high-pressure chambers, within electrochemical cells, or as precipitates within a host matrix. As intensities increase, time-resolved spectroscopy is being developed so that a structural determination of a transient phase

may be determined. A few of these experimental areas will be reviewed in more detail in Chapter 4.

Ideally, a census of users should not be just a head count, because of the varying amounts of beam time that the different types of users require. However, a simple number does suggest how much the use of SR has diffused into the scientific community. A similar assessment of the use of SR is the number of published papers based in whole, or in part, on its use. Both of these assess quantity. Quality assessments require a detailed view of a given field, the rate of production of new ideas, and their adoption in other areas. We attempt this in Chapter 4 with a few illustrations.

The growth in use of SR facilities in the United States is shown graphically in Figure 1. A user in



FIGURE 1 Total annual number of users at U.S. synchrotron radiation facilities.



FIGURE 2 Annual numbers of synchrotron publications .

Figure 1 is a scientist who appeared at a SR facility at least once during the year on the abcissa to take data. Those for whom beam time was unavailable are not counted. A distinction between "committed" and "general" users was not made on a year-by-year basis. The increase between 1981 and 1982 is due to the beginning of operations at CHESS and NSLS .

The scientific output, as measured by annual publications, has increased substantially since the 1976 report and shows a long-term growth rate of about 30 percent per year. Figure 2 shows the number of annual publications reported by the following institutions: United States: CHESS, SRC, SSRL, and SURF; world: U.S. facilities and Ha sylab (West Germany) , SRC ( United Kingdom) , and LURE (France). The figure does not include publications from SR facilities in Italy, Japan, and the Soviet Union. ( Data for 1981 are incomplete at the time of this report.) The current annual rate of publications based on SR exceeds 550 .

10

In 1981, about 40 percent of the SR user community came from universities, 30 percent from National Laboratories, and 30 percent from industry. Those from industry came not only from the large industrial research laboratories with prominent basic research efforts but also from many other companies with relatively narrow interests. The university-based users who had funding from NSF were distributed across several disciplines: condensed-matter science, 30%; chemistry, 25%; biology, 15%; materials science, 15%; miscellaneous, 15%. Such figures fail to show the remarkable number of collabor ations that have occurred among users. These go far beyond collaborative research and include joint industryuniver sity and university-National Laboratory funding of beam lines and experimental stations .

An important aspect of the user community is graduate education. Many graduate students do all or part of their thesis research at SR facilities. All told, about 200 graduate students have earned Ph.D.s with work partly done at SR facilities. This number is growing rapidly. These students are not just from nearby institutions. For example, at the SRC in Wisconsin, Ph.D. students from Cornell, Pennsylvania, Georgia Tech, Chicago, Illinois, Iowa State, and Montana State have carried out much of the experimental part of their research with SR. These students, as well as postdoctoral students, often take positions at new academic institutions or in industry and become users themselves or encourage others at their institutions to become users .

The availability of more SR facilities allows the development of new types of experiments, e.g., pulsed x-ray diffraction and far-infrared spectroscopy. These methods, especially pulsed diffraction, which can be used by many people in a transient mode, should have wide application and should draw large numbers of users. This type of growth of the user community is expected but is hard to quantify.

Another change in the character of the user community is expected when more beam lines are functioning in the 500-3000 eV spectral region, making it more easily accessible. Part of this region can be reached with grating monochromators, e.g., the "grasshopper." The remainder can be reached with grating-crystal monochromators, e.g. , •jumbo• at SSRL. Once more high-quality beam lines are more widely available in this spectral range, the K edge of the important elements carbon and oxygen can be utilized more widely, as can the L edges of

Facility	Supply			Demand		
	PRT	General	Undeveloped	PRT	General	
<b>CHESS</b>						
X-ray	-	24			24	
UV	-					
<b>NSLS</b>						
X-ray	240	168	96	240	$\frac{b}{b}$	
UV	132	120	48	132		
<b>SRC</b>						
X-ray	$\qquad \qquad \blacksquare$	$\overline{\phantom{0}}$	۰	-		
UV	132	120	168	132	72	52
<b>SSRL</b>						
X-ray	16	140	192	16	280	
UV	24	72	≗	24	144	
Total						
X-ray	256	332	288	256	304	
UV	288	312	216	288	216	
	Developed		Undeveloped			
	Supply		Supply		Demand	
X-ray	588		288		560 <sup>°</sup>	
UV	600		216		504 <sup>°</sup>	

TABLE 1 Supply and Demand for Synchrotron Radiation (units are average users, as defined in the text)

 $\overline{a}$  Any number of the ports listed as  $x$ -ray ports could be developed as UV ports.

 $\Delta$  The projected number of NSLS general users is discussed in the text.

 $C$  Does not include NSLS general users.

Copyright © National Academy of Sciences. All rights reserved.

calcium and potassium. The former is of great interest in studies of oxidation of metals and semiconductors, as well as in far more complex processes, and the latter three are of biochemical interest, thus increasing the diversity of the user community.

#### SIZE OF THE USER COMMUNITY AND COMPARISON WITH 1976 PROJECTION

In this section, the user demand is compared with the predictions of the 1976 report. In that report, the number of x-radiation users was predicted to grow from 85 in December 1976 to 675 in 1986, with a corresponding g rowth in exper imental stat ions f rom 7 to about 60. The corresponding growth in UV users and stations was from 120 to 480 and from 16 to about 40, respectively. In the 1976 report, a "user" was defined as an advanced-degree U.S.-based scientist who is directly involved with experiments requiring the use of SR. The report made "the somewhat arbitrary definition that three average users are equal to one full-time equivalent user (FTE) " and that four full-time users would fully utilize an experimental station. For consistent comparison purposes, we have followed these definitions. It was also assumed that stations would have photons available for the equivalent of at least 10-12 hours per day, 6 days per week, as is consistent with operating patterns at existing facilities. We have followed these definitions.

Subsequent to the 1976 report a substantial construction program took place, leading to new capability. Table 1 summarizes the current status. First the user capacity of SR facilities in the United States, which will be available when NSLS and Aladdin are fully functioning, is summarized, using the same algorithm as in the 1976 study, i.e., 12 average users are assumed to utilize an experimental station. Furthermore we have categorized the available capacity in terms of beam lines already constructed for use by PRTs, beam lines available for general users, and ports available but not yet developed .

In determining the current demand for the existing capability we assume that the PRTs will use their time allocations completely. The general users constitute those people who have currently active proposals. In addition, the anticipated decrease in demand on SSRL,

SRC, and CHESS was taken into account in these projections. It was, however, only partially added back into the NSLS numbers through the PRT figures. Because that facility is not at present available to general users, hard numbers for general users are not obtainable. A recent NSLS survey specifically designed to assess general user demand indicates approx imately 1,000 people interested in using the facility, 70 percent of whom have not previously used SR.

A few general conclusions can be drawn from Table 1. First and foremost is that, even without the group indicated in the NSLS survey, there is close correspondence between the existing demand and the supply that will be realized when NSLS and Aladdin reach normal operation. We also note that the UV user demand, 480, that was predicted to exist in 1986 already has been realized in 1982 and that this is almost the case for the x-ray demand. It is also clear that, as predicted in 1976, there is greater demand for  $x$ -ray capability than for UV. Namely, the x-ray demand is 560 , almost equal to the developed supply, 588, and the UV demand is  $504$ , while the supply is 600.

The remaining question is how rapidly the undeveloped port capacity will be required. To this end, we note that there has been a long-term average yearly growth rate of just over 20 percent in identifiable users and 30 percent in annual publications (see Figures 1 and 2). Assuming that this user growth rate continues, demand will approximately equal total supply by 1985. Such growth may not occur as a result of limited funding of users by funding agencies, either through budget constraints or the normal proposal refereeing process .

In summary, these numbers indicate that the 1976 report contains a marked underestimate of the demand for SR capabilities. In fact, the projections of 1976 were explicitly labeled "Minimum Predicted Growth." In addition, however, there have been a number of significant scientific and source developments (see Chapter 4), which were unforeseen in 1976 and which have tended to increase the demand for SR facilities .

#### 3. OVERSEAS SYNCHROTRON RADIATION FACILITIES-STATUS AND PROJECTIONS

Since 1976 several storage-ring facilities have been designed as sources of synchrotron radiation (SR) in a number of countries. Existing facilities have been expanded at other sites. The newly designed and constructed facilities are SRS at Daresbury, England, BESSY in West Berlin, and the Photon Factory, in Tsukuba, Japan. These are described in more detail below. In addition, the European Science Foundation has proposed a very large European SR facility, also described later. Expansions of SR facilities at LURE, Orsay, France, at HASYLAB, Hamburg, and at ADONE, Frascati, Italy, have taken place. Several small storage rings have been built in Japan, all for a limited number of SR users. In the Soviet Union, VEPP-2M is largely dedicated to SR g eneration, and VEPP-3 is so dedicated 6 weeks per year . In addition, a new storage ring for SR research is under construction at the Kurchatov Institute in Moscow.

LURE ( Laboratoire pour !'Utilisat ion du Rayonnement Electromagnetique émis par l'Anneau de Collisions d'Orsay) is a laboratory for the use of SR from the 540-MeV s torage r ing ACO ( used in a dedicated mode but not designed as a source of SR), from the 1.8-GeV storage ring DCI (used parasitically) and from the super-ACO, and 800-MeV ring designed specifically for SR, now under construct ion . In addition, if the proposed European SR facility is not to be built, France probably will opt to build her own dedicated x-ray source. ACO has 8 experimental stations, to increase to 10 by the end of 1982, and DCI has 14. Use of these facilities is saturated, and the demand is continuing to grow at about 20 percent per year. Super ACO, with 6 to 7 undulators, should alleviate the user pressure, since up to 30 new experimental stations will be available. There are over

15

350 users, working on a large variety of research programs .

SRS (Synchrotron Radiation Source) Daresbury, England, is the first major purpose-build synchrotron light source to become truly operational as a research device. Its first year of regularly scheduled operation began in March 1981. While the design of the ring results in a rather larger electron-beam cross section than those expected of the machines currently being commissioned, it now has reached its design object ive of 380 mA at 2 GeV , and thus it is now the most powerful dedicated SR source in the world. A high-field superconducting wiggler has recently been commissioned, and the spectral capabilities of this device when the ring is operating at full current and energy are impressive. There are at present nine experimental stations in operation. Nine more stations are expected to come on line during the 1982-1983 period. A total of more than 450 investigators are expecting access to these stations as soon as scheduling and/or completion permits. Single-bunch operation for time-resolved studies is now being developed and is expected to become a normal operating procedure shortly. Future developments include an increase in beam current at full energy, multipole wigglers, and a modified magnet lattice. These will give this machine capabilities quite comparable with its more modern contemporar ies . Over 15 0 FTE users will be involved in this operation.

BESSY (Berliner Synchrotronstrahlungslabor) is an 8 00-MeV storage r ing designed as a source of SR. It is now operating for users but not yet at full current and beam lifetime. There are 21 ports not yet all in use. A unique feature of BESSY is that German industry is involved in the organization and operation of the facility. One quadrant of the ring is devoted to UV and soft X-ray lithography by groups from the West German electronics industry. Two of the 10 possible beam lines in this section are being constructed, separated from the rest of the ring by clean-room walls. In all, 20,000  $ft<sup>2</sup>$  of clean space are available for exposure and processing of photoresists. Another section of the ring is available for use of the PTB (Physikalisch-Technische Bundesanstalt) for cal ibrations and for standards and instrumentation development. The remainder of the ring is for the general scientific user community. There are 11 experimental stations now in operation for experiments in surface and interface science, atomic and molecular spectroscopy, and x-ray microscopy. The users are partly

local (BESSY and Fritz-Haber Institut) and partly from many institutions from the remainder of West Germany . BESSY has been designed to have extremely short (3 psec ) pulses in the single-bunch mode, but this capability will not be implemented in the near future.

HASYLAB (Hamburger Synchrotronstrahlungslabor) is a laboratory using SR from the 5 . 6-GeV storage r ing DORIS in Hamburg. There is a large experimental hall fed from 5 ports on DORIS . Rad iat ion from 5 eV to 100 keV is provided to 24 experimental stations, most of which are newly instrumented. Many support facilities exist on the site. This laboratory is a continuation of the one that began us ing SR from the synchrotron DESY some 15 year s ago. There is a large user community from West Germany and regular participation by groups from Denmark, Finland, France, Sweden, and Israel. The storage ring is used parasitically, as well as in a mode dedicated to SR. The relative fractions of the two modes has varied over the recent past, as the usefulness of the parasitic beam time.

The Photon Factory at Tsukuba, Japan, became available for experimenters in March 1982. It is a 2.5-GeV storage ring designed as a SR source. Phase I, now in operation, has 4 ports with 11 experimental stations. Phase II, already under way, will add 4 more ports with 10 new stations in an expanded experimental hall. Completion is e xpected by March 1983. Approximately 60 percent of the stations are for x-ray use; the rest are for VUV and soft x-ray users. Future plans include a 1-GeV storage ring and a 400-MeV storage ring, both on the photon factory site, and parasitic use of an 8-GeV ring being built for high-energy physics. There is a large user community in Japan, with a great diversity of research interests. There are two other smaller storage rings in Japan. One for lithography and calibration of standards is in operation, while the other is being built at the National Institute of Molecular Science in Okazaki for its own use.

There are other SR facilities abroad, but these either s erve smaller user communities or are built around older storage rings. There are six experimental stations on the beam line of the 1.55-GeV storage ring ADONE at Frascati, Italy, and six stations on five beam lines at the 400-MeV INSOR storage ring in Tokyo. Both of these storage rings now have insertion devices. The INSOR ring has a very large user community, which has produced 117 publications based on work at INSOR, as of February 1982. There is also a 550-MeV storage ring, MAX, under construction at Lund, Sweden, with 8 bending magnet ports and one wiggler port.

The European Synchrotron Radiation Facility was originally designed in 1977-1979 as a 5-GeV storage ring, but such a machine has not been built. The European Science Foundation is organizing a new study to plan a different facility, based on wigglers and undulators.<sup>2</sup> The site for the facility has not yet been chosen, although several countr ies have made tentative offers of substantial funding if they are chosen to host the facility. The decision to build such a facility appears to be more than a year in the future, since it will depend on the result of the design study. A rough estimate of the cost of this facility is over \$100 million.

#### 4. RESEABCH WITH SYNCHROTRON RADIATION

The report in 1976 outlined a number of areas in which extensive applications of synchrotron radiation (SR) were anticipated. For some of these areas, progress has been faster and more extensive than previously envisioned. A f ew areas have been slow to develop and are still not widely pursued. Several unforeseen applications of SR have already appeared. In the following sections we cover some of the techniques that one can use with SR, g iving a br ief descr iption of each ( more extensive descriptions are found in the 1976 report), an assessment of the applications in light of the 1976 report, and an assessment of future developments. These sections are organized by method rather than by field of application.

#### X-RAY SPECTROSCOPY : EXAFS , SEXAFS , AND XANES

While the power of x-ray absorption spectroscopy was certainly realized in 1976, the breadth and depth of technical and scientific ach ievement was only h inted at in the study of that year. With the conversion of the Stanford Synchrotron Radiation Laboratory (SSRL) from parasitic to semidedicated operation, this field has advanced markedly. The simple act of measuring the transmission of x rays through a sample as a function of energy to determine its absorption spectrum has been transformed in many cases to a complex measurement of the secondary products of absorption: fluorescence (photon), Auger ( electrons) , and photon stimulated desorption (ions), whose spectra resemble the absorption spectrum. These secondary detection techniques have extended the range of absorption spectroscopy to greater dilution ( 1-10 ppm) , the surfaces (1/10 monolayer), and to

19

more-complex materials. The testing of EXAFS itself has been extensive and thorough with a clear understanding result of the strengths and limitations of the techniques.<sup>3</sup> Analysis of the data has been standardized, and results on the same system taken by various groups are in agreement.

The many uses of EXAFS were speculated on in the 1976 report, and even the early results on rubredoxin and Cu-Ru catalysts mainly ind icated the promise of the technique. Sine then, virtually hundreds of systems have been studied, many of which have been important in their respective fields. The following brief description of several significant accomplishments in various disciplines gives a sense of the magnitude of the impact of EXAFS.

Biology has emerged as one of the major beneficiaries from EXAFS. Studies on nitrogenase and its various  $cofactors  $1^4$  on the oxygen-binding proteins, cytochrome$ oxidase and hemoglobin,  $5$  as well as studies of the photosynthesis process, including Mn chloroplasts<sup>6</sup> and Fe reaction centers,  $7$  have significantly contributed to our understanding of the metal coordination in these important systems. Experts in this field look to the future with continued enthusiasm. In fact, EXAFS is probably the most significant advance in structural biology since diffraction, although it is not a substitute for complete single-crystal diffraction analysis.

In catalysis, the other field in which early results were mentioned in the 1976 study, there have also been significant developments but at a slower rate than in biology. The early work on Ru-Cu has been extended to a general study of bimetallic systems, including the  ${\tt commut}$  is a material  $\sim$   $1$  cannot  $\sim$   $1$  and  $\sim$   $\sim$   $3$  The future trend in EXAFS and catalysis is to perform in situ studies of real catalysts under actual operating conditions .

The role of EXAFS in disordered systems like amorphous and glassy materials has been mixed. The in-depth study of the technique itself revealed some difficulties with EXAFS and high structural disorder, which have been shown to limit the applicability of the technique for disordered systems to nearest neighbors with limited local disorder. In spite of this limitation, beautiful work on TiO<sub>2</sub>-doped SiO<sub>2</sub> and Cu-doped As<sub>2</sub>Se<sub>3</sub> has been performed.<sup>9</sup> As will be discussed briefly in the following section, the outlook for EXAFS applications to disordered materials is that by combining it with

21

dif ferential anomalous scattering (DAS) one should be able to have a significant impact on the study of disordered materials.

Within the limited scope of this review one cannot begin to cover the various individual studies in the f ield of solution, ionic conductors, and geology and in general sol id-state problems such as mixed-valence , layered, and impurity systems. Also, the use of EXAFS in more-complex systems such as coal and oil has proven fruitful and will be increasingly important in the future. What one can say is that the breadth of EXAFS u tilization has certainly been beyond that expected in 1976.

The development of surface-extended x-ray absorption spectroscopy (SEXAFS) has been a major accomplishment since 1976. Merely hinted at in the 1976 study, it has blossomed into a field of its own. The early workers have shown that by use of electron detection (Auger or total yield), or ion detection, one can make the EXAFS technique have the requisite submonolayer sensitivity and also be completely compatible with ultra-high-vacuum conditions. $^{10}$  Until now, this technique has been extensively practiced by only a limited number of groups, but many groups at the new facilities are planning to have SEXAFS capability. It is hard to imagine this t echnique not being a permanent part of any substantial surface-sc ience program where structural characterization is important.

The technique of x-ray absorption near edge structure (XANES) was essentially nonexistent in 1976 but has grown into a subfield of EXAFS since then. The basic idea is that the transitions to the low-lying unoccupied states gives one information on those states and thus on the local bonding. Edge structure has been used in several studies, together with model compounds, to ascertain the oxidation state and local geometry of a site. Also, cor relat ions of edge features with d character and catalytic activity have been successfully made. A major h indrance to the successful utilization of XANES has been the difficulty of theoretical interpretation. Recent progress in the theory looks promising  $11$  and suggests that in the future XANES will provide local chemical and structural information not obtainable by other<br>-----------------spectroscopies .

In summary, it is fair to characterize the field of absorption spectroscopy as having more than fulfilled the promise seen in 1976. It is currently a vital technique

be ing appl ied to an extremely broad range of problems . The use of EXAFS in situ for a whole range of biological and chemical processes will be greatly expanded. The general future outlook is for continued growth in the number of practitioners as well as the range of problem s impacted .

#### X-RAY SCATTERING AND DIFFRACTION

At the time of the 1976 study there was only a limited demonstration of the possibilities for scatter ing with SR, through studies of anomalous scatter ing effects from single crystals of rubredoxin and dynamic small-angle scattering from muscle contraction, as well as limited inelastic scattering studies. Since that time there have been many developments, and while the view of the future is extremely positive, the growth is expected in ways not antic ipated in 1976. Before descr ibing those developments it should be pointed out that the delayed development of SR scattering is due to several factors, including the experimental complexity, the need for higher intensity than required by EXAFS to make real breakthroughs, and the need for source stability. The development of improved facilities at SSRL has resulted in all three of these points being addressed successfully, and it is expected that a vigorous and expanding scattering community is being developed to the extent that the new x-ray facilities will have about equal numbers of scatter ing and EXAFS exper iments .

In 1976, anomalous scattering studies, which are intended to solve the phase problem, were presented as having the largest potential impact on crystallographic studies conducted with SR. While anomalous scattering data have been collected on gramicidin and parvalbumin, the current outlook is for a much more restricted impact. The reason for this is both the difficulty of interpretation and the availability of other approaches, most importantly the use of isomorphous der ivatives . However, the more restricted outlook, expressed in 1976, of limited applicability (i.e., small crystals with few derivatives) for anomalous scattering has been replaced by an enthusiastic outlook for the general utilization of SR for protein crystallography owing to increased br ightness . Increased br ightness has been shown to allow one to get more data before a sample dies from radiation (i.e., rate can be important as well as dose). In

addition, smaller samples can be measured at higher re solution in a shorter time. All this has recently created a rebirth in macromolecular crystallography with SR. The observation of increased dosage before degeneration, if that dose is at a high rate, is probably the s ingle most important development in attracting the interest of crystallographers. Once involved, they have discovered, e.g., that in three days they can accumulate data on deoxyhemoglobin with 30 percent better resolution than in the original study, which took months to perform.<sup>12</sup> Also it has been found that, with SR, crystals of about 25 t imes smaller volume can be used than would be needed to get comparable data with a conventional source. Further reductions in crystal size will be feasible with new sources. All these developments portend increased use of SR for regular protein c rystallography.

As important as these developments are, they are further enhanced by the development of surface c rystallography. Conventional x-ray sources are not intense enough to allow the study of the crystallography of the two-dimensional structure on the surface of a material. Previously, one depended on low-energy electron diffraction (LEED), which has all the well-known diff iculties of interpretation because of multiple scattering. With the use of the wiggler beam lines at SSRL, not only has surface Bragg crystallography been demonstrated, <sup>13</sup> but the count rate is large enough that one can expect the method to be generally applicable to a wide range of surface and interface structural studies. Several groups are already planning to perform similar experiments. One can speculate confidently that this technique, regular Bragg diffraction, will be used routinely to characterize structurally the two-dimensional world of surfaces and the solid-solid and liquid-solid interfaces.

While much of the emphasis in the 1976 study was on crystallography, the perspect ive in 1982 is that thermal diffuse scattering in the small- and wide-angle regime will be extremely important in the future. In the 1976 study, the use of SR for such studies was only speculated on with no real accomplishments. Since that time there has been a virtual explosion in activity, such that it is probably fair to character ize it as the fastest-growing field. Studies already completed span phase-transition studies of thin liquid-crystal films, 14 adsorbed atoms on graphite,  $15$  and adsorbates on single-crystal

surfaces.<sup>16</sup> They also include radial distribution function studies of amorphous and glassy materials. $^{17}$ The technique of differential anomalous scattering (DAS) has been developed successfully, which enables one to use anomalous scattering to interpret radial distributions measured in binary and ternary disordered materials. As mentioned previously, this appears to be more useful in many cases than EXAFS for studying disordered mater ials . Finally, small-angle diffuse scattering is providing exciting results in the solution and assembly properties of macromolecular systems.<sup>18</sup> The results to date span the range of the study of solution properties of heavy oils to biological systems. These studies, as in the case of EXAFS, are beginning to be performed under conditions of temperature and pressure in which real processes are carr ied out .

An important component in following real processes is the observation of their time dependence. The intensity provided by SR is beginning to make this possible. Several experiments have been completed, in addition to the preliminary results on the time-dependent scattering from muscle reported in 1976. In a recent experiment at CHESS the structural changes during the laser annealing of a silicon surface were observed with a time resolution of 10 nsec, <sup>19</sup> permitting comparison with theoretical models for laser annealing. Such measurements require the time structure available with single-bunch operation of a storage ring. The time dependence of spinodal decomposition has been followed similarly at SSRL. New detector developments should make many more timedependent studies possible. Recent activity suggests that the in-situ small-angle-scattering studies of solutions and porous materials are likely to incorporate time-dependent studies in the future.

The field of scattering is in the midst of a rapid expansion. The short-term future is extremely bright, with the initial experiments described in this section creating many opportunities for scatter ing that were not envisaged in 1976. These opportunities have many of the features that character ized the EXAFS era of SR. Namely, x-r ay scatter ing is becoming i ncreasingly important to many disciplines, both scientifically and technologically. The information provided is in many cases unique, not available by other techniques, and utilizes the unique properties of SR. If this promise is fulfilled, then even the significant SR resources that we possess today will not be adequate to address effectively the

scientific and technological opportunities. Considerable advances in the development of ultra-high-resolution x-ray monochromators have taken place, and millivolt (meV) resolution has been achieved. These backscattering Bragg reflection devices permit the study of low-level collective excitations an phonons in crystalline solids, but intensities greater than those available from bending magnets will be needed. Undulators presumably will meet this need .

#### PHOTOEMI SSION

The 1970s witnessed two major advances in the technique of photoemission: (1) exploitation of the polarized SR continuum and (2) introduction of angle-resolved photoelectron spectroscopy (ARPES). Initially these developments proceeded independently. At the time of the 1976 report they had just recently been combined, and the future promise was clearly evident. We now have a versatile spectroscopy with which we can measure not only the energies, E, of photoemitted electrons but also their momenta,  $\vec{k}$ , and this can be done over a continuous range of photon energies. The photon polarization has been exploited to determine level symmetries and molecular orientations. In the lower end of the UV range,  $\hbar\omega$  < 50 eV, emphasis is on investigation of valence electronic states; in the intermediate range, 50-800 eV, attention turns more to studies of core levels, including chemical shifts, resonant photoemission, photoelectron diffraction, and near-edge structures; in the x-ray range, SR-based photoemission assumes the name SEXAFS.

In choosing examples from among the large number of experiments done in the last five years, we shall focus on nickel. The work done on this metal is particularly rich since it makes contact with a number of important topics in condensed-matter physics: band theory, ferromagnetism, and many-body satellites and resonances. Nickel is also a favored substrate in surface adsorption exper iments .

The band structure of Ni, i.e., its  $E(\vec{k})$  dispersion, has now been determined with considerable precision. $^{\mathbf{20}}$ Since E and  $\vec{k}$  are experimental variables, it is possible to tune in on any desired point in  $\vec{k}$ -space. The continuum nature of SR permits one to i solate unambiguously optical transitions at critical points. This has eliminated the guesswork associated with the more traditional techniques

of optical absorption. A principal discovery is that the width of the d band in Ni is considerably smaller (by about 25 percent) than predicted in the best theoretical band calculations. Likewise, the ferromagnetic exchange splitting, which can be resolved in the vicinity of the Fermi level, is found to be less than 50 percent of the theoretical values. The temperature dependence of the exchange splitting has been followed through the Curie temperature. Work of this kind goes to the heart of the phenomenon of ferromagnetism and has renewed theoret ical activity and controversy on this long-standing problem. (Indeed this is a good example of how an increasingly substantial number of theoreticians, not generally counted as "users," are looking to SR spectroscopists for inspiration and for verification of their ideas.) The prevail ing view on Ni is that the discrepanies in d-band width and exchange splitting arise through the need for a many-body correction owing to hole-hole correlation.<sup>21</sup> They can be linked theoretically to the "6-eV satellite" (or two-d-hole shake-up peak) seen just below the valence band. Much excitement was generated in 1977 when a group at LURE took photoemission data on passing through the Ni 3p core-level edge (67 eV) and discovered a resonance when the 6-eV satellite comes into energy coincidence with an Auger peak that leaves the Ni atom in the same two-d-hole configuration.<sup>22</sup> This observation has spawned an unanticipated subsidiary school of study called "resonant photoemission." The two-holecorrelation picture in Ni has recently received further support from work by a German group working at LURE, which has accomplished the formidable feat of measuring not only E and  $\vec{k}$  but also the photelectron spin.<sup>23</sup>

While photoemission is the technique par excellence for electronic structure determination, it has also enjoyed use in the determination of atomic structure, specifically of surfaces and adsorbates. The 1976 report made mention of the then-recent ARPES work, which used polarization selection rules in the valence region to determine the orientation and polarity of the molecular axis of CO adsborbed on Ni. (CO stands up on a Ni surface, with its C end down.) Since then, three new photoemission structural tools have been been developed that focus on core-level rather than valence-level emission: photoelectron diffraction, surface-extendedx-ray-absorption fine structure, and x-ray absorption near-edge structure. (The latter two are treated in a preceding section.) Photoelectron diffraction is

e xper imentally the most sophisticated and can be thought of as an angle-resolved version of SEXAFS in which one detects core photelectrons emitted in specific directions and monitors directly the effects of interference between the outgoing electron wave and the waves scattered from neighboring atoms. Photoelectron diffraction has been applied successfully to a number of systems. Perhaps most impressive is recent work done on CO on Ni, since this was carr ied out in the extremely difficult experimental range above the C K-edge.<sup>24</sup> Analysis of t he data is more cumbersome than in SEXAFS since it requires a full-blown multiple-scattering calculation . An important discovery, however, is that the problem is piecewise separable. Because of the dominance of backscatter ing , the C ls photoelectron diffraction is sensitive primarily to the C-Ni distance, whereas the O ls photoelectron diffraction is sensitive to the c-o distance.

Other outstanding achievements in SR-based photoemission over the last five years include determination of  $E(\vec{k})$  dispersion relations for surface states and adsorbate levels, observation of surface-atom core-level c hemical shifts , core-level monitor ing of the formation of semiconductor interfaces , studies of laser annealing and molecular-beam epitaxy, and photon-stimulated desorption of ions and their subsequent fluorescence.

Even with present capabilities we foresee a strong continuing role for SR-based photoemission studies. Of special technological importance will be more extensive investigations of various semiconductor interfaces. Such studies are under way already and include work on semiconductor-metal interfaces, i.e., Schottky-barrier formation, semiconductor-insulator interfaces relevant to metal-oxide-semiconductor (MOS) devices; semiconductorsemiconductor interfaces, i.e., heterojunctions; and new materials produced by molecular beam epitaxy. This field will profit greatly from the forthcoming new highintensity, high-resolution monochromators for the region above the carbon K-edge. This will enlarge the range of elements available for study, as well as increase the precision with which local surface chemistry can be infer red through core-level chemical shfts .

There will also be a number of qualitatively different exper iments that will be critically dependent on the performance of the new high-brightness sources. ARPES exper iments with an order-of-magnitude improvement in  $\bar{k}$ -space resolution are quite feasible and could uncover a

new layer of phenomena that probe surfaces on a scale comparable with the much smaller Br illouin zones assoc iated with surface reconstruct ion and charge-density wave formation. Time-resolved photoemission experiments could monitor surface chemical reactions in real time. High-resolution, high-intensity monochromators for the region above the C K-edge promise to extend core-level c hemical-shift spectroscopy. Small illuminated spot size offers the possibility of photoemission with fine spatial resolution .

This record of continuing achievement and advances in condensed-matter photoemission has been paralleled by similar successes in gas-phase photoemission studies of atoms and molecules, both angle-resolved and angleintegrated studies. The richness of the line spectra permits a more detailed study of many-body correlation effects. To quote but one example we mention the study of the various autoionization channels of the Ba+ ion after excitation of the 6s level. $^{25}\,$  The many-body shake-up lines are frequently more intense than the usual "one-electron" 6s line. The work is additionally noteworthy in that it exploited the pulsed nature of SR by utilization of time-of-flight energy analysis of the photelectrons. More-refined time-domain experiments include detection of various particles (photons, photoelectrons, photoions) in coincidence. These have already begun<sup>26</sup> and are expected to be a major activity in the future.

#### X-RAY LITHOGRAPHY, MICROSCOPY, TOPOGRAPHY, AND OTHER X-RAY TECHNIQUES

Soft x-ray lithography has been demonstrated. Structures as small as 70 Å have been produced. Little additional work has been carried out at the current SR sources since these demonstrations, but interest in x-ray lithography has not diminished. One beam line at NSLS is devoted to lithography, as are several on BESSY. It is premature to predict whether soft x rays will be the radiation of choice in future commercial applications of lithography. The German electronics industry has made a limited bet that it will. X-ray lithography is a field not advanced much further than its status in 1976, but it still seems to have a potentially promising future.

The same is true of x-ray microscopy. Lithographic m icroscopy has been demonstrated but not yet widely used. Scanning x-ray microscopes have been demonstrated , a nd a beam l ine at NSLS is devoted to improved microscopy of this type. Imaging microscopy has advanced over the past years in the hands of the Göttingen group, but it is not yet at a state where it is used by anyone other than its developers. Soft x-ray lithography may aid in producing higher-quality zone plates, and smaller source sizes just becoming available will provide additional progress, but at this time, one cannot be sure that there will be widespread applications of x-ray microscopy, and if so, when they may appear .

X-ray topography is an area in which the gains from SR are already spectacular. Not only may data be taken much faster than with conventional sources, the apparatus is far simpler and cheaper. Considerable work has been carried out at the Daresbury synchrotron (now replaced by a storage ring) and at DCI. With video imaging systems, dynamic topography allows stress propagation studies to be carried out in crystals. At the moment, the collection of data with the present sources (not even the new ones) takes far less time than their interpretation.

In the United States significant progress has been made by a number of researchers in the area of dichromography around the iodine edge to perform noninvasive angiography.<sup>27</sup> With the aid of significant technical development and the high intensity provided by SR from wigglers, the angiogram can be taken quickly enough, ~20 msec, so that there is little blurring due to time-dependent changes. Plans are under way to study human subjects .

#### NUCLEAR PHYSICS

Compton scattering of photons from a laser by the oncoming electrons in a storage ring can give a beam of monochromatic gamma rays, tunable by varying the electron energy, laser wavelength, or angle of scattering. The bandpass in an actual exper iment can be far less than that from the monochromatized bremsstrahlung normally used. Such radiation was produced in the late 1960s but not really used. A recent attempt to increase the flux by including a storage r ing (ADONE) straight section inside the laser cavity was successful.  $28$  An 8-W Ar+ laser gave 5 x  $10<sup>4</sup>$  linearly polarized Compton gamma

÷.  $\mathcal{L}$ 

photons per second with a bandpass of a few percent . Their energy was tunable from 5 to 80 MeV, and they were used to measure the asymmetry in neutron photodisintegration.<sup>29</sup>

#### FUTURE RESEARCH PATTERNS

The potential of SR research is sufficiently large and its growth so rapid that we must plan for the future at the same time that we bring the new sources into operation. While it is hard to predict how much longer the current growth rate of about 20 percent per year will continue, it is certain that it will depend on further developments in sources and in scientific investigations. The past has shown that with each increase in intensity, new possibilities with existing exper imental techniques have been created, which, in turn, have opened new opportunities and created new demands. Also, increased intensity has opened up new fields that did not exist previously. An example of the former is the EXAFS technique, which was originally carried out with SR in a transmission mode with x radiation from a bending magnet. It was then limited to concentration ranges of about 1 part in  $10^3$ . The development of focusing elements to collect more radiation from a bending magnet led to the development of fluorescence EXAFS detection and extended the dilution range to 1 part in  $10^4$  to 10<sup>5</sup>, thereby greatly expanding the biological applications of EXAFS. Finally, with the development of wiggler sources, the technique of surface EXAFS (SEXAFS) has become practical and has developed into an important surface-science tool.

A parallel history can be discerned in the VUV range with the development of angle-resolved photoemission spectroscopy (ARPES) . Initially, low intensities permitted only angle-integrated photoemission measurements whose novelty resided in the use of the continuum nature of SR. As more intensity became available it was possible to resolve other experimental variables, namely the three components of the photoe lectron momentum. The ARPES technique now has yielded precision information on the electronic band structures of bulk solids, clean surfaces, and adsorbate systems. Photon polar ization has been fully exploited to determine symmetr ies of electronic states and the or ientations of molecules. Most recently, the UV flux has been

31

sufficient to resolve photelectron spin, an experiment that incurs a  $10^{-4}$  loss in detection efficiency. In the future we envisage ARPES experiments carried out with higher momentum resolution, sufficient to detect a new range of phenomena associated with superlattices and long-r ange order .

An example of the creation of entire new research fields by the availability of higher fluxes is surface scattering. Wigglers were necessary to obtain sufficient intensity to investigate the structure of surfaces and thin layers. This new capability has begun to attract scientists with interests in phase transitions, interfaces, and surfaces. Future improvements in intensity would signif icantly broaden the user community in this area.

This pattern of increased capability with existing techniques should continue into the future. Scattering techniques, in particular, can be expected to exhibit a growth similar to that of EXAFS and ARPES. Each increase in intensity will enable smaller samples to be studied with higher resolution. In that regard, a major new opportunity is the development of very-h igh-energyresolution (1-10 meV) x-ray scattering capacity, which opens up the utilization of SR for the study of phonons . S ignif icant breakthoughs in other areas can be expected with future intensity increases that will result from wiggler and undulator developments. This study is not intended to review these in any depth. The major ones are likely to be time-dependent x-ray and UV studies of reactions, x-ray holography, and x-ray microscopy and microprobe analysis. If successful, these would attract new communities of scientists with interests in biology, chemistry, and the solid-state sciences. These, and other scientific developments, will not only depend on the increased intensity that wigglers and undulators provide but also on other machine and instrumentation parameters. Issues of time structure, brightness, and beam-line optics will affect significantly the scientific possibilities achievable with SR.

Increasing amounts of research will be directed toward topics of technological relevance. The characterization a nd control of semiconductor interfaces will continue to improve our understanding of Schottky barriers, silicon/ silicon-oxide device interfaces, and the entire process of molecular-beam epitaxy mater ial fabrication. Microfabrication of integrted circuits by means of x-ray

 $\mathcal{C}_{\mathcal{A},\mathcal{A},\mathcal{A}}$ 

lithography will receive renewed attention. EXAFS work relevant to the operation of supported catalysts is expected to extend further into studies in real time. Finally, some medical applications, such as noninvasive angiography, should become prevalent.

The scientific possibilities that are confronted successfully, and consequently the new members of the scientific and technological community who will be attracted to SR facilities, will depend strongly on the development of wigglers and undulators.

Unforeseen in 1976 were the order s-of-magnitude increases in SR intensity and brightness, compared with those from bending magnets, which are obtained from insertion devices (wigglers and undulators, see Appendix). These increased brightnesses and intensities already have had a substantial impact in condensed-matter and materials science. They make possible experiments not possible with the radiation from bending magnets. It seems certain that there will be increasing demand for the radiation from these devices. Here we summarize the present status of these devices and discuss research on insertion devices that we believe should be performed.

Two 8-pole, 18-kG wigglers have been in operation routinely and reliably at SSRL for over a year. They have been used as sources of SR in a number of experiments by users. At low energies, the intensity gain is about the expected factor of 8. Because the magnetic fields exceed those in the bending magnets, the wiggler critical energy is increased significantly, g iving hundredfold to thousandfold increases in intensity at photon energies above the critical energies of the bending magnets .

In contrast, the undulator yields a hundredfold to thousandfold increase in brightness at photon energies that are generally less than the normal bending-magnet cr itical energy. Based on the rel iable operation and utilization of an undulator with its first-order peak near 1 keV, there is no doubt that these devices can be used to produce extremely bright radiation in the soft x-ray and VUV spectral reg ions .

During the past year it has become apparent that characteristics of these devices and their radiation may influence strongly the design of future storage rings for SR. It is imperative that an increased understanding of them and of their interaction with the storage rings in which they are embedded be obtained. It has been proposed that relatively low-energy storage r ings with

33

very low emittances may be used to obtain high photon e nerg ies with permanent-magnet undulators having extremely small gaps and correspondingly short undulator wavelengths. If these are realizable, substantial cost savings could be achieved in a new generation of storage r ings, because they could operate at relatively low electron energies. There are, however, two problems that s hould be investigated to determine whether such utilization of these rings can be realized in practice. First, there is concern that the presence of several such insertion devices will increase the emittance of the ring to such an extent that the small-gap insertion devices cannot be utilized. The other problem is that the minimum gap may not be determined by the emittance, which represents the phase-space spread of the majority of the e lectrons. Instead, it may be limited by the spread of the small numbers of electrons in the tails of the d istr ibution in phase space . Both factors would increase the minimum gap and, therefore, the highest photon energy achievable. These limitations might lead to the need for higher-energy storage rings in order to cover the x-ray spectrum with undulators.

Similarly there is concern that it will not be possible to achieve another order-of-magnitude increase in x-ray intensity over that from existing wigglers. The calculated power dens ity in a 54-pole permanent-magnet wiggler, currently under construction, is about 10  $kW/cm<sup>2</sup>$ . The heat-transfer problems associated with such a high power density are barely manageable. They must be overcome if still higher intensity gains are to be obtained through wigglers.

Thus the two least expensive approaches to achieving one to two orders-of-magnitude gains in intensity or brightness at x-ray energies, multipole wigglers and small-gap undulators, have significant uncertainties associated with them that should be resolved. With the recognition of these problems comes the realization that there may be other problems with the utilization of many insertion devices on storage rings. These known and unknown problems are most likely to be resolved by aggressive insertion device programs in the near future on existing storage r ings.

 $\sim 10$ 

#### APPENDIX: INSERtiON DEVICES

#### H. Winick, SSRL

An insertion device is a periodic array of dipole magnets or a bifilar-wound solenoid placed in a straight section of a storage ring.<sup>30-35</sup> The magnets may be conventional electromagnets , superconducting magnets , or permanent magnets , and they may be located inside the electron-beam vacuum tank or outside it. For illustrative purposes, we consider an array of 2N electromagnets of alternating polarity, forming N periods of a spatially periodic magnetic field. The spatial period is  $\lambda_{\mathbf{u}}$ , and the peak field is  $B_0$ . The spatially alternating magnetic f ield causes an electron of energy E to oscillate about its original (straight) path, but with no net deflection or displacement on exciting the device. To distinguish between wigglers and undulators, the parameter  $K =$  $0.934B_0$  (kG)  $\lambda_{11}$  (cm) is very useful. When the magnetic field is sinusoidal,  $K = \gamma \delta$ , where  $\gamma =$  $E/$  (m $_{0}$ c $^{2}$ ) and 2 $\delta$  is the full angular excursion of the electron beam traversing the magnet.

For  $K \leq 1$  the device is called an undulator. The angular excursion of the electron beam is less than, or comparable with, the natural opening angle of synchrotron radiation (SR) emission  $(-\gamma^{-1})$  and hence the radiation emerging from the device is concentrated in the smallest possible opening angle. Thus an undulator produces radiation with very high brightness. For an undulator with a large number of periods, interference effects in the radiation produced at a large number of essentially collinear source points result in a spectrum with quasi-monochromatic peaks at wavelengths given by

$$
\lambda = \frac{\lambda_{\rm u}}{2\pi\gamma^2} \quad 1 + \frac{\kappa^2}{2} + \gamma^2 \theta^2, \tag{1}
$$

34

where  $\theta$  is the angle of observation relative to the average electron direction and n is the harmonic number . For  $K \leq 1$ , only the fundamental peak  $(n = 1)$  is important. For  $K \approx 1$  the power in the fundamental is a maximum and the first few harmonics have appreciable intensity (see Figure 3 for an example). The suppression of radiation at most wavelengths and the concentration of the radiation into one or a few quasi-monochromatic peaks results in radiation of very high spectral brightness.

The spectral width of the peaks is determined by the number of periods in the undulator, the transverse size and divergence of the electron beam, and the angular acceptance of the detector. For an electron beam of negligible size and divergence, and for a detector of very small acceptance , the fractional bandwidth of the peaks is given by  $\Delta \lambda / \lambda_n = 1/(nN)$ , where N is the number of periods. In this case the spectral brightness increases as  $N^2$ . A device with 100 periods could therefore produce a brightness that is 4 order of magnitude greater than that produced by r ing-bending magnets. When beam size and divergence and detector acceptance are taken into account the brightness gain is less than  $\mathbb{N}^2$  but still large.

For  $K > 1$  the wavelength of the fundamental becomes longer [see Eq. (1)] and more harmonics appear. For K >> 1 the fundamental has a very long wavelength and there are many closely spaced harmonics. In this limit the device is called a wiggler, and the envelope of the spectrum approaches the familiar continuous SR spectrum characteristic of bending magnets. However, interference effects are still present in devices with  $K > > 1$ , especially at long wavelengths and in devices with many periods. At the shorter wavelengths, where these devices are used more frequently, interference effects, although still present, produce only very small variations about the normal continuous spectrum. For devices with  $K \geq 1$ the spectrum can be characterized by the critical energy calculated in the usual way [i.e.,  $\varepsilon_c$  (keV) = 0.0665B (kG)  $E^2$  (GeV<sup>2</sup>)]. The intensity is enhanced owning to the superposition of radiation from individual poles. Depending on the design of the wiggler and the emittance of the electron beam, this enhancement factor can be as large as the number of poles in the wiggler. The beam-line optics and the details of the spectral-angular distribution from an extended source must be considered in calculating the actual intensity delivered to an exper imental station.

 $\gamma$ 



<sup>F</sup> IGURE 3 Calculated photo spectrum for a permanent-magnet undulator at SSRL for three different undulator magnetic-fields (gap widths). As the magnetic field increases, the peak of the fundamental shifts to lower energy, and the harmonics increase in intensity. The electron kinetic energy in the beam is 3 GeV.

Copyright © National Academy of Sciences. All rights reserved.

w G\

Devices with 1.5  $\tilde{\zeta}$  K  $\tilde{\zeta}$  5 represent a transition reg ion between wigglers and undulators. These are also being considered as radiation sources.<sup>36</sup>

High-f ield wigglers offer extended spectral range compared with ring-bending magnets. Extension of the spectral range can be achieved with a very simple 3-pole wiggler producing only one oscillation of the electron beam. Additional poles producing additional oscillations would provide higher intensity. As an example, consider an 800-MeV ring with typical bending-magnet fields of about 12 kG. The SR spectrum has a critical energy of 5 11 eV and a maximum useful photon energy of 2-2.5 keV. A 50-kG superconducting wiggler in the same ring produces a spectrum with a critical energy of 2.13 keV and a max imum useful energy reaching the important 8-10 keV region. Thus, a relatively low-energy ring could provide radiation over an extremely broad spectral range. This means that a single moderate-sized ring can serve as a high-intensity source in both the VUV and x-ray parts of the spectrum.

It may be possible to modify existing rings or build new r ings to permit the use of undulators with smaller gaps than used at present, with correspondingly shorter periods. This would extend undulator high-brightness peaks to energies above 7 keV in existing rings and make it possible for even lower-energy rings (<2 GeV) to reach x-ray energies with such devices.<sup>37</sup> Permanentmagnet undulator technology has developed to the point where a storage ring with permanent-magnet bending magnets, hence low power consumption, may be possible.

Carrying wigglers and undulators one step further by introducing reflectors to create an optical cavity for the radiation results in a free-electron laser. Such devices may be based on either linear accelerators or storage rings and may indeed be built into an existing storage ring. They have been studied by a recent subcommittee<sup>38</sup> and are considered no further in this report.

Insertion devices not only have the capability of changing the character of research at a SR facility, they also offer a different way of thinking about the SR source. In future SR sources, the emphasis may be on insertion devices in the straight sections, with the bending magnets being secondary sources of radiation at best. Several such storage rings have been designed. This report will not address the role of "all-wiggler" machines, but we emphasize that in the near future, panels should consider ser iously their design and mode s of use .

#### **REFERENCES**

- 1. 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. D. J. Thompson, R. Colsson, J. LeDuff, F. Dupont, M. Erickson, A. Hoffman, D. Husman, G. Mülhaupt, M. Poole, M. Renard, M. Sommer, V. Suller, S. Tazzari, and F. Wang, IEEE Trans. Nucl. Sci. N5-28, 2153 ( 1981) .
- 3. P. A. Lee, P. H. Citrin, P. Eisenberger, and B. M. Kincaid, Rev. Mod. Phys. 53, 769 (1981).
- 4. S. P. Cramer, K. O. Hodgson, W. O. Gillum, and L. E. Mortenson, J. Am. Chem. Soc. 100, 3398 (1978); S. P. Cramer, W. O. Gillum, K. O. Hodgson, L. E. Mortenson, E. I. Stiefel, J. R. Chisnell, W. J. Brill, and V. K. Shah, J. Am. Chem. Soc. 100, 3814 (1978) .
- 5. L. Powers, B. Chance, Y. Ching, and P. Angiolillo, Biophys. J. 34, 465 (1981).
- 6. J. A. Kirby, A. S. Robertson, J. P. Smith, A. C. Thompson, S. R. Cooper, and M. P. Klein, J. Am. Chem. Soc. 103, 5529 (1981); J. Kirby, D. B. Goodin, T. Wydrzynski, A. S. Robertson, and M. P. Klein, J. Am. Chem. Soc. 103, 5537 (1981).
- 7. P. Eisenberger, M. Y. Okamura, and G. Feher, Biophys. J. 37, 523 (1982).
- 8. J. H. Sinfelt, G. H. Via, and F. W. Lytle, J. Chem. Phys. 76, 2779 (1982); E. Stern, University of Washington, to be published.
- 9. D. R. Sandstrom, F. W. Lytle, P. S. P. Wei, R. B. Greegor, J. Wong, and P. Schultz, J. Non. Cryst. Solids 41, 201 (1980); S. Lademan and A. Bienenstock, Bull. Am. Phys. Soc. 27, 177 (1982).

39

- 10. P. H. Citrin, P. Eisenberger, and R. C. Hewett, Phys. Rev. Lett. 45, 1948 (1980).
- 11. P. J. Durham, J. B. Pendry, and C. H. Hodges, Comput. Phys. Commun. 25, 193 (1981).
- 12. K. O. Hodgson, Stanford University, personal communication.
- 13. P. Eisenberger and W. C. Marra, Phys. Rev. Lett. 46, 1081 ( 1981) .
- 14. R. Pindak, D. E. Moncton, S. C. Davey, and J. W. Goodby, Phys. Rev. Lett. 46, 1135 (1981).
- 15. D. E. Moncton, P. W. Stevens, R. J. Birgenau, P. M. Horn, and G. S. Brown, Phys. Rev. Lett. 46, 1533 (1981); P. A. Heiney, R. J. Birgenau, G. S. Brown, P. M. Horn, D. E. Moncton, and P. W. Stevens, Phys. Rev. Lett. 48, 104 (1982).
- 16. W. C. Marra, P. H. Fuoss, and P. E. Eisenberger, Phys. Rev. Lett. 49, 1169 (1982).
- 17. P. H. Fuoss, P. Eisenberger, W. K. Warburton, and A. Bienenstock, Phys. Rev. Lett. 46, 1537 (1981).
- 18. K. Liang, Xerox Corporation, personal communication.
- 19. B. C. Larson, C. W. White, T. S. Noggle, and D. Mills, Phys. Rev. Lett. 46, 337 (1982).
- 20. F. J. Himpsel, J. A. Knapp, and D. E. Eastman, Phys. Rev. B 19 , 2919 ( 1979) ; E. Eberhardt and E. w. Plummer, Phys. Rev. B 21, 3245 (1980).
- 21. L. c. Davis and L. A. Feldkamp, Solid State Commun . 34, 141 (1980); G. Treglia, F. Ducastelle, and D. Spanjaard, Phys. Rev. B 21, 3729 (1980); A. Liebsch, Phys. Rev. B  $23$ , 5203 (1981).
- 22. C. Guillot, Y. Ballu, J. Paigne, J. Lecante, K. P. Jain, P. Thiry, R. Pinchaux, Y. Petroff, and L. Failicov, Phys. Rev. Lett. 39, 1632 (1977).
- 23. R. Clauberg, W. Gudat, E. Kisker, E. Kuhlman, and G. M. Rothberg, Phys. Rev. Lett. 47, 1314 (1981).
- 24. S. D. Kevan, R. F. Davis, D. M. Rosenblatt, T. G. Tobin, M. G. Mason, D. A. Shirley, C. M. Li, S. Y. Tong, Phys. Rev. Lett. 46, 1629 (1981).
- 25. R. A. Rosenberg, M. C. White, G. Thornton, and D. A. Shirley, Phys. Rev. Lett. 43, 1384 (1979).
- 26. E.-E. Koch and B. Sonntag, Chapter 6 in Synchrotron Radiation, C. Kunz, ed. (Topics in Current Physics, Springer, Berlin, 1978).
- 27. E. R. Hughes, H. D. Zeman, L. E. Campbell, R. Hofstadter, V. Meyer-Berkhart, J. N. Otis, J. Nolfe, J. P. Stone, E. Rubenstein, D. C. Harris, R. S. Kernoff, A. C. Thompson, and G. S. Brown.
- 28. M. P. De Pascale, G. Giordano, G. Matone, P. Picozza, R. Caloi, L. Casano, M. Mattioli, E. Poldi, D. Prosperi, and C. Schaerf, Appl. Opt. 21, 2660  $(1982)$ .
- 29. W. Del Bianco, L. Federici, G. Giordano, G. Matone, G. Pasquariello, P. Picozza, R. Caloi, L. Casano, M. P. De Pascale, L. Ingrasso, M. Mattioli, B. Poldi, C. Schaerf, P. Pelfer, D. Prosperi, S. Frullani, B. Girolami, and H. Jeremie, Phys. Rev. Lett. 47, 1118 (1981) .
- 30. H. Winick, G. Brown, K. Halbach, and J. Harris, Phys. Today, May 1981, p. 50.
- 31. J. Spencer and H. Winick, in Sychrotron Radiation Research, H. Winick and S. Doniach, eds. (Plenum Press, New York, 1980), p. 663.
- 32. Y. Farge, Appl. Opt. 19, 4021 (1980).
- 33. B. M. Kincaid, J. Appl. Phys. 38, 3684 (1977).
- 34. A. Hofmann, Phys. Rep. 64, 253 (1980).
- 35. F. Dikman, Nucl. Instrum. Methods 195, 349 (1982).
- 36. R. Z. Bachrach, I. Lindau, M. H. Hecht, W. E. Spicer, L. E. Swartz, and S. B. M. Hagström, Nucl. Instrum. Methods, to be published.
- 37. G. Brown, P. Eisenberger, and H. Winick, Nucl. Instrum. Methods, to be published.
- 3 8. The Free Electron Laser , report of the Free Electron Laser Subcommittee of the Solid State Sciences Committee (A Resource Paper) , National Academy Press, Washington, D.C., 1982.

l,

 $\hat{\boldsymbol{\theta}}$ 

 $\ddot{\bullet}$ 

 $\ddot{\phantom{1}}$ 

 $\bullet$ 

 $\hat{\mathbf{x}}^{(i)}$ 

 $\lambda_{\rm{max}}$ 

 $\ddot{\phantom{0}}$