Synthesis and Characterization of Advanced Materials

Solid State Sciences Committee, Commission on Physical Sciences, Mathematics, and Resources, National Research Council

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PREFACE

Are the human and material resources allocated to the scientific and technological development of the synthesis and characterization of advanced materials (SACAM) sufficient to meet the needs of the coming decades? This question has been of continuing concern to the Solid State Sciences Committee (SSSC) of the National Research Council over the past several years. Although an appreciable portion of the SSSC's activity during this time has been related to various aspects of SACAM, its concerns in this regard were first brought into focus at a SACAM Workshop held on December 11-13, 1978, in Washington, D.C. A substantial number of solid-state chemists and other scientists from closely related disciplines participated in this workshop, which stimulated considerable subsequent discussion of SACAM throughout the solid-state chemistry community--discussion that continues.

This report is based on the SACAM Workshop and the discussion it engendered; thus it is principally an assessment of the status and future directions of SACAM from the perspective of solid-state chemists and of other scientists who interact closely with solid-state chemists. In a very real sense, this report has grown beyond the bounds of the original SACAM Workshop; a major portion of it, notably Part I, the SACAM Summary Report, has been written in its final form during 1983, and the entire report has been reviewed and updated as appropriate. Accordingly, we believe that this report presents an accurate picture of the current status of SACAM.

The SACAM Workshop was sponsored by the SSSC and was planned in consultation with representatives of the Solid State Chemistry Subdivision of the American Chemical

Society (ACS). Advice on subjects to be included in the workshop was sought from representatives of the funding agencies and from senior researchers and managers in materials preparation and characterization. The purpose of the workshop was to provide an evaluation of the achievements, strengths, future directions, and needs of solid-state materials synthesis and characterization in the United States on the basis of the views of practitioners in the field. The participants were drawn principally from the solid-state community, with emphasis on solid-state chemists and other scientists who have collaborated with solid-state chemists. Every effort was made to assure the widest possible participation in the workshop by members of this community.

The SACAM Workshop opened with four introductory talks:

1. N. B. Hannay, Bell Laboratories, "SACAM: A Technological View"
2. J. R. Goodenough, Oxford University, "SACAM: A View from Another Country"
3. D. A. Shirley, University of California, Berkeley, "SACAM: An Academic View"
4. D. K. Stevens, U.S. Department of Energy, "SACAM: The Government Agency"

Section V of Appendix A contains some of the highlights of these talks.

Five panels then convened to evaluate various aspects of SACAM. The panel topics were

1. Problems Related to the Character of SACAM Research
2. Scientific Challenges Arising from Technological Needs
3. Interdependence of Synthesis and Characterization
4. Training and Orientation of Personnel for the Advanced Materials Field
5. Instrumentation and Facilities

Scientific and Technological leaders from industry, universities, and the federal government, covering a broad range of geographical locations and scientific interests, served on these panels. Panel chairmen and members are listed in Section II of Appendix A. A number of additional people who attended and participated in the deliberations are listed in Section IV of Appendix A.

Each panel met for three half-day sessions and then presented a report on its deliberations to all the workshop participants.

Following the SACAM Workshop, each panel prepared a first draft of its report and circulated it among the workshop participants and the solid-state chemistry community. The ensuing discussions were both extensive and substantive and led to considerable revisions of the panel reports. The five panel reports constitute Part II of this document.

The Report Committee (See Section III of Appendix A) abstracted and summarized the five panel reports to provide an initial draft of a summary of the workshop. This initial draft was then also circulated among the workshop participants and the solid-state chemistry community. The consequent discussions were again extensive and substantive and resulted in revision and expansion of the summary to encompass a greater variety of concerns than had been addressed by the SACAM Workshop. Therefore, the SACAM Summary Report (Part I), presents the conclusions and recommendations of the Workshop and of the discussion it engendered, as well as the accomplishments, strengths, resources, and opportunities of SACAM.

As this report goes to press, four recent developments indicate growing awareness of some of the needs it discusses and of the attempts being made to deal with them: (a) there have been numerous symposia on solid-state chemistry at recent ACS meetings; (b) the first and second Gordon Research Conferences on Solid State Chemistry were held in the summers of 1980 and 1982, and a Gordon Research Conference on the Physics and Chemistry of Solids was held in the summer of 1981; (c) the August 1980 issue of the Journal of Chemical Education contained 14 papers from a symposium, Solid State Chemistry in the Undergraduate Curriculum; and (d) the Department of Defense (DOD) has announced a 5-year, $150 million DOD-University Research Instrumentation Program. Further discussion of these recent developments appears in Chapter 2 of Part I, Section VI of the Panel 4 report, and Sections III and IV of the Panel 5 report.

We wish to emphasize that this report is the result of the deliberations and efforts of a large number of people and, as such, undoubtedly does not fully represent the views of any individual participant. Moreover, it is intended primarily for informational purposes.

We thank the SSSC for its sponsorship. We are also grateful to W. F. Brinkman, Martin Blume, E. Burstein, D. E. Eastman, and R. M. Thomson for advice before and during the writing of this report and to the panel chairmen, H. F. Franzen, N. Bartlett, G. A. Somorjai, R. A. Laudise, and L. Eyring, and the panelists and other participants in the SACAM Workshop.

Murray Robbins, Chairman
Steering Committee for SACAM Workshop

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PART I. SACAM SUMMARY REPORT

1. INTRODUCTION

Scientific and technological efforts in the synthesis and characterization of advanced materials (SACAM) are carried out by an interdisciplinary community whose contributions have been at the heart of progress in materials science and technology and whose future achievements will be central to the accomplishment of many technological goals. This community includes researchers in solid-state physics; metallurgy; ceramics; materials science; geoscience; electrical engineering; and inorganic, physical, organic, and solid-state chemistry. Only recently has awareness of group identity begun to develop within this community.

Synthesis, as used in modern solid-state science, includes not only the preparation of novel and well-characterized materials but also the precise control of microstructure and extrinsic properties. Characterization is the measurement of chemical and physical properties of materials, with the goal of achieving understanding of the same and similar materials based on their chemical bonding, atomic structure, and microscopic and macroscopic perfection. Characterization also provides a basis for specifying and improving materials for particular applications. By the term "advanced materials" we mean those materials that are at the forefront of science or technology at the time they are being studied. That is, advanced materials are those with novel properties that command interest from a variety of scientific and technological communities. Such materials now include the A-15, Chevrel phase, and ternary compound superconductors; bimetallic cluster catalysts; intercalation compounds; silicon, gallium arsenide, TTF-TCNQ, and other quasi-one-dimensional materials; and metallic glasses.

The development of SACAM has differed significantly from that of most other areas of physical science. In these other areas, the majority of important advances in basic research have been made in universities, whereas for SACAM, industry and the national laboratories have been the sources of many of the important basic advances. This difference results from the interdisciplinary nature of SACAM, which calls for substantial research interaction among scientists working in materials preparation, characterization, and theory. Such interaction has been more readily achieved in industrial and national laboratories than in university laboratories. Though collaborative, interdisciplinary research is developing in universities, industry and the national laboratories will undoubtedly continue to play a major role in this field.

SACAM has been essential to the electronics revolution. The basic techniques for making Si and III-V compounds, for example, zone refining, float-zone crystal growth, crystal pulling, and liquid-phase epitaxy, have provided the materials foundation for transistors, solid-state lasers, light-emitting diodes (LEDs), and magnetic bubbles. SACAM has also contributed substantially to advances in a wide variety of technologies, including luminescent materials (the basic building blocks of the lamp industry), "super" ceramics (Lucolox and Pyroceram being noteworthy examples), materials for superconducting wire (which is used in making superconducting magnets and eventually, perhaps, motors, generators, and transmission lines), and families of heterogeneous catalysts essential for the modern conversion of petroleum feed stocks to fuels, petrochemicals, and polymeric materials.

Current problems associated with advanced communications, data processing, process control, energy production and storage, automation, catalysis, environmental improvement, and materials conservation and substitution, among others, comprise a set of challenges for the preparation and characterization of sophisticated new materials. In many cases, progress in these areas will be paced by the timely availability of well-characterized advanced materials.

In addition to these "need-driven" challenges, an equally compelling group of "opportunity-driven" challenges can be identified. Scientific progress in understanding real surfaces, the connection between chemical bonding and structure and useful properties of solids (for the design of new materials), the nature of the amorphous state, and the control and optimization of the properties and effects of grain boundaries are all dependent on highly sophisticated materials preparation and characterization and theoretical understanding.

The urgent need of society for the new and improved technologies that could be based on advanced materials, and the scientific opportunities that well-characterized advanced materials would offer, clearly indicate the desirability of an increase in the size and sophistication of the interdisciplinary community dedicated to the preparation and characterization of such materials. The challenges and opportunities associated with SACAM can be met adequately only if significantly greater numbers of scientists with diverse perspectives are trained in the areas relevant to SACAM. This increase will occur only as a broader awareness of the accomplishments, challenges, and opportunities of SACAM develops within the entire scientific community.

In the future, new materials with greater perfection and purity and more stringent characterization requirements will be increasingly needed. The facilities for the preparation and characterization of such materials will necessarily be more complex and expensive than present facilities. Thus, while it is important to attract researchers to SACAM in larger numbers, it is also important that these scientists be provided with adequate resources, especially support personnel and state-of-the-art instrumentation.

As we have already noted, SACAM is intrinsically interdisciplinary in nature, and the kind of collaborative interaction among researchers from diverse but related fields that is required is currently found to a much greater extent in industry than in academia. For the continuing healthy growth of SACAM, university researchers must be encouraged to participate in such interdisciplinary and collaborative research. Concomitantly, university-industry communication and interaction for the purpose of such research must be improved.

In this report emphasis is placed on university-industry relationships. However, it must be recognized that the national laboratories provide an excellent environment for a cross-disciplinary role in condensed-matter science and will become even more important in this area with the establishment of major facilities such as synchrotron light sources, high-intensity neutron sources, and high-voltage electron microscopes. A study of the role of national laboratories in SACAM is being carried out by the Department of Energy.

In the following four chapters we summarize the conclusions and recommendations resulting from the SACAM Workshop and the extensive discussion it engendered (Chapter 2), the scientific and technological accomplishments of SACAM (Chapter 3), the societal needs and future opportunities that SACAM will face (Chapter 4), and human and material resource needs for effective SACAM (Chapter 5).

2. CONCLUSIONS AND RECOMMENDATIONS

I. CONCLUSIONS

Based on the considerations outlined in Chapter 1, we conclude that to facilitate the timely response of the SACAM community to the variety of challenges and opportunities we expect it to encounter, it is necessary to

- Attract potentially able researchers into SACAM and ensure that they receive rigorous, in-depth training in one of the disciplines central to the field. Training should be sufficiently broad to allow them to communicate and interact effectively with collaborators in related disciplines.
- Improve educational opportunities in the disciplines relevant to SACAM, especially solid-state chemistry.
- Encourage interdisciplinary research at the interuniversity and intrauniversity levels and increased industry-university cooperation.
- Establish centers where state-of-the-art materials characterization capability is available to the SACAM community on an ongoing basis.
- Encourage and broaden joint research efforts with other countries, especially in solid-state chemistry and advanced materials, in which other countries have much to offer.

II. RECOMMENDATIONS

Based on the SACAM Workshop Panel Reports (Part II), the extensive discussion that accompanied their preparation, and the resulting conclusions, we developed three categories of recommendations.

The first, self-help, includes steps that the materials research community should take to strengthen SACAM to meet future challenges, opportunities, and needs. The second, institutional measures, deals with university and industry actions that could help to ensure a consistent flow of high-quality research in the basic sciences and technologies relevant to SACAM, improve interdisciplinary and collaborative interactions, and attract and train new generations of solidly grounded, innovative researchers and technologists in SACAM and related fields. The third, funding, suggests some modifications of funding practices that could strengthen selected portions of SACAM research, thus helping to provide a solid base of research, technology, and pedagogy for the challenges of the future.

Self-help. The consensus of the SACAM Workshop participants and the ensuing discussion was that SACAM could be improved through self-help measures that do not require significant new funds or institutional rearrangements. Specifically, for the continued development of SACAM it is necessary to attract highly qualified students in increasing numbers and able researchers in disciplines related to the field. This objective can best be achieved by the concerted actions of the SACAM community. On the basis of the SACAM Workshop Panel Reports and the consequent discussion, we offer the following recommendations for such actions by the SACAM community:

1. Speakers from industry, national laboratories, and academia, representing a variety of research and technology areas within the general field of SACAM, should be made available to universities and colleges for seminars and short courses. A central file of SACAM speakers and topics should be maintained and well publicized.
2. The publication in educational journals of tutorial articles and descriptions of undergraduate laboratory experiments convering the various aspects of SACAM should be strongly encouraged.
3. The publication of texts and monographs for use in introducing the variety of subjects relevant to SACAM should be encouraged.
4. SACAM workshops, short courses, and symposia for researchers in the field and related disciplines should be made available on a regular basis by the appropriate scientific societies.

We note that implementation of some aspects of these recommendations has already begun. There have been numerous symposia on solid-state chemistry at recent American Chemical Society (ACS) meetings. The first and second Gordon Research Conferences on Solid State Chemistry were held in the summers of 1980 and 1982, and a Gordon Research Conference on the Physics and Chemistry of Solids was held in the summer of 1981. In its August 1980 issue, the Journal of Chemical Education published 14 papers from a symposium on Solid State Chemistry in the Undergraduate Curriculum.

Institutional measures. Universities and colleges should be encouraged to initiate, maintain, and improve high-quality research activities in SACAM-related disciplines. It was the view of the participants in the SACAM workshop that solid-state chemistry is particularly in need of such attention. It provides the scientific foundation for synthesis and chemical characterization leading to new materials; however, as a distinct subject of study and research it is represented in only a few universities in the United States. Therefore, we propose the following activities:

1. Invite SACAM scientists to be regular seminar speakers, visiting lecturers, and visiting professors, particularly on joint appointments from industry.
2. Include SACAM topics and laboratory experiments in undergraduate and graduate courses and offer introductory solid-state chemistry as an integral part of the curriculum. Examples of such activities are the laboratories at the University of California, Berkeley, and the Massachusetts Institute of Technology (MIT), where students prepare an integrated circuit starting with a Si chip, and the introductory solid-state chemistry course offered at MIT, which is described in Appendix E.
3. Encourage the addition of scientists in the various disciplines relevant to SACAM to university staffs in tenure track positions.
4. Establish mechanisms to encourage and facilitate the participation of faculty members in collaborative university-university, university-industry, university-national laboratory research projects relevant to SACAM.
5. Introduce students in SACAM to the interdisciplinary nature of the field as early as possible.

Funding. Funding is potentially a powerful instrument for change. The following recommendations are directed principally toward development of interdisciplinary research in the various aspects of SACAM:

1. Funding agencies should encourage the establishment of the new state-of-the-art SACAM thrust areas and centers and the upgrading of existing facilities. This stimulus is desirable because effective research in modern synthesis and characterization generally requires an interdisciplinary program, which in turn requires a critical core of instrumentation, synthesis capabilities, and characterization skills. Funding agencies must carefully monitor the materials research laboratories (MRLs) and regional centers to ensure that their efforts are appropriately focused and that needed interdisciplinary team interactions occur.

2. Proposals for SACAM research are generally interdisciplinary or interinstitutional or both in nature. Such proposals often fall between the cracks in the deliberations preceding funding decisions. The funding agencies should make a conscious effort to prevent this situation and, in fact, should strongly encourage interdisciplinary and interinstitutional research. The National Science Foundation (NSF) Industry/University Cooperative Research Projects program appears to be a useful vehicle for encouraging the academic-industry exchanges so vital to SACAM research.

3. Interaction and cooperation with selected foreign laboratories, especially those conducting research in solid-state chemistry, where local strengths could benefit U.S. activities, should be encouraged by provision of funds for this purpose and by appropriate modifications to institutional arrangements where necessary. The NSF Cooperative Science program seems to be a useful effort of this sort.

4. Funding should be targeted to young faculty members in SACAM. The usual criteria of excellence, originality, and career potential would be fully appropriate for use in making decisions on support. Sabbatical and exchange support by funding agencies could be particularly important in SACAM, because exciting new basic research is often performed at foreign and industrial institutions.

5. Particular attention should be given to providing adequate support personnel and state-of-the-art instrumentation. The provision of adequate support personnel invariably results in an increase in program productivity

much beyond its cost. State-of-the-art instrumentation frequently also leads to increased program productivity beyond its cost, particularly for lower-priced (below $50,000) and moderately priced ($50,000-$250,000) equipment. Judicious equipment support in these ranges by the funding agencies could result in significant improvements in the quality and quantity of SACAM research, particularly that conducted at universities. In this regard, the DOD-University Research Instrumentation Program is a noteworthy development. This program began in fiscal year 1983 and is budgeted at $30 million per year for 5 years. Approximately 25 percent of this funding is for instrumentation related to advanced materials research.

3. SUMMARY OF SCIENTIFIC AND TECHNOLOGICAL ACCOMPLISHMENTS

We now briefly discuss the accomplishments of SACAM and show that SACAM activities are beginning to change from the past emphasis on electronic materials to a broader effort encompassing materials for advanced communications and automation and development of new materials for energy conversion and conservation.

I. ELECTRONIC MATERIALS

Semiconductor science has been at the heart of modern electronics since the invention of the transistor. The development of the basic preparative techniques for making semiconductors, especially single-crystal Si and III-V compounds, was a landmark achievement of SACAM. This work took place over more than 20 years and included the development of such methods as zone refining, float-zone crystal growth, crystal pulling, and liquid-phase epitaxy. Advanced synthesis and characterization research is still needed to achieve the degree of perfection and crystal size required for very-large-scale integrated-circuit devices, advanced light-emitting diodes (LEDs), solid-state lasers, and magnetic bubbles.

Several activities allied with preparation have played key roles in semiconductor materials advances. Characterization of the chemical purity and electrical properties and careful studies of point and extended defects have been essential for progress at every stage, as have the theoretical description of impurity and dopant partition and the interaction of defects. Thus in semiconductor materials research and development, advances have depended on the interdisciplinary activities of metallurgists, chemists, and solid-state physicists.

Another important SACAM contribution to electronics is the preparation of magnetic materials. The descriptive and structural chemistry of these materials was developed through decades of continuous work. As a result, a reasonably complete picture of the crystal chemistry of single-crystal spinel and garnet structure materials is now available. Indeed, the magnetic interactions have become so well understood that it might be argued that these materials have been the "fruit flies" of magneto-chemistry. These successes depended heavily on the invention and exploitation of single-crystal techniques, such as flux growth, for the preparation of refractory oxides. The capability for producing single crystals made it possible to gain a thorough understanding of intrinsic properties. Controlling microstructure and understanding the connection between magnetic properties and extrinsic structure have also been essential to progress. The present families of important materials include polycrystalline ferrites, which are used in cores and memories, and single-crystal magnetic garnets, which are used in bubble-domain memories.

Luminescent materials play an essential role in modern instrument and appliance displays, TV picture tubes, and fluorescent lighting. (Of course, these materials could be classified as either electronic or optical materials, depending on whether the basic mechanism or the application is of primary concern.) The careful preparation and control of the chemistry of II-VI and $ZnSiO_4$ phosphors and the discovery of the luminescent properties of Eu, which is now used extensively in color TV picture tubes, are examples of the contributions of SACAM to these technologies.

II. OPTICAL MATERIALS

SACAM has made substantial contributions to the development of the optical materials that are widely used in modern technology. Such materials include yttrium aluminum garnet, which is used in solid-state lasers, and a variety of nonlinear optical materials, such as $LiNbO_3$. These are examples of the contributions of synthesis chemists, ceramists, and metallurgists to the preparation of carefully controlled single crystals of high complexity, high reactivity, and high melting points. Another notable contribution is the discovery and perfection of the techniques now used for the routine preparation of optical fibers. These techniques, which are based on rapid, controlled, vapor-phase chemical reactions, permit technologists to make materials with only a few parts per billion of critical, optically absorbing impurities. With such high-purity materials, the optical losses at the wavelengths of interest for optical communications are sufficiently low that repeater spacings can be many kilometers. These techniques also allow the careful control of deliberately added impurities over dimensions of micrometers, so that the index of refraction can be tailored to produce the desired waveguide characteristics. It is clear that glasses for fiber transmission constitute a crucial and challenging opportunity for additional SACAM contributions.

III. CERAMIC MATERIALS

Cost considerations have dictated that, wherever possible, ceramic systems be used in electronics. Accordingly, the ability to control the microstructure of ceramic materials is among the most significant accomplishments of SACAM. Electronic ceramics, such as piezoelectric lead zirconate titanate, doped ZnO and related nonlinear resistance (varistor) materials, and the complex ceramic conductors used in thick-film hybrid integrated circuits are examples of contributions of ceramic science to modern technology where SACAM has been instrumental. We also mention, as an additional example, the processing techniques that have made possible the preparation of ceramics for electronic substrates and autocatalyst bed applications.

IV. HETEROGENEOUS CATALYSIS

The efficient conversion of petroleum into the variety of fuels needed by modern industry and the conversion of petroleum feedstocks to petrochemicals and polymeric materials depend on the availability of highly specific solid catalysts. For example, zeolite catalysts, Ziegler-Natta catalysts, and metal-alloy catalysts are vital in modern technology. All of these catalysts and many more have resulted from extensive synthesis programs. However, only now are fundamental investigations beginning on the effects of composition and structure of catalysts, their characterization, and the understanding of their role in breaking and forming chemical bonds in petroleum-based and other materials. The effort directed toward the cleaning and conversion of coal for energy and chemical applications is barely under way. This program will require the application of the most advanced tools and techniques available to the SACAM community.

V. ELECTROCHEMICAL MATERIALS

The efficient and pollution-free production of elemental chlorine by electrochemical processes is a key part of current industrial chemistry. Thus, the discovery that ruthenium-titanium oxides can replace mercury anodes was of great importance. These new dimensionally stabilized anodes permit higher current efficiencies, thus conserving energy and, at the same time, eliminating mercury pollution.

The development of advanced batteries has progressed considerably during the last decade or so through preparation and characterization research in the solid-state sciences. First, a solid electrolyte, β-alumina, was found to exhibit ionic conductivities at 300°C as high as those of aqueous solutions. Then excellent reversibility was discovered for the layered materials, such as TiS_2, in lithium cells at ambient temperatures. There are now extensive research and development programs based on these findings, and, in addition, lithium-alloy anodes are playing a critical role in the development of molten-salt batteries.

VI. ADVANCED MATERIALS THROUGH CONTROLLED PREPARATIVE TECHNIQUES

The ready availability of high pressures has made it feasible to produce a number of new materials with application to advanced technologies. Two of the most important of these are synthetic quartz and diamond. As a consequence, the United States has become independent of overseas sources of these two materials.

Selective leaching before final consolidation has yielded comparatively inexpensive, thermally shock-resistant families of glasses. Careful control of recrystallization has produced even more remarkable thermal properties in the Pyrocerams. Rapid quenching has opened the glassy state to metals, resulting in new materials with remarkable mechanical strength and unusual magnetic properties. All of these achievements have resulted from controlled synthesis and careful characterization.

Amorphous materials play a role in a number of technologies. One of the best-known examples is selenium for xerography; a second is the use of amorphous silicon for solar cells. The development and exploitation of this material, production of which relies on arc discharge synthesis techniques, is just beginning. The SACAM community can be expected to play a central role in the continuing development of amorphous silicon, as well as other materials, for solar cells.

VII. RESEARCH IMPLICATIONS

In areas as diverse as ferromagnetism, the band structure of semiconductors, superconductivity, defect solids, and layer and chain structures, the observation of unusual properties in a novel material has been the initial stimulus for new theoretical and experimental research, which has opened broad areas of science. Thus advances in materials preparation frequently precede and stimulate theoretical activities and are often the precursors of the effort to establish the scientific bases of new fields. Advances in understanding the connections between useful properties and chemical bonding and crystal structure have been closely coupled to the availability of well-characterized classes of materials that are difficult to synthesize. For example, our understanding of the magnetochemistry and spectroscopy of the magnetic and nonmagnetic garnets required the availability of well-characterized single crystals of scores of garnet compositions. The technological fruits of these scientific acievements included bubble garnet memories and low-threshold optically pumped lasers.

One of the strengths of materials science is the close coupling between research and technology. This relationship is particularly true in SACAM. Thus, many of the specific achievements that we have listed were closely associated with and heavily dependent on basic research and could be discussed again here, with a slight change in viewpoint, as research accomplishments. For example, the accurate characterization of carefully prepared single-crystal semiconductors led to the understanding that holes and electrons obey the law of mass action, which was an important scientific finding and a key step in the advance of semiconductor technology. Another example of an important basic scientific advance, which resulted from semiconductor studies and stimulated technological progress, is the conceptualization of the Frank-Read source, the dislocation mechanism whereby basic crystal growth kinetics can be understood.

4. SOCIETAL NEEDS AND FUTURE OPPORTUNITIES

The examples of achievements presented in the previous chapter are but a prelude to those that SACAM can yield in the future. Advanced materials are increasingly important to the development of new technologies, and the preparation of well-characterized advanced materials is the limiting factor to progress in many critical areas. In addition to these technology-driven opportunities, there are also science-driven opportunities. Frequently, strong basic interest in new materials and techniques for synthesis and characterization leads to advances in understanding the chemical and physical properties of solids.

Here, we discuss some of these technology- and science-driven opportunities.

I. TECHNOLOGY-DRIVEN OPPORTUNITIES

A. Energy

It is increasingly clear that an ever-larger fraction of our resources is going into the production, conversion, storage, and conservation of energy. The survival of our technological society depends on the more efficient use of energy resources and the development of environmentally sound new resources. Some opportunities in energy research and development where advanced materials can be expected to play a key role are the following:

o Heterogeneous Catalysis. In spite of the critical role catalysis plays in many processes, for example, petroleum refining, polymerization, and processes relevant to autocatalysis and fuel cells, little is known about the active sites or species in commercial catalysts. If we are to develop advanced catalysts to handle the feed stocks of the future, which will include dirtier crudes, tar sands, the products of coal liquefaction, and shale, a well-planned, rapidly moving program in catalyst characterization must be undertaken. The methodology for the effective synthesis of new materials must advance concurrently. Catalysts are required to convert carbonaceous residues to useful liquids, crack large molecules, remove sulfur and nitrogen, and convert bad oxygen (e.g., phenol) to good oxygen (e.g., tertiary alcohols, ethers). To be effective, catalysts must be highly selective, so that, for example, hydrogen consumption is minimized and environmentally and economically undesirable byproducts are not formed. Heterogeneous catalysts that will minimize undesirable combustion products, such as NO_x and SO_x, are needed. The efficient production of chemicals, such as ammonia and propylene oxide, also depends on superior catalysts, as does the conversion of coal-gasification products to useful products.

o Electrochemical Material. Electrochemical processes, such as those used in chlorine and aluminum manufacturing, consume large amounts of electrical energy; therefore, more efficient processes should be developed, and some of these (e.g., air cathodes in the chloralkali cells) require new materials. In addition, whole technologies, such as those on which electric vehicles are based, are limited by the lack of suitable batteries, which, in turn, stems from a lack of appropriate electrolyte materials. Much effort has been expended in the last few years on such exotic materials as β-alumina and TiS_2. These and related efforts must be continued if high-power and -energy density batteries are to be developed. The electrochemical synthesis of organic chemicals also requires improvements in the activity and selectivity of electrocatalytic materials.

o Solar Energy. Progress in solar photovoltaic and photothermal devices is critically dependent on SACAM. In particular, the development of low-cost solar cells of sufficiently high efficiency through the perfection of new processing techniques for the active components is crucial to the achievement of a practical and economical photovoltaic power system. Improvements are also needed in inactive construction materials and mirrors to achieve cost reductions and longer lifetime while maintaining or improving system efficiency.

o <u>Hydrogen Utilization and Storage</u>. The use of hydrogen as a fuel depends in part on the development of improved storage media. These must have the attributes of the lanthanum nickel materials ($LaNi_5$) without their weight and cost limitations. Also, to facilitate the routine use of hydrogen as a fuel, containment (piping) materials that are impervious to hydrogen and resistant to embrittlement must be found.

o <u>Materials for Energy Conservation</u>. There are many areas where energy conservation could be achieved through weight reduction and more efficient processes. Vehicle efficiency could be substantially increased if lighter materials meeting present engineering criteria could be developed without significant cost increases. One example is new synthetic routes to graphite-reinforced plastics and a variety of other composites.

Other opportunites in energy conservation, such as improved lamp envelopes and phosphors, also depend on the availability of new advanced materials.

Materials that will withstand high temperatures and hostile environments have many potential applications, particularly in the construction of turbines for use in magnetohydrodynamic, geothermal, and nuclear power generation and ocean thermal energy conversion. Operation at high temperatures can lead to increased thermodynamic efficiency, and operation in hostile environments is a necessary part of these comparatively exotic power-generation technologies. The availability and characterization of materials such as nitrides, carbides, silicides, super alloys, and composites could well determine future advances in these technologies.

B. Electronic Materials for Communications, Data Processing, Control, and Automation

Synthesis and characterization of advanced electronic materials have played and will continue to play a key role in communications, data processing, process control, and automation. Probably the foremost driving force is the continuing increase in the scale of integration of integrated circuits. Less costly dataprocessing and increased processing capabilities will result from putting more circuit functions on a single chip. At present, large-scale integration (LSI) circuits have brought 262-kbit memories close to being standard commercial items. The packing density in silicon integrated circuits has been doubling approximately every 2 years. For this trend to continue, advanced materials will be required, and it is not clear that the materials now used, such as the SiO_2 insulator and photoresist families, will be adequate.

There is a need for insulator materials less subject to pinhole formation, that is, materials that can be made in thinner layers more reproducibly and that have lower imperfect ion densities. Extensive investigation of silicon-nitrogen chemistry might result in the synthesis of such materials. Silicide chemistry and preparative activities in general are ripe for SACAM contributions, which could be the key to a new generation of very-large-scale integration. In the case of photoresists, chemical properties can be controlled by radiation exposure. However, as sizes decrease, the diffraction limit of light will become increasingly restrictive. Accordingly, much SACAM research is directed toward the development of organic polymeric materials with properties that are altered by exposure to light, x rays, and electron beams. The hope is that appropriate resist materials for integrated-circuit features in the micrometer and sub-micrometer regions can be realized from these studies. All of these activities require careful synthesis and characterization; they appear to be essential to future progress in integrated-circuit technology.

The role of SACAM in the development of low-loss and high-bandwidth optical fibers is well known. However, new families of materials might have losses and dispersion orders of magnitude lower than the silicate-based glasses now used for optical fibers. The impact would be substantial if repeater spacings could be much greater than is now possible.

The new need for conservation of and substitution for critical materials increases in electronics and other areas. Shortages and prohibitive costs affect the users of materials as varied as Sn, Co, Hg, and Au. As an example of the contribution SACAM can make, recent alloy research has provided magnetic alloys that use half as much Co while retaining the magnetic properties of alnico.

Other opportunities for SACAM in electronics include high-speed circuit elements, such as Josephson logic junctions, and new display materials, such as liquid crystals, which could provide cheaper interfaces and open a much larger market for optical fibers and large-scale integration. In spite of its remarkable contributions, the impact of electronics on technology is just beginning, as is the impact of SACAM on electronics.

II. SCIENCE-DRIVEN OPPORTUNITIES

In the last two or three decades, much of the progress in the study and application of advanced materials originated in industrial laboratories; examples include semiconductor materials, intercalation compounds, and ionic conductors. In these and other cases, the materials involved were relatively simple solids, and, accordingly, one might have expected academic research to play a larger role. Apparently the amount of university-based research was limited because, in many cases, the opportunities in SACAM research appeared to be technology-driven. The situation now is quite different; of the great variety of opportunities in SACAM research, many are substantially science-driven. Thus the prospects for SACAM research to be recognized as a legitimate and intellectually exciting area of academic research and, concomitantly for high-caliber faculty and students to be attracted to it, are much greater than in the past. What is needed is a broader awareness in the scientific community of the challenges and opportunities of SACAM.

The basic science underlying many areas of interest to SACAM is poorly understood; examples include catalytic activity, diffusion in superionic materials, the band structure of amorphous materials and defect solids, surface and interfacial properties of solids, the properties of very small particles, and the basis of phase stability and bonding in binary and ternary solids. In addition, there is need for new and more powerful theoretical and computational tools to provide greater interpretive and predictive capabilities in SACAM.

Let us consider one of these challenges--solid-state ionics--where the implications are manifold. Solid-state ionics is the study of the role of ionic properties, in particular ionic motion, in determining the overall properties of a solid. Little is known about (a) why ions in some solids show ionic conductivities orders of magnitude higher than others, (b) what can be predicted about diffusion in coupled solids of known structure, and (c) how to produce a solid through molecular engineering that will give a desired level of ionic mobility. Ionic mobility is critical in synthesis and in many technologically important areas, including corrosion of metals, hydrogen embrittlement, semiconductor composition, solar-cell junctions, hydrogen storage materials, oxidation catalysts, battery electrodes and electrolytes, and electrochromic devices.

There are many examples of new materials that had little obvious application when initially investigated. It is in just such areas of basic research that break-throughs can yield immense technological benefits. Some of the areas in which there is substantial basic interest and that show promise for future applications are less-than-three-dimensional solids, anisotropic solids in general, metal-organic compounds, particularly those of interest to the organometallic chemistry community, very small clusters of atoms, grain boundaries, interfaces, and other sources of inhomogeneity. Often the generation of new approaches and tools for synthesis is critical to the force that science can exert; the same can be said of new techniques and tools for characterization. Thus, for example, low-temperature techniques, including quenching and reactive sputtering, have not been exploited for many classes of materials, and more extensive use of these techniques by the SACAM community should be encouraged. The synthesis and characterization of totally new and unforeseen types of solid-state materials is important not only for providing the source materials for future applications and devices but for developing further the intellectual and scientific framework of materials chemistry. The few current programs directed along these lines are comparatively small and isolated.

It is generally acknowledged that many of the problems that today endanger our standard of living, and perhaps our physical well-being, will be solved only by advanced research and technology. SACAM offers the possibility of giant advances in many fields.

5. HUMAN AND MATERIAL RESOURCES

SACAM has developed primarily in industry in the United States, but elsewhere it has been actively pursued in universities, especially in Germany, the Scandinavian countries, the Netherlands, France, and Austria. Growing interest in SACAM characterizes material resources efforts in the Soviet Union and Japan. For a variety of reasons, in the United States basic research on advanced materials has not kept pace with basic research in many other fields. The magnitude of the academic effort in the United States lags behind that of other advanced countries and proportionately behind that of other scientific disciplines. Here we suggest ways to improve the development and utilization of resources for SACAM in the United States.

I. HUMAN RESOURCES

Experience has shown that SACAM usually involves a synergistic interaction among scientists with skills in synthesis (often, but by no means always, chemists) and characterization (often, but not always, materials scientists and physicists). The growth of the field depends on the interaction of people from different disciplines who work at the frontiers of knowledge in their own disciplines and are also conversant with the vocabulary, approaches, and techniques of related disciplines. Accordingly, the fostering of fruitful interactions between scientists from different disciplines is a major concern. The prime requisites for such interactions are that they lead to a high degree of intellectual stimulation and that the resultant collaborative programs be recognized as bona-fide professional activities.

In the United States, the less-well-recognized activity in the interaction of synthesis and characterization is generally synthesis. This situation weakens the whole field of solid-state science. At present, solid-state chemistry, a key synthesis discipline, is generally perceived by other chemists to be a peripheral and ill-defined area, whereas in terms of the needs and opportunities of SACAM it has the potential of providing much-needed ideas and techniques. Many of the important materials and concepts of solid-state science are rarely dealt with in the courses routinely offered by chemistry departments. In this respect, universities in the United States differ markedly from European universities where preparative solid-state chemistry is a well-recognized and accepted discipline. The French and German university systems have a long history in the training of solid-state scientists in both synthesis and characterization. For example, unlike universities in the United States, European universities have emphasized solids rather than solutions and molecular materials. In most cases, the main centers of solid-state science receive government support and funding and at the same time are an integral part of chemistry training programs. In Norway and Sweden, the emphasis historically has been directed toward the crystal-chemical characterization of solids, but the synthesis aspects of solid-state science have received considerable attention as well. In the United Kingdom, synthesis and characterization have been noted features of inorganic chemistry at Oxford and, more recently, of physical chemistry at Cambridge. Such encouragement within chemistry departments and by governments results in sufficient numbers of trained, synthesis-oriented scientists to satisfy the industrial, government, and university needs of many of these countries.

To tap and increase the human resources devoted to SACAM in academia, it is necessary to

- Encourage interdisciplinary collaborative research in SACAM by equitable funding of such collaborative research projects;
- Upgrade training in solid-state chemistry, particularly at the undergraduate level, where basic courses in solid-state chemistry are needed.

II. MATERIALS RESOURCES--INSTITUTIONAL

The establishment of dedicated, well-staffed, continuously updated facilities outside the exclusive domain of any one department would greatly promote interdisciplinary research in SACAM. One of the more important aspects of such facilities should be service or support, specifically state-of-the-art instrumentation and skilled support personnel.

Many of the basic personnel and equipment resources needed for a dynamic program in SACAM in educational institutions could well be funded, at least in part, by joint university-industry research grants. This method would benefit both universities and industry, particularly the smaller industrial firms. A greater level of university-industry interaction would also help to keep university researchers abreast of the current industrial scientific challenges and problems, as well as assist in keeping industrial personnel abreast of the latest ongoing academic research.

III. MATERIALS RESOURCES--EQUIPMENT

The problem of the growing sophistication and cost of apparatus used in the characterization and occasionally the synthesis of materials is of great concern. Much of this apparatus is too costly for most universities. In some instances, even the largest companies cannot afford valuable modern facilities (e.g., a synchrotron and the associated instrumentation). More major centers for sophisticated state-of-the-art instrumentation, permanently staffed by dedicated and expert personnel, should be established. Industrial scientists should be encouraged to use such centers. More and expanded materials-research-type laboratories centered on major campuses might be appropriate to develop.

Different problems are associated with the instrumentation in different cost brackets. For example, it is a widely held view that a large proportion of instruments costing up to about $50,000 are poorly maintained and deteriorating. Frequently, funds are not available for service contracts or other forms of maintenance. Generally, funds are needed to maintain and upgrade existing equipment and instruments.

For the efficient operation of a piece of equipment costing from about $50,000 up to approximately $250,000, a full-time technician is frequently necessary. Funds for the training and employment of such technicians are difficult to obtain. In addition, although maintenance is a major need, it is often not appropriately budgeted or anticipated. Funding for these purposes is essential. It is also desirable for research centers having specialized equipment to offer short courses and training programs to educate potential users. The provision of support for visiting scientists to learn how the instrumentation operates should also be considered.

PART II PANEL REPORTS

PANEL 1. PROBLEMS RELATED TO THE CHARACTER OF SACAM RESEARCH

I. INTRODUCTION

Basic research in the synthesis and characterization of advanced materials (SACAM) has been the principal source of new materials, structural information, bonding models and theories, thermodynamic data, and synthesis techniques and, as such, has provided the materials community with the scientific base on which materials technology has flourished. This area has been actively supported in universities, especially in Germany, the Scandinavian countries, the Netherlands, France, and Austria, during much of this century, and interest is growing in the Soviet Union and Japan.

For a variety of reasons, basic research in advanced materials in U.S. universities has not kept pace with other areas of basic research. Some of the obstacles that are frequently identified by members of the materials community are the following:

1. The prevalent structure of academic departments along the lines of individual research groups staffed by graduate students and postdoctoral researchers of short tenure;
2. The tradition of evaluating principal scientists primarily in terms of their individual contributions;
3. The emphasis on molecular science in undergraduate curricula, especially in chemistry, which is a key discipline in advanced materials synthesis and characterization;
4. The lack of a sense of identity and coherence among the members of the synthesis and characterization research community.

These obstacles have the following effects:

1. The short tenure of postdoctoral personnel and graduate students results in difficulties in maintaining continuity, which is particularly serious in those research areas of materials synthesis that require skills and techniques that are generally developed only with considerable experience.

2. The evaluation of scientists primarily on the basis of their individual contributions makes it difficult to establish a research program based on collaboration, yet collaborative efforts are crucial to research in materials.

3. The emphasis on molecular science in undergraduate education makes it significantly more difficult to attract graduate students, and, concomitantly, future faculty, into research groups doing solid-state preparation and characterization.

4. The lack of a feeling of community among the materials chemists, ceramists, metallurgists, and other scientists involved in synthesis and characterization makes it difficult to develop the interaction and cross-fertilization so important to the development of this field.

Our approach to these problems is to consider the status of a variety of materials research areas with the aim of providing an overview of the field and a synopsis of current and near-future research problems. This overview and synopsis, together with the scientific importance of the research problems discussed, provide the background and basis for the panel's recommendations and for a number of those in the Summary Report (Part I).

It should be recognized that studies of novel materials should not be limited to the synthesis of materials in the sense that a chemist ordinarily uses the term "synthesis." The preparation and study of materials that are of interest for their mechanical properties, especially durability, present a broad range of problems in basic research. Materials such as fiber composites, ultrahard boron compounds, high-temperature alloys, and spinodal compositions deserve basic study by metallurgists, ceramists, and chemists. In addition, the study of low-energy-cost materials processing is of obvious importance.

It should also be noted that there are fundamental problems in the chemical bondings and mass-transport processes that are operative in growing interfaces and passivating surfaces. For example, the understanding and chemical control of surface oxidation, surface-bonding defects, transport of atoms along grain boundaries, and impurity diffusion to surfaces are of growing importance for electronic devices, magnetic materials, corrosion, fracture, and radiation-hardened coatings. These areas, which have direct bearing on many technological needs, offer substantial challenges and opportunities for basic research in the synthesis and characterization of solids.

We consider the current status of basic research in advanced materials synthesis and characterization using the following breakdown: electronic structure of solids, inorganic solids: new classes of compounds and their impact on solid-state concepts, highly conducting molecular solids, ceramics and amorphous solids, and predicting the lifetimes of materials. We then present our conclusions and recommendations.

II. ELECTRONIC STRUCTURE OF SOLIDS

In the electronic structure of solids, the interaction between those concerned with theory and with the development of synthesis and the resultant impact on characterization of materials are increasingly important. This interaction is largely a result of the availability of computers and relatively large-scale experimental facilities. Modern research efforts in materials frequently take the following form:

1. A structural or physical effect of potential interest is observed.
2. The effect is studied in detail by any one of a number of modern techniques [e.g., nuclear magnetic resonance (NMR), x-ray absorption field spectroscopy (XAFS), Auger spectroscopy, photoelectron emission (XPS)].
3. A rigorous quantitative theory of the effect is developed.

The requirements for collaboration are obvious. Among the benefits is that theory generally provides insight, guidance, and incentive for additional synthesis efforts.

Modern theoretical approaches include empirical and semiempirical approaches, such as the Brewer-Engel correlation of gaseous atom electronic states and alloy structure, Phillips and Van Vechten dielectric electronegativities, and the Mediema model of intermetallic solids, as well as ab initio calculations, such as augmented plane wave (APW) and linear augmented plane wave (LAPW), which are becoming increasingly available to support the work of synthesis scientists. The theoretical framework is being extended to more complex materials; these extensions are essential for the systematic development of advanced materials. This theoretical development is, in turn, being accelerated by the synthesis of completely new classes of compounds that are expanding our awareness of possibilities for chemical interactions and of the limited nature of the concepts with which we have circumscribed our thinking.

Descriptions of electronic behavior in solids are based primarily on two extreme models: the localized model applies to electrons about discrete atomic centers, and the intinerant model applies to electrons distributed over the entire solid. Many materials exhibit intermediate behavior, thus efforts are under way to establish a theoretical bridge between the extremes of localized and itinerant electron behavior. The general problem is known as the "narrow-band" problem; its solution requires the introduction in zero order of electron-lattice interactions and electron-electron correlations. Successful treatment of the narrow-band problem is essential to our understanding of the relationship between phase instabilities, high-temperature superconductivity, and the appearance of spontaneous magnetization. Narrow-band effects are responsible for the disproportionation reaction, $2Fe^{+4} = Fe^{+3} + Fe^{+5}$ in $CaFeO_3$ (not found in isostructural $SrFeO_3$), for the semiconductor-metal transition in VO_2 (which forms V-V pairs at low temperatures), and for the unusual phase transitions found in NiS.

Other areas of theoretical development that will have an impact on synthesis and characterization are the effects of disorder, that is, the conceptual passage from the ordered solid to the amorphous state, and the electronic structure of surfaces and interfaces. The former is relevant to the study of defect formation and migration, and the latter is necessary in the investigation of the numerous surface properties of materials, of which catalysis and corrosion are two of the most important. The interplay of theory and synthesis benefits both areas. Systematic chemistry delineates the boundaries of applicability for the simplifying assumptions, either implicit or explicit, in the phenomenological models. Furthermore, inadequacies of models that emerge in the attempt to predict synthesis behavior or properties of materials in new configurations frequently lead to the application of more rigorous or *ab initio* methods; these then provide a basis for the evaluation and refinement of the empirical theories. This interplay leads to feedback between theory and experiment and results in a rapidly developing area of scientific understanding. It merits strong support and encouragement.

III. INORGANIC SOLIDS: NEW CLASSES OF COMPOUNDS AND THEIR IMPACT ON SOLID-STATE CONCEPTS

In the area of synthesis per se, two extreme situations can be identified. One is the preparation of known and relatively well-characterized materials in higher purity, special form, or with specific doping or atomic distributions. The other, the subject of this section, is the creation of totally new classes of compounds exhibiting novel structures and bonding. The latter situation exemplifies the need to reconsider many of our traditional ways of thinking about chemistry, structure, and bonding, particularly in expanding our horizons about what is possible and what must be taken into account. Thus, the concepts associated with isotropic bonding, structure, and electronic properties, which have been so well studied for traditional metals, are now being tested for one- and two-dimensional metallic arrays. Some of these new types of compounds are expected to display new phenomena. Examples, most of which have been known for less than 10 years, make it clear that new and exciting types of compounds are to be found even in binary metal-halogen and metal-chalcogen compounds; ternary systems are much less well explored, although the remarkable Chevrel phases and their relatives that are now being reported suggest that such studies will be productive.

Nearly all of what may be classified as structurally "remarkable" and "novel" phases have the highly anisotropic metal-metal bonding associated with the unusual low-oxidation states of many metals. The reduction in the formal nonmetal-to-metal ratio is usually accompanied by some degree of metal-metal bonding, apparently to accommodate orbital-electron requirements already recognized for the metals and their more normal compounds. Metal-metal bonding often appears to control the resulting structure rather than occurring as a secondary, weak effect. Some examples are as follows:

1. Alkali metal-rich oxides have recently been found, Cs_7O and $Cs_{11}O_3$, for example, in which structured metal-oxygen clusters appear in a sea of metal.

2. Isolated metal tetrahedral or octahedral clusters occur in halides and chalcides, for example, the Chevrel phases $Pb_xMo_6S_8$, $Mo_4S_4Br_4$, Nb_7P_4, and $CsNb_6I_{11}$.

3. Infinite chains of metals are found in the form of (a) metal octahedra sharing adjoining edges in Nb_2Se, (b) metal octahedra sharing opposite edges in M_2Cl_3 (M = Y, Gd, Tb), Sc_7Cl_{10}, and Gd_5Br_8, (c) metal dodecahedra in Ta_6S, and (d) metal octahedra sharing verticles in Ti_5Te_4-type phases. Indeed, the last structure occurs with so many transition metal-posttransition nonmetal combinations that one wonders what remarkably flexible electronic requirements pertain.

4. Infinite double metal sheet structures in the monohalides of Zr, Hf, Sc, Y, and many rare earth elements and in Hf_2S, PtTe, Ag2F, and Ba_2N provide the first really two-dimensional metals for study, for example, in the areas of band theory, properties of interstitial impurities such as hydrogen, conduction, and catalytic behavior.

Nontransition elements also share in the structural and bonding significance:

5. Complex chains of tellurium occur in Te_3Cl_2 and Te_2Br and of phosphorus in many polyphosphides.

6. Metal clusters, chains, and ribbons are even found in a remarkable class of intermetallic phases involving metals of widely different electronegativities, for example, square Bi_4 units in $Ca_{11}Bi_{10}$, angular Sn_3 in Li_7Sn_3, ribbons in NaHg, and tin tetrahedra in KSn.

Obviously, these phases provide new horizons for what is possible, if not immediately explicable, in chemistry. The metal-metal bonding and low-dimensional electronic conductivity provide strong challenges to both the theorist and the experimentalist for explanation, interpretation, and characterization. Not only do these compounds imply the occurrence of new phenomena, but they also promise direct use as catalytic substrates, media for hydrogen storage, new electronic environments for nonmetals or for metal ions in electronic and magnetic applications, and as intermediates potentially important in corrosion of active and refractory metals and significant for their mechanical properties (e.g., stress corrosion cracking of zirconium by iodine).

There are some special conditions and circumstances that allow for such discoveries in what have sometimes been thought to be "sterile" systems. Surface blockage and kinetic limitations, even at 800°C, have made vapor-phase transport reactions invaluable and higher temperatures, melt-solvent reactions, and longer reaction periods increasingly necessary. Tantalum and similar container materials, high-quality (space-age) drybox facilities, and metal fabrication and welding equipment are often necessities. Characterizational tools such as microprobes, Guinier powder and single-crystal x-ray diffraction facilities, and photoelectron emission (XPS) equipment with high-quality drybox entrance capability are essential. Synthesis using molecular-beam epitaxial methods is promising. Most, if not all, academic institutions find it difficult to provide these sophisticated facilities without considerable assistance, yet these capabilities should not be limited to national laboratories and industrial firms.

IV. HIGHLY CONDUCTING MOLECULAR SOLIDS

During the past 10 years or so, a new area of materials synthesis and characterization emerged. It deals with the preparation and measurement of properties of molecular solids that are good electronic conductors. This area has undergone rapid development as a result of strong interactions among synthesis chemists, materials scientists, and solid-state physicists. The motivation for synthesizing and characterizing these molecular solids stems in part from the desire to obtain materials with unusual or unprecedented properties, some of which might be of technological importance.

The new phenomena already discovered have stimulated the advance of theoretical concepts of electronic conduction in solids. We expect that other new phenomena will be found that will further stimulate advances in this area. The results of work in this field have played a crucial role in developing concepts related to one-dimensional band theory, charge density waves, Peierls instability effects, Coulomb interactions, incommensurate lattice effects, and effects of defects.

Electronically conducting molecular solids fall into two broad categories: highly conducting substances (conductivity >1 ohm^{-1} cm^{-1} at 25°C) and semiconducting molecular solids, including some photoconductors and photoresists. The first category, which includes the new and potentially important molecular metals, is one of vigorous basic research activity. We give it special attention.

The first example of a covalent polymer, which contains no metal atoms, is highly conducting ($\sigma \sim 5 \times 10^3$ ohm^{-1} cm^{-1} at room temperature) and is a superconductor (T_c = 0.3 K), is polymeric sulfur nitride, $(SN)_x$. Potential future research includes synthesis efforts to produce substances isoelectronic with $(SN)_x$, for example, $[(CH_3PN]_x$, $[S(CH)]_x$. Another example is polyacetylene, $(CH)_x$. This material can be prepared in the form of large thin, free-standing, and flexible silvery films. Polyacetylene can be p- or n-doped to yield a series of semiconductors and the first examples of organic polymeric metals. In the semiconducting forms it has been used to fabricate p/n junctions and Schottky barriers, which act as rectifying diodes. In certain systems these exhibit a photovoltaic effect and, accordingly, have a potential for application as solar-cell materials. The use of different dopants and the replacement of hydrogen by organic or inorganic groups could result in new molecular metals and semi-conductors.

Another class of materials in this category is the intercalation compounds of graphite. Through intercalation with a variety of electron-donating or electron-attracting species, the conductivity of graphite can be spectacularly modified. By doping with AsF_5, conductivities in excess of that of copper have been obtained. It seems likely that further studies will result in the discovery of interesting and useful electronic behavior.

The materials exhibiting marked anisotropy of electronic conduction and significant one-dimensional effects should also be mentioned. In this category fall the TTF derivatives (e.g., (TTF)(TCNQ) and $(TTF)Br_{0.6}$, the platinum chain compounds (KCP), the mercury chain compounds ($Hg_{2.84}AsF_6$), and the charge-transfer complexes, of which (TTF)(TCNQ) is an example. These compounds have already resulted in new concepts of electronic conduction in solids, which will undoubtedly continue as new materials are prepared and studied. The discovery in $Hg_{2.84}AsF_6$ of a sublattice that is incommensurate with the main crystal lattice has evoked considerable theoretical interest. New types of charge-transfer complexes, such as the iodine complexes of certain phthalocyanin and porphyrin derivatives, with single-crystal, room-temperature conductivities up to 500 $ohm^{-1}\ cm^{-1}$, have been reported.

Research on highly conducting molecular solids is advancing at an extraordinary rate. The synthesis of new chemical systems is essential to the continued growth of this field. The potential for increasing scientific knowledge through the synthesis of new compounds, the better characterization of known materials, and the theoretical analysis of new phenomena is great. The field presents a challenge and an opportunity for collaborative interaction among chemists, physicists, and materials scientists. Present knowledge suggests that in the next few years many new materials with unusual properties will be discovered, if the appropriate scientific climate can be fostered.

V. CERAMICS AND AMORPHOUS SOLIDS

Ceramics and specially designed amorphous solids are attractive for use in advanced energy, electronic, magnetic, and optical systems. Examples of opportunities for significant new developments in ceramic materials include metallic oxides for use as electrode materials in electrochemical cells, for example, oxygen electrodes in fuel/electrolysis cells and solid-solution electrodes in high-specific-energy batteries; catalytic substrates and mixed ceramic-metal catalyst systems; high-temperature structural materials for heat engines and turbines; radiation-hardened and corrosion-resistant materials for nuclear fusion containment; photosensitized ceramics for photography and photoelectrolysis of water; controlled surface-reactive glasses and glass ceramics for replacement of bones or teeth; and tailor-made crystal chemicals for long-term encapsulation of nuclear wastes.

Because of the multicomponent and polyphase nature of these materials, characterization and synthesis are often highly complex and difficult. Consequently, research in this class of materials has been unduly influenced by applications, mechanical performance criteria, and consumer products, all of which have tended to limit innovation and the development of new processing and materials concepts. Several kinds of long-term basic research required to advance the fundamental science of these materials are the following.

Structural and physical characterization at the intermediate range of order (10-100 Å) and a physical theory including such order are needed for ceramic and amorphous materials. Information is needed to provide insight into the statistical distribution of molecular species, bond types, bond angles, and relaxation times. Such research has been made possible by the recent development of a variety of new experimental approaches, including Fourier transform NMR, laser Raman spectroscopy, and XAFS. Such studies would lead to a better understanding of a variety of materials: amorphous solids with solutions of second and third components, for example, hydrogenated amorphous silicon and selenium hybrid crystalline materials with amorphous sublattices, such as β-alumina with an ordered AlO lattice and disordered Na^+; stabilized unusual oxidation states in invert glasses; meta stable solubility gap materials; and microphase separated oxide and chalcogenide glasses.

A basic theory relating environmental sensitivity of mechanical properties to structural flaws and kinetics of reactions at interfaces is required for improving and developing new structural ceramics and glasses. High-temperature creep of Si_3N_4 and SiC materials, fatigue of single and polycrystalline oxides, and surface deterioration of glass optical fibers are examples of areas where such basic research is needed.

Quantitative characterization of the structure, composition, and phase state of grain boundaries and surfaces is essential to understanding of the properties of many advanced ceramic materials. Amorphous grain-boundary phases of 10-50 Å thin films cannot generally be analyzed by present instrumental methods, which is a basic limitation to progress in this class of materials. For example, electron-beam techniques result in structural alteration of grain boundaries and surface films.

Control of particulates used in processing of many types of ceramics requires improved theories of agglomeration, mixedness, liquid-particulate interactions, specific surface-adsorption and electrochemical effects, composition and defect gradients, and organic-inorganic interactions. A general theory of ceramic particulate systems needs to be related to the rheology, forming, drying, and subsequent firing steps in achieving tailored microstructures required for new energy systems, biomaterials, and electronic applications.

Several novel techniques are now being used for fabricating metastable alloys and structures with unique chemical, physical, and mechanical properties. Amorphous metal sheets, ribbons, fibers, and powders may be produced by rapid cooling and subsequently consolidated into bulk structures. The chemical homogeneity and lack of the normal (crystallographic) deformation modes in these solids provide unique properties that have not been fully identified and exploited. In addition, amorphous, ultrafine, crystalline, or epitaxial surface layers on bulk metals are being formed by laser-quenching, electron-beam quenching, and ion implantation. These processes are of significant utility in coping with a variety of surface-related phenomena such as corrosion, friction, wear, fatigue, and catalysis. Moreover, ion implantation permits the formation of alloys that are unobtainable by other techniques and makes possible studies of diffusion, oxidation, and decomposition involving atom species that were not previously accessible. A new generation of instrumental analysis methods of dramatically greater resolution and sensitivity was developed during the last decade. Opportunities are many for the use of this new instrumentation for the characterization of surfaces and interphase boundaries, intermediate-range order, and the environment-structure interactions of ceramics and amorphous solids. The complexities that result from the polyphase and multicomponent nature of ceramic materials often make the new characterization techniques difficult to apply; however, the understanding of dynamic mechanisms in structural and atomic detail probably will yield new ceramic materials and improvements in properties and processing of existing materials.

VI. PREDICTING THE LIFETIMES OF MATERIALS

Prediction of the structural reliability of materials exposed to high-performance conditions for long periods of time is a scientific problem of great practical importance. Nuclear waste encapsulants will be required to isolate radioactive constituents from the ecosphere for thousands of years. Such materials must withstand harsh combinations of thermal, chemical, mechanical, and radiation stresses. Basic research on the synergistic interaction of such complex factors during surface chemical reactions and microstructure evolution is needed to extrapolate from laboratory-time-scale experiments to geologic-time-scale needs.

The effort to ensure the reliability of isolated defense and energy-generating and -conversion facilities requires prediction of the long-term performance of electronic and optical components exposed to combinations of severe thermal, chemical, mechanical, and radiation environments. Fracture mechanics theories that lead to lifetime predictions are currently based on empirically derived relationships involving environment-sensitive factors. Basic research to develop a molecular theory underlying the origin and magnitude of the environment-sensitive parameters in these fracture mechanics theories is urgently needed to assure accuracy of lifetime predictions. Synthesis of new structural materials with improved lifetimes and development of protective coatings cannot proceed on other than a trial-and-error basis without an improved physical understanding of materials degradation.

The problems of lifetime predictions in severe environments require a synthesis of theories of molecular structure, mechanical behavior, and surface chemical reactivities coupled with accurate characterization of flow distributions, heterogeneous surface states, microstructural parameters, and composition gradients.

VII. CONCLUSIONS AND RECOMMENDATIONS

Based on accomplishment and research potential, we conclude that SACAM is a healthy field of endeavor. A wide variety of materials is being synthesized in response to a diversity of scientific motivations; the materials are being characterized with a growing set of powerful experimental techniques; and the results of the synthesis and characterization have potential applications to a broad range of pressing national problems. Accordingly, there are many opportunities for the development of substantial and meaningful research programs. However, there are some aspects of materials synthesis and characterization that lead to special problems. Our perception of the problems and our recommendations follow.

1. The techniques required for synthesis research are generally sufficiently demanding and specialized that efforts to develop a synthesis program frequently preclude the development in the same group of the expertise required for the incisive investigation of properties or front-line theoretical analysis. Therefore, <u>we recommend that collaborative efforts be encouraged, not only between different departments in the same institution but</u>

also between different institutions. This objective can be accomplished by increased funding for domestic travel and for intermediate-term exchange appointments, especially across the industrial-academic interface.

2. There is concern about the attractiveness of solid-state science to students. We recommend that an effort be made to attract first-rate minds into the area by emphasizing the intellectually stimulating character of the problems and by better disseminating news of the field and the continuing substantial accomplishments and applications of solid-state research.

3. There is widespread agreement that research in synthesis and characterization requires more continuity than is generally possible in university-based basic research groups under current funding arrangements. We recommend that continuing efforts be made to ensure that research groups remain large enough so that all the diverse aspects of SACAM research are represented in these groups. We also recommend increased support for senior research technicians and postdoctoral research personnel. The creation of postdoctoral fellowships in solid-state science, to be awarded for from 3 to 5 years and in a research group of the fellow's choosing, is one possible way of accomplishing some of these goals.

PANEL 2. SCIENTIFIC CHALLENGES
ARISING FROM TECHNOLOGICAL NEEDS

I. INTRODUCTION

The synthesis and characterization of advanced materials (SACAM) are carried out by an interdisciplinary community whose contributions have been at the heart of progress in materials science and technology. This community includes researchers in solid-state physics; metallurgy; ceramics; materials science; geoscience; electrical engineering; and inorganic, physical, organic, and solid-state chemistry. Only recently has awareness of group identity begun to develop within this community.

We will begin with some definitions: first, the word "synthesis" as used in the SACAM Workshop and this report. Although synthesis is generally used, "preparation" might be preferable, for it would include both the careful control of microstructure and extrinsic properties of materials, which are in the province of the ceramist and metallurgist, and the *ab initio* preparation or synthesis of materials, which is in the domain of the chemist. In this sense, both synthesis and preparation and, concomitantly, their synergistic interaction, have been essential to many achievements in solid-state science and technology. We believe that they will continue to be the driving forces of progress in materials science and technology.

Second, "characterization" refers to the measurement of the chemical and physical properties of materials. The purpose of characterization is generally twofold: to understand closely related materials on the basis of their chemical bonding, atomic structure, and microscopic and macroscopic perfection and to improve and specify materials for particular applications.

Third, "advanced materials," which can best be defined briefly by examples, such as the following:

- o Semiconductors (excluding "routine" Si and GaAs)
- o Magnetic materials
- o Ferroelectric materials
- o Piezoelectric materials
- o High-strength and electronic ceramics
- o Metallic organic materials, especially those with established connections between bonding, structure, and properties, where synthesis of desired structures is critical, for example, linear chain conductors and layered compounds
- o Inorganic polymers, for example, SN_x
- o Active organic polymers, such as resists and piezoelectric materials
- o New superconducting materials, particularly binary and ternary compounds, alloys, and solid solutions
- o High-performance composites
- o Amorphous materials for which the preparation requirements are unusual, such as amorphous metals and fibers
- o Alloys and composites for which specialized care in preparation and processing control is essential
- o Some single-crystal materials
- o Various other inorganic materials such as oxides, layered materials, tunnel junction materials, intercalation compounds, chalcogenides, and pnictides

Advanced materials are those at the forefront of science and technology at any given time, the materials critical to improvements in the technologies at the heart of our economic system.

Because of the overlap between charges to Panels 1 and 2, there is a degree of duplication between the reports of the two panels. There were somewhat different emphases in the two groups, however, so it has seemed useful to include both accounts.

II. ACHIEVEMENTS IN SACAM

To assess the importance of SACAM to future technology and to explore the strengths and needs of the present SACAM community, it is helpful to consider past achievements. Such an exercise provides models for future efforts and shows how obstacles have been overcome.

A. Achievements in Electronics and Related Fields

Semiconductor science and technology have been central to modern electronics since the invention of the transistor and the development of the basic preparative techniques for making semiconductors, especially single-crystal Si and III-V compounds. This work took place over more than 20 years and included the development of such methods as zone refining, float-zone crystal growth, crystal pulling, and liquid-phase epitaxy. Si and GaAs were once exotic advanced materials. Indeed, at the degree of perfection and crystal size needed for very-large-scale integrated-circuit devices, advanced LEDs, solid-state lasers, and magnetic bubbles, they are still advanced materials, and substantial synthesis and characterization research is still needed.

Several activities allied with preparation have played key roles in the development of semiconductor materials. Characterization of the chemical purity and electrical properties and careful studies of point and extended defects have been essential for progress at every stage.

The theoretical description of impurity and dopant partition and of the interaction of defects has also been essential. Thus, in semiconductor materials research and development, advances have depended on the interdisciplinary activities of metallugists, chemists, and solid-state physicists. The interactive style of research developed in the work on semiconductor electronic materials has pervaded and been a model for much of materials science.

Another area of SACAM contributions to electronics is the preparation of magnetic materials. The descriptive and structural chemistry of oxide magnetic materials, alloys, and intermetallic compounds was developed through decades of continuous work. As a result, an understanding of spinel and garnet structure materials has been achieved. The magnetic interactions have become so well understood that these materials might be regarded as the "fruit flies" of magnetochemistry. These successes depended heavily on the development and exploitation of single-crystal techniques, such as flux growth, for the preparation of refractory oxides. Studies of properties of single crystals have resulted in a basic understanding of intrinsic properties. Controlling microstructure and understanding the connection between magnetic properties and extrinsic structure have been essential to progress.

The newest addition to the family of magnetic materials, the transition metal/rare earth intermetallic compounds, benefited from the measurement of the anisotropic properties of single-crystal materials. The exploitation of this crystalline anisotropy required the development of powder-metallurgy techniques for the consolidation of these highly reactive materials and the exploitation of new chemistry to produce fine powders at reasonable cost from inherently inexpensive rare earth oxides. Although these materials are intrinsically more expensive than oxide materials, their high coercive force makes them extremely resistant to demagnetization and thus cost effective for many device applications.

Techniques have been developed for the routine preparation of optical fibers for communications. These methods, which are based on rapid, controlled, vapor-phase chemical reactions, permit technologists to produce materials with only a few parts per billion of critical, optically absorbing impurities. With such high-purity materials, the optical losses at the wavelengths of interest for optical communication are sufficiently low that repeater spacings can be many kilometers. These techniques also allow the careful control of deliberately added impurities over dimensions of micrometers so that the index of refraction can be tailored to produce the desired waveguide characteristics. Glasses for fiber transmission provide a continuing need and stimulus for additional SACAM contributions.

B. Ceramic Materials

Cost considerations have dictated that, wherever possible, ceramic systems be used in electronics. Accordingly, the ability to control the microstructure of ceramic materials is among the most remarkable accomplishments in controlling the properties of inorganic substances of technological importance. The emphasis in much of electronic materials synthesis has been on the preparation of materials in a state of sufficient purity and perfection that they exhibit their intrinsic properties. These properties are often unique and result in entire families of devices based on single crystals, where the quantities of materials required per device function are quite small. The unique challenges of ceramic SACAM research have been to control the grain structure and the state of grain boundaries. The roles of solid-state chemists in providing background understanding of defect chemistry and of physicists and engineers in characterization and end-use guidance have been significant. Luculox and its relatives--optically transparent ceramics for lamp envelopes and windows--are typical of the technological achievements. The key to these advances was the discovery that MgO inhibited grain growth in Al_2O_3 and the subsequent careful exploitation of this discovery so that it could be used under actual processing conditions. Other examples of SACAM achievements based on detailed understanding of ceramic processing include the efficient fabrication of UO_2 fuel rods for fission reactors, ZrO_2 ceramics for oxygen detectors, which find use in emission control in internal combustion engines, ballistic armor for military and civil police applications, tungsten carbide tool tips for high-speed machining, and β-Al_2O_3 and related ceramic materials for solid-state battery electrodes. The key has been the careful control of grain structure to make a useful polycrystalline material at a cost low enough to permit exploitation.

Electronic ceramics, such as piezoelectric lead zirconite titanate and its cogeners, doped ZnO and related nonlinear resistance (varistor) materials, and complex ceramic conductors and their relatives, which are essential in thick-film hybrid integrated circuits, are all examples of additional SACAM contributions. The set of innovative processing techniques that permit the rapid and cheap preparation of Al_2O_3 ceramics for electronic and autocatalyst bed applications is an additional example.

C. High-Pressure Materials

High-pressure synthesis is an important area of scientific research and has produced a number of high-technology materials. A key element in these successes was the timely exploitation of modern engineering materials to produce the experimental conditions necessary for new syntheses; for example, high-pressure autoclaves, pumps, and gauges. Two of the most important products of this work are synthetic quartz and diamond. As a result, the U.S. electronics industry is now independent of foreign sources of natural quartz, and the U.S. machine tool industry is independent of foreign sources of industrial-grade abrasive diamond.

D. Heterogeneous Catalysis

The efficient conversion of petroleum into the variety of fuels needed by modern industry and the conversion of petroleum feedstocks to petrochemicals and polymeric materials depend on the availability of highly specific solid catalysts. The synthesis of these catalysts, their characterization, and the understanding of their role in breaking and forming chemical bonds in petroleum-based materials have been major successes of modern science and technology. The role of solid-state chemistry and synthesis is often overlooked in these achievements. For example, controlled zeolite catalysts, Ziegler-Natta catalysts, and metal-alloy catalysts are vital in modern technology; all of these have resulted from extensive SACAM efforts.

E. Dimensionally Stable Anodes

The efficient and pollution-free production of elemental chlorine by electrochemical processes is a key part of present industrial chemistry and provides an essential industrial chemical, Cl_2, for scores of industrial syntheses. The discovery, through preparative techniques and characterization, that ruthenium-titanium oxides can replace mercury anodes had great impact on our chemical industry. These new anodes not only increase efficiency, thus conserving energy, but also eliminate mercury pollution.

F. Controlled Preparation of the Glassy State

Control of glass "structure" by selective leaching before final consolidation has given us comparatively inexpensive, thermally shock-resistant families of glasses, such as vycor. Careful control of recrystallization has produced even more remarkably controlled thermal properties in, for example, the pyrocerams. Rapid quenching has opened the glassy state to previously non-glass-forming materials, such as metals. Indeed, glassy metals have remarkable mechanical strength and unusual magnetic properties. All of these achievements resulted from controlled synthesis and careful characterization.

G. Controlled Preparation of Alloys and Composites

With the notable exception of semiconductors, polycrystalline solids are the basis of much of our technology. In these materials it is extrinsic structure (grain boundaries, impurities, inclusions, and dislocations) coupled with the intrinsic molecular or crystal structure that determine the technological importance of the material. Materials that are appropriate for a variety of complex functions generally have higher intrinsic value.

Technically sophisticated systems (gas turbines, nuclear power plants, space capsules) require the simultaneous optimization of several properties, such as strength, density, and chemical stability. Accordingly, the materials employed usually have coupled chemistry and microstructure.

The key to developing new alloys and composite materials is to understand and manipulate the microstructure and thereby the properties of the materials. Four classes of tools are required for progress: (1) theoretical models of the structure and binding of localized states of matter, (2) computational procedures and equipment to evaluate the models and suggest experiments to validate them, (3) observational techniques and equipment to provide structural and compositional information on a local scale, and (4) an extensive and precise quantitative data base for phase equilibria.

All of these tools have been and are being applied to the development of technologically important materials. Examples of past accomplishments and areas of particular promise for the future are phase state and phase equilibria; transport phenomena; and interface, surface, and grain boundary phenomena.

Historically, the major body of phase-state information has been obtained by measurement and computation of bulk properties, augmented, when appropriate, with simple rules for predicting phase type from electron concentration and pre-existing knowledge of crystal structure. Crystal structure cannot be predicted *a priori* except in the simplest of cases. One example of a simple rule is the PHACOMP calculation of phase stability from knowledge of a specific alloy composition and multiple regression analysis of previous data relating composition to volume fraction of constituent phases. This method has been applied successfully to superalloy design and specification. These superalloys are critical for the efficient power generation and propulsion devices necessary for a modern industrial society.

The recently developed theory of atomic clusters, coupled with powerful computational techniques, shows promise for improving the prediction of phase stability. Clearly this is an area of opportunity.

In service, materials are often subject to changes that are diffusion-controlled, and product life is limited by time and temperature under stress. Nevertheless, detailed analysis of diffusion mechanisms and their relation to composition are rarely a part of an alloy-development program.

A recent report demonstrates that in 25 years of high-temperature alloy development, the prime factor accounting for the 50 percent increase in allowable operating temperature has been the decrease of the diffusion coefficient. This analysis includes the recent spectacular improvement resulting from fiber and lamellar eutectics represented by TaC- and Mi_3Nb-reinforced, nickel-base superalloys.

Another example of the importance of transport phenomena in technologically significant materials is identification and development of structural materials for fast breeder reactors. The extensive swelling of austenitic alloys caused by a fast neutron flux can be drastically reduced by control of both the major alloying elements, Fe, Cr, and Ni, and a host of minor impurities. The effects can be understood from a knowledge of the changes in diffusion rates that accompany these changes in composition.

Grain boundaries and internal interfaces frequently limit the structural performance of metals, alloys, and composites. The strength and ductility of the boundaries and interfaces are, in turn, controlled by the structures produced at these interfaces where segregation occurs. Modern analytical tools, such as the electron microscope, microprobe, and Auger spectrometer, which permit chemical and structural analysis on a localized scale, are now being effectively used in studying structure and composition of grain boundaries and other internal interfaces in solids.

Primary and secondary recrystallization of metals and alloys, such as copper, nickel, and transformer steels, are controlled in part by segregation of minor additives, both intentional and inadvertent. The amelioration of temper embrittlement in steels will require understanding and control of the segregation of impurities at grain boundaries, which controls the embrittlement kinetics. Corrosion phenomena, particularly those associated with stress corrosion, are influenced by local chemical conditions in the solid and solutions. Both, in turn, are modified by segregation of alloying elements and impurities on a local scale.

Multiphase composite materials, which permit new levels of performance and allow materials to be tailored to specific needs, depend for their mechanical properties on the transfer of load between the phases. Bond strengths at interfaces are markedly influenced by phase stability, local structure, and composition. Opportunities exist to develop phase-compatible fibers, coatings, and matrix materials for new composities. The boron-aluminum composites and carbon-reinforced polymers are two examples of synthetic composites that have unique properties for aircraft skin and engine use. Natural composites, such as eutectic superalloys produced by directional solidification, are currently under development for use as blading in aircraft turbine engines. Composites offer a unique opportunity for improved efficiency and reduced weight in aircraft applications and are finding use in consumer products in the less sophisticated form of glass-fiber-reinforced polymers.

III. TECHNOLOGY-DRIVEN OPPORTUNITIES

The achievements that we have discussed are merely a prelude to the achievements that SACAM can yield in the future. Trends in technology point to increased importance of advanced materials and the likelihood that SACAM will pace progress in many critical areas. Some major opportunities are the following.

A. Communications and Data Processing

Electronic materials will continue to play a key role in many areas of technology, especially communications and data processing. Several driving forces important to the future of the electronic materials industries have as their central feature the need for improved advanced materials. Probably foremost is the continuing increase in the scale of integration of silicon integrated circuits (SICs). Automata of all sorts, such as inexpensive small personal computers (the hand-held calculator) and distributed computation and control devices (the microprocessor), will have increasing impact on society. Super-large-scale computers, which will make possible real-time calculations for a variety of problems, notably meteorological equilibria and kinetics necessary for the accurate prediction of weather, will also become a reality. These developments will come about only as a result of increases in the memory and calculating power obtainable per unit investment. Less costly data processing results directly from putting more circuit functions on a single Si chip. At present, large-scale integration (LSI) has brought 262-kbit memories close to everyday use. The packing density in SICs has been doubling approximately every 2 years as feature sizes become smaller. It is currently possible to fabricate LSI circuits with feature sizes of the order of a micrometer. Submicrometer featured sizes or less are expected within a few years. However, advanced materials will be required. The conventional conductors and dielectrics used in SICs will require improvement or replacement. Thus, SiO_2 may not be adequate as the insulator in semiconductor circuits as the feature size becomes smaller. We need materials of higher dielectric constant, materials less subject to pinhole formation, materials that can be made in thinner layers more reproducibly, and materials that have a smaller likelihood of imperfections over a small area. Perhaps detailed study of silicon-nitrogen chemistry could lead to the production of such materials. The techniques for preparation of new Si dielectrics should be compatible, insofar as possible, with semiconductor processing as currently carried out with respect to times, temperatures, and pressure, since there is an immense investment in processing equipment and procedures. The same is true of improved conductors. Thus, silicide chemistry and preparative efforts in general are ripe for SACAM contributions, which could be the key to the next generation of very-large-scale integration (VLSI).

To pattern smaller feature sizes, families of improved resists are needed. Resists are materials for which solubility can be changed by exposure to radiation and that can thus be patterned to produce the circuit features desired in SICs. Optical resists are the mainstay of the semiconductor industry for direct processing, although master masks for patterning many devices are regularly made using electron-beam resists. As feature sizes become smaller, the diffraction limit of light will become increasingly restrictive. Accordingly, much SACAM research is concerned with organic polymeric materials for which solubility is altered by exposure to light, electron beams, and x rays, with the hope that from these studies resist materials for the micrometer and submicrometer regime can be developed. All of these efforts require careful synthesis and characterization and are essential to future progress in integrated-circuit technology.

The role of SACAM in the development of low-loss and high-bandwidth optical fibers is well known. However, new families of materials might have losses that are orders of magnitude lower than the silicate-based glasses now used for optical fibers. There are classes of non-oxide glasses in which, with careful synthesis and control, such low losses might be achieved. The impact would be substantial if repeater spacings could be much greater than is now possible.

There are many other opportunities for SACAM in electronics. Examples include high-speed circuit elements, such as Josephson logic junctions, and new display materials. The latter could result in cheaper interfaces, which, together with the broad bandwidths of optical fibers and the cheap computational and control power of VLSI, could lead to a much larger market. Electronics, in spite of its remarkable impact on communications and computation and the key role of advanced materials in its development, is in many ways just beginning to show what it can do for technology and what SACAM can do for it.

B. Energy

An ever larger fraction of our resources is going into the production, conversion, storage, and conservation of energy. Survival of our technological society and improvement of less-developed societies will depend on the more efficient use of energy resources and on environmentally sound new resources. Here we discuss some SACAM opportunities in energy research and development.

- Heterogeneous Catalysis. Petroleum fuels require expensive pollution-control devices. Efforts will be directed toward the development of catalytic processes to eliminate the pollutants at the refinery. These efforts will require advances in understanding catalytic activity. Efficient catalysts for shale, coal, and other abundant sources of hydrocarbons are needed for both breaking chemical bonds to produce useful fuel and feedstocks and for forming bonds for property modification.

o Electrochemical Materials. Electrochemical processes such as those used in chlorine and aluminum manufacturing consume large amounts of energy. The opportunity exists for the development of new electrode materials using the Yi-Nb-Cl_2 electrode as a model.

o High-Temperature Hostile-Environment Materials. New energy sources, including fission, fusion, geothermal energy, and ocean thermal energy, and new approaches to higher-efficiency energy generation, such as magnetohydrodynamics, all involve demanding temperature, corrosion, or radiation environments. The ability of the SACAM community to provide nitrides, carbides, silicides, superalloys, and composites for these critical areas could well determine the extent and reliability of advances in these technologies.

o Solar Energy and Hydrogen Utilization and Storage. Progress in photovoltaics, liquid-junction solar cells, solar batteries, solar collectors, photodissociation techniques for producing hydrogen, and hydrogen storage is tightly tied to SACAM. Key contributions to energy production can be made in all of these areas. Both new advanced materials and older materials prepared by innovative lower-cost techniques are needed.

o Lighting Materials. Further opportunities in energy conservation through improved design of lamp envelopes, phosphors, and the like are closely coupled to the availability of new advanced materials.

o Materials Substitution. Increased vehicle efficiency through weight reduction depends on the development of new lighter materials meeting the requisite engineering criteria.

C. Environment

Advanced materials can play a vital role in improving the quality of the environment and making it possible to pursue desirable technologies without adverse environmental effects. In regard to efficient and environmentally satisfactory energy production and utilization, solar energy, fission, and fusion will depend for their ultimate success on yet-to-be-developed advanced materials. Photovoltaic solar energy requires low-cost solar-cell materials; fission requires inexpensive encapsulants for spent fission products that are environmentally stable for hundreds of years; and fusion requires materials that maintain their structural integrity under intense neutron irradiation.

Improved heterogeneous catalysts for vehicles and boiler stacks could result in significantly improved emission control. Heterogeneous catalysts could also make possible the reduction of high sulfur content of some fuels, notably petroleum and coal, before their use. Clearly, catalysts that facilitate the more-efficient and less-expensive removal of sulfides and other pollutants from stack gases would be a boon.

D. Opportunities Presented by Research

So far we have considered the opportunities for SACAM arising from societal and technological needs; the research itself generates additional opportunities.

The significantly lower cost of polycrystalline materials usually dictates their choice over single-crystal materials when they meet requirements. Consequently, ceramic materials have found many applications. However, improvement in mechanical properties, such as strength, ductility, and durability, and improved control of electronic properties over wider ranges would greatly increase the economic attractiveness and utility of ceramic materials. Research techniques, many of them originally used in physical metallurgy, are unraveling many of the mysteries of grain growth and control during densification and sintering in ceramics. Much basic progress is possible in the area of grain-boundary, interface morphology and microstructure characterization and control. Characterization of impurities in grain boundaries by the use of the analytical scanning transmission electron microscope (STEM), studies of the basic mechanisms of sintering, and studies of the relationship of the properties of ceramics to those of single crystals are examples in which progress in fundamental science driven by SACAM can lead to great benefits.

In the study of solids with interactions in less than three dimensions, theory and SACAM interact vigorously. Metal-organic chemists, solid-state chemists, solid-state physicists, and theorists have made this a fruitful field in U.S. university research. The theoretical results often suggest classes of materials and particular materials that would be worth synthesizing. Theories with predictive capability stimulate synthesis. Technological results have already come from such materials, for example, intercalation compounds for battery electrodes. We believe that this area will continue to be productive and should be pursued for the intellectual challenge it presents, to advance the connection between solid-state theory and synthesis, and for the likely technological spin-offs.

New techniques of synthesis are in many respects the life blood of SACAM. Emphasis on developing new techniques, exploiting techniques developed in other branches of science, and extending older techniques to new classes of materials should accelerate progress. Molecular beam epitaxy (MBE) and ion implantation have been applied to comparatively limited classes of materials. Their extension to the synthesis of more diverse materials should be productive, especially in view of the sensitive control of properties over small dimensions that MBE makes possible. Low-temperature techniques, including quenching from both the vapor and the liquid, have not been exploited for many classes of materials, and their further use by the SACAM community should be encouraged.

We believe that with respect to catalysis the characterization and understanding of real surfaces could be the next area where scientific opportunities will become a driving force for technological progress. The materials on which these studies should be made will have to be provided by SACAM techniques. SACAM researchers would like to begin to look at catalytic material with a complexity approaching that of catalysts used in technology; however, it is essential that these materials be prepared reproducibly with stoichiometry and defect chemistry well characterized and understood.

The need for theoretical work of many sorts is obvious. One aspect of theory that tends to be overlooked is the development of qualitative models to help the synthesist choose the most promising classes of materials and compounds to work with. Clearly, this kind of qualitative modeling, which permits classes of materials to be investigated for interesting properties without always being synthesized, can increase the effectiveness of synthesis.

IV. NEEDS AND SUGGESTED ACTIONS

U.S. industry is conducting a great deal of excellent research and development in SACAM. Tutorials based on this activity could be valuable to university programs. Universities are conducting some of the best fundamental research in SACAM; therefore, more interaction would benefit both industry and academia. To increase academic-industry coupling, we recommend that the exchange of personnel be encouraged as much as possible. Such exchanges could range from seminars to permanent movement of people from industry into university teaching appointments. Sabbaticals of from several months to 1 or 2 years could be particularly useful. The NSF Industry/University Cooperative Research Projects program could provide an effective means of encouraging cooperative ventures between universities and industries.

A large fraction of the sabbaticals taken by SACAM researchers in U.S. industry involve substantial interaction with the European SACAM community. There is a vigorous SACAM community in Europe with which U.S. researchers should interact; however, there is a possible problem in that the U.S. SACAM academic community is smaller and less active than the European, which could hamper reciprocal interaction.

The panel agreed that more solid-state chemists are needed in SACAM research. Solid-state chemistry is crucial to many SACAM activities.

The Panel also believes that the unique contributions of the national laboratories to SACAM should be studied. Further, the Panel found that data are lacking on the number of individuals in SACAM, the number being trained in SACAM, and similar demographic information. Such data are essential for future planning in the field.

PANEL 3. INTERDEPENDENCE OF SYNTHESIS AND CHARACTERIZATION

I. INTRODUCTION

The development of new materials usually involves a synergistic interaction between researchers with preparative skills (often chemists) and researchers with characterization skills (often physicists). We must continue to depend on this interaction of people, often from different disciplines, who are trained at the frontier of knowledge in these disciplines. A major concern is how to foster fruitful interaction between scientists from different disciplines; this chapter addresses this problem.

We consider various ways to foster such synergistic interaction. First, we examine the collaborative enterprise, particularly the key impediments to collaboration between scientists with differing backgrounds. Second, we briefly consider how education can facilitate interaction. Next we consider other means of encouraging interaction between the "preparers" and the "characterizers." We then discuss the problem of funding interdisciplinary research, new funding needs, and more effective use of funds. Last, we present our major observations and recommendations.

II. NATURE OF THE COLLABORATIVE ENTERPRISE AND IMPEDIMENTS TO IT

The preparation and utilization of advanced materials usually involves an interplay of individuals, each of whom has a distinctive background and set of skills. Figure 1 illustrates the usual situation, where S represents the synthesizer, C the characterizer, T the

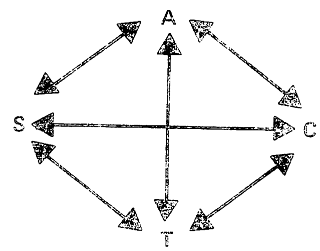

FIGURE 1 Elements in the SACAM collaborative enterprise.

theorist or other provider of the intellectual stimulus for the interaction of S with C, and A the applications. Although the interaction of any two of the components can initiate the eventual tetrahedral clustering represented, such collaboration can proceed only if it is adequately funded.

We shall concentrate on the relationship between synthesizer and characterizer, S and C, although other, perhaps equally important, analyses could be made for the other one-to-one interactions. The first question is why the components of the situation need be as they are. For example, why not train an interdisciplinary individual who is both synthesizer and characterizer? There may be circumstances in which this would be practical, but usually the creation of new advanced materials depends for many reasons on the interaction of researchers trained in separate disciplines. Perhaps the most important is that the preparation and characterization of advanced materials is carried out most effectively when the latest knowledge and expertise from each of the parent disciplines is applied. The range of possible advanced materials is virtually unlimited. Even for a specific application, a material developed on the basis of capabilities in one discipline, say metallurgy, might be inferior to a material that calls for capabilities in another discipline, such as biochemistry. Moreover, a given class of new materials might benefit from a thorough survey by characterizers from a variety of disciplines. Usually, the best course is to bring the specialists together.

Perhaps the single most important impediment to interdisciplinary collaboration is the peer review effect. Status, rewards, and funding are usually determined by the evaluations of knowledgeable specialists. Therefore, each individual will strive to maintain the greatest possible freedom of action for his research. To be a mere supplier or supporter in the work of another is to run the risk of being perceived as without a program, without initiative, uncreative, a technician, and so on. Consequently, any collaboration should be so arranged that each participant can cope effectively with these peer pressures.

Another major impediment is the language barrier. The specialized languages (jargon) of science are increasingly a barrier to communication between disciplines and subdisciplines. The language barrier that limits communication between preparers and characterizers of materials is often substantial. In dealing with this impediment, as with peer pressures, organizational and funding arrangements can help, but the essential requirement is the education of each specialist in the essentials of the disciplines of the other specialists. The theoretician can play a key role here. Theoreticians (model builders, knowledgeable interdisciplinary entrepreneurs, and other providers of intellectual stimuli), if they are "multilingual" and have the ability to explain the intellectual challenges inherent in an interdisciplinary program, can provide the greatest help in overcoming impediments to interdisciplinary interaction.

Other impediments are largely institutional and organizational and involve provision of appropriate technical support. External funding is usually also crucial. Suggestions on how to surmount these impediments follow.

III. EDUCATION

Universities provide the major opportunities for educational efforts to foster the synergistic interaction of preparers and characterizers of advanced materials. Yet, university researchers are usually subject to peer-pressure effects to a higher degree than researchers in other organizations and institutions. Special organizational efforts and funding arrangements are necessary to provide a favorable university setting for interdisciplinary work.

Where there is active interdisciplinary research, young scientists being trained in the individual disciplines can be brought into a collaborative effort while their attitudes are still in a formative stage. Such experience would expose the trainee to the dynamic interplay among the preparative and characterization disciplines and, as already noted, would usually involve intellectual challenges to the participants from each of the disciplines. Again, it is clear that a theoretician, conversant in the language of each discipline and aware of problems in the activities of each specialist, could help to initiate and foster such collaborative ventures.

The major aim should be to overcome the language barrier. The first requirement is to provide the incentive to make the effort, probably best done by involving the participants (students, postdoctoral researchers, and faculty) in mature and detailed investigations (i.e., in learning by doing). This kind of activity should be backed up with an appropriate curriculum. Since the most forbidding language barrier is that between chemistry and the solid-state sciences, particularly physics, the needs of the chemist and the experimental solid-state physicist provide examples. Texts that translate or interpret the language of solid-state physics into the language of chemistry, and vice versa, are urgently needed and should be helpful. Interpretative courses in solid-state physics (which would, in part, amount to language courses) should be provided for students with a standard background in inorganic and physical chemistry. These courses should require the same standards expected of physics students. The aim would be to provide the chemist with fundamental understanding of the operating principles of his physicist counterpart and so enable him to participate creatively in collaborative research. For the same reasons, and in a similar way, the physicist should be trained in the language and operating principles of the synthesis chemist.

The organizational and funding arrangements to foster interdisciplinary work on advanced materials in universities should be directed toward the cooperation of researchers in disciplines ranging from metallurgy to biochemistry and for the widest possible range of physical studies. The science of advanced materials may eventually benefit from contributions by the biological sciences as much as it has already from chemistry.

IV. INSTITUTIONAL AND ORGANIZATIONAL ASPECTS

Since industrial organizations are usually oriented toward specific goals and must make a profit to survive, collaborative enterprise usually lies at the heart of their efforts. The situation is different in academic institutions, where the emphasis is on the encouragement of the individual and the unique contributions he or she can make.

The smaller industrial laboratory faces the need to keep its scientists who are engaged in applied research aware of the latest developments in their parent disciplines. One way of dealing with this need is for industrial laboratories to develop relationships with academic institutions, such as the equivalent of the university professor's sabbatical leave. An industrial scientist would also bring new viewpoints and awareness of practical needs to the university research group. Joint industry-university research projects should be encouraged, and industrial researchers should be invited to participate in and give university seminars.

The growing sophistication and cost of apparatus used in the charaterization, and occasionally the preparation, of materials also present problems. In some instances, not even the largest companies can afford valuable modern facilities (e.g., a synchrotron and its associated instrumentation). More major centers for sophisticated state-of-the-art instrumentation, permanently staffed by dedicated and expert personnel, should be established. Industrial scientists should be encouraged to use such facilities. However, the need for an industrial laboratory to protect its proprietary interests must receive recognition when user contracts are drawn up. Again, cooperation between academic and industrial groups in sponsoring, funding, and using common facilities and instrumentation should result in benefits to all. More and expanded materials research laboratories (MRLs), centered on major campuses, might be an appropriate step.

Of particular concern are institutional and organizational innovations that might be applied in academic institutions to foster the interaction of preparer and characterizer. Given the importance of peer pressure and the all-too-common interdepartmental competition, special efforts are necessary to encourage collaboration. Funding arrangements can be especially helpful, but institutional and organizational improvements can also be made.

Setting up dedicated, well-manned, and continuously updated facilities (e.g., MRLs) outside the exclusive domain of any department or speciality group would overcome many difficulties. Such facilities would probably be of greater benefit to the synthesizer than the characterizer. In most cases, they would provide sophisticated and costly instrumentation on a routine service basis that would otherwise be largely unavailable. These facilities would also provide instrumentation for the characterizer. Such facilities should be administered with advice from a committee of users. Probably the most important aspect of such facilities would be service.

High-quality services require that the individuals providing the services have well-defined roles. It is particularly important to recognize that the success of a collaborative enterprise may depend more on routine or repetitive operations being well done than on intellectual input. Thus, a dependable person in a supportive role should be recognized as a valuable component of the enterprise.

Although most support personnel in a collaborative facility would be experts in instrumentation, in some centers it might be desirable to have a person whose province is preparative work. (Preparative work can be defined as the production of a known material in a particular form--single crystal, thin film, ultrapure specimen, control-doped specimen--as well as synthesis of a novel material.) This suggestion reflects recognition of the long-term nature of most synthesis enterprises. There is still much art, as well as science, in preparative activities. Time is needed for the frequently necessary trial-and-error process, and some synthesis reactions, even when the conditions are well defined, are inherently slow, because the kinetics for the growth processes are slow. Moreover, the skills and experience built up with the development of one material often will be of little value in the synthesis of another. These considerations discourage many from specializing in the preparative or synthesis aspect of research in advanced materials. Further, the low status frequently accorded those who do preparative work makes recruitment even more difficult. This situation could be the major reason for the lack of vigor and status of solid-state chemistry compared with solid-state physics in many U.S. universities.

Sound management, both in industry and academia, is crucial to the success of the collaborative enterprise. The good manager will look for compatible personalities as well as complementary knowledge and skills. The manager should also emphasize the appropriate incentives for the collaboration, be these profit or intellectual challenge. In the healthiest arrangement, the management position would be viewed as a service position to be filled by the person best able to provide the required services or expertise for a given period. A change in the required services or expertise could bring a change in management. With such an arrangement, industrial laboratories would be more responsive to changes in corporate goals, and universities would be more responsive to changes in research directions. An added benefit would be the improved situation of the working scientist whose relationship with his supervisor would be more nearly a peer relationship.

An appropriate professional organization, perhaps a division of the American Chemical Society, the American Physical Society, or the Materials Research Society, could do much to bring together scientists with the diversity of backgrounds needed in the study and development of advanced materials. Such an organization could also fulfill an important educational role with its scientific meetings and publications. It could enhance awareness of and encourage support for the interdisciplinary activities that it represents by arranging for the funding of prizes and awards for excellence of research.

V. EXTERNAL FUNDING

Funds, properly disbursed, can foster the desired collaboration between synthesizer and characterizer. Providers of support should encourage (or even require) the following characteristics of SACAM collaborative groups:

1. A group should be of sufficient size to provide the breadth of expertise needed for solution of the problems under investigation.
2. Each of the participants in the collaborative enterprise should be willing to play a dual role of active research and of service to collaborators.
3. Because research on advanced materials requires a broad-based approach to both preparation and characterization, a variety of experimental capabilities should be available. Theoretical expertise should also be available, for theory is crucial in providing intellectual stimuli for collaboration and sustaining collaboration.
4. Technicians, staff personnel, postdoctoral researchers, and graduate students should be included in

a working SACAM group to ensure a well-balanced, self-sustaining operation. The proper combination of participants should provide for

(a) Sample preparation for various physical measurements,

(b) Routine characterization,

(c) Continuity of broad-based programs,

(d) Sufficient flexibility to explore problems in new areas.

Some of the obstacles to this kind of interdisciplinary research could be overcome by different funding arrangements. These obstacles include the following:

1. Funding agencies often are not organized to handle large-group interdisciplinary proposals.
2. Peer review of collaborative interdisciplinary proposals is often unsatisfactory within the usual discipline-oriented funding structures.
3. Isolated investigators and small institutions are unable to mount efforts of critical size.
4. Larger programs often require partial support from several different agencies.
5. The total funding available for basic SACAM research is less than is commensurate with the potential scientific and technological benefits.

The particularly serious aspect of present funding policy is its generally short-term nature. It is difficult to provide guarantees of job security for the technical support staff. The requirement of funding renewal on a short-term basis also discourages those ventures that require a long-term investment. Many preparative projects are of this type. Some possible solutions are as follows:

1. Multi-investigator, interdisciplinary grants should be encouraged. In SACAM, such programs are likely to be more efficient and productive than the traditional single-investigator project. Specifically,

(a) Collaborative efforts within a single institution should be encouraged.

(b) Interinstitutional grants (with travel funds) should be available to help solve the problem of isolated investigators.

(c) Because technicians and staff personnel require longer-term funding, grants of longer duration, (at least 3 years) are needed. Grants that are not renewed should be phased out gradually over a period of a year or so rather than abruptly.

2. Interdisciplinary units should be established within the funding agencies. The NSF Division of Materials Research is a successful example of an attempt to encourage such endeavors. The peer review process employed by such units should include advisory panel representatives of the involved disciplines.

3. Partial support from several sources should be allowed and encouraged.

4. There should be an increase in overall support commensurate with the current growth and potential rewards of the field.

5. Centralized instrumentation centers should be kept up to date and manned by dedicated personnel. Provision should also be made in funding for the travel costs of the users of such facilities.

VI. CONCLUSIONS

The synthesis and characterization of advanced materials will continue to depend on the synergistic interaction of specialists in preparation and characterization. We believe that the barriers to interaction can largely be overcome by the following steps:

1. Funding should be specifically earmarked for interdisciplinary projects in SACAM and should provide for long-term preparation projects and long-term support personnel.
2. Peer review procedures appropriate to the interdisciplinary character of the work, including an advisory panel that is representative of the involved disciplines, should be employed.
3. Centralized instrumentation centers oriented toward service should be established and maintained at the state of the art.
4. Institutional and organizational changes should be made to facilitate the interaction of characterizer and preparer. Such changes should recognize the prime importance of incentives, such as profitable applications, particularly for industrial scientists, and intellectual stimuli and challenges to overcome the barriers to collaborative interdisciplinary research in SACAM.

5. Efforts should be made to improve communications, that is, lower the language barriers, among the disciplines involved in SACAM. Some possibilities for doing this include the following:

(a) Involvement of scientists, at the earliest practical stage of their training, in interdisciplinary projects.

(b) Encouragement of the preparation of texts to educate the synthesis chemist in the principles and language of solid-state physics and to educate the solid-state physicist in the principles and language of inorganic and physical chemistry.

(c) Organization of interdisciplinary seminars in which industrial scientists present material or participate in discussion.

6. Industrial laboratories, particularly the smaller ones, should consider encouraging their scientific personnel to spend periods of leave in academic institutions. This policy would help to keep industrial personnel scientifically up to date and would also bring academic personnel into greater contact with the problems of the industrial world.

PANEL 4. TRAINING AND ORIENTATION OF PERSONNEL FOR THE ADVANCED MATERIALS FIELD

I. INTRODUCTION

This panel was concerned with the training and orientation of scientists for research in SACAM. For three reasons we focus primarily on solid-state chemistry: first, chemical synthesis and characterization are major components of SACAM research; second, solid-state chemistry is a comparatively neglected field that is much less well established than solid-state physics, metallurgy, ceramics, and materials science and, therefore, requires particular attention; and third, almost all members of the Panel (see Appendix A) and others participating in the discussion at the time of the SACAM Workshop and afterward were either solid-state chemists or were concerned with hiring and working with solid-state chemists. In this chapter, we analyze the changes that must occur if sufficient numbers of persons are to be trained in the chemical aspects of research on advanced materials. We offer a caveat concerning the restriction of our consideration largely to solid-state chemistry: it is our impression that the ignorance of chemistry among solid-state physicists and other researchers in SACAM who are not chemists is as profound and inimical to the needs of SACAM research as is the ignorance of the solid-state among chemists. Most of our suggestions for increasing awareness and enhancing the regard of chemists for the solid state could be employed, with some modifications, to deal with the ignorance of chemistry among solid-state physicists and other nonchemist researchers in SACAM.

II. SCOPE OF CONSIDERATIONS

Solid-state chemistry has not yet become well defined through long practice, in contrast to, for example, organic chemistry, even though a great variety of solid materials is indispensable to modern science and technology. Industry has borne most of the task of training people to deal with chemical problems involving solids, partly because the relevant university-based training has been inadequate and research in advanced solid materials is inherently multidisciplinary in character and so can be easily organized in an industrial laboratory.

By solid-state chemistry we mean the preparation and chemical characterization of solids; such solids are largely inorganic but not exclusively so. Solid-state chemists traditionally have dealt with semiconductors and ionic inorganic solids, but many organic materials should be included in this field.

To exploit the potential of solid structures, extensive exploration of materials with coupled electronic and crystal structures and coupled stoichiometries should be undertaken. Imaginative research is needed, and it requires sound training. Chemistry curricula focus primarily on the principles underlying the behavior and synthesis of molecular systems, with little attention to extended solids. Nevertheless, chemists will continue to play a central role in pioneering research in advanced solid materials, for scientists whose specialities are in other disciplines are unlikely to have the background and orientation required for chemical synthesis and characterization. We propose modifications of the present educational system that would lead to a more balanced division of emphasis between molecule-oriented and solid-oriented thinking.

Why is a greater emphasis on solid-state chemistry desirable? There are many phenomena displayed by crystalline and amorphous solids that are not found in molecular systems. The essence of the difference is that the long-range order in a solid gives rise to conditions and properties not found in molecular systems. Furthermore, many solids lack molecular analogs. Although the study of chemical phenomena in solids is interesting, challenging, and important, it is largely ignored in undergraduate chemistry curricula and only occasionally treated in graduate courses in chemistry. In fact, solid-state physics evolved to handle certain aspects of solid-state chemistry. The development of the solid-state sciences has not benefited substantially from the uniquely chemical view of the interplay between structure and electronic configuration; for example, adequate and useful models of chemical bonding in solids are not available. The value of the chemical viewpoint is verified by the contributions of chemists to fields initiated by physicists, such as spectroscopy and crystallography. The panel believes that the study of solids would benefit substantially from greatly increased emphasis on chemical modeling and theory.

The phenomena unique to solids often involve long-range and collective effects, and an appreciation of these effects requires specialized training. Superconductivity is a good example. Advances in this field are closely tied to the synthesis of novel materials, and so depend significantly on the contributions of chemists. Many of the possible binary compounds have already been explored, and the opportunities for the future lie in ternary and more complex systems requiring a high level of chemical inguenuity. Charge-density waves in the layered compounds, incommensurate lattices, and metal-to-insulator transitions illustrate the richness of behavior to be expected in compound solids. Surface studies supply an important link to such applied problems as catalysis, electroplating, and corrosion, while at the same time they provide a link between the solid-state sciences and the complementary fields of organic and physical chemistry.

Studies of solids also yield new insight into basic chemical and physical principles. Studies of mixed valence compounds, cluster compounds, nonstoichiometric materials, and extended defects are examples where the fundamental nature of the chemical bond in a solid results in behavior not predicted by traditional chemistry. Frequently such effects can be analyzed in depth most effectively with the use of solid-state probes. In addition, the diffusion of ions in solids may provide model systems that will enhance our understanding of transport processes in general while aiding in the development of novel ionic conductors for electrochemical applications.

In addition to the intellectual challenges of solid-state chemistry, there is an industrial demand for solid-state scientists. The energy industry is concerned with numerous problems related to hydrogen embrittlement, catalysis, friction, wear, solar energy (thermal and photovoltaic), and energy storage, all of which require chemical ingenuity. The communications and computer industries need new and improved optical communications devices and high-speed computer components. The development of the next generation of optical storage, recording, and signal-processing technology will require a substantial solid-state effort. The automotive industry needs novel materials that are lightweight, durable, and do not require copious amounts of energy for their production.

Against the background of these pressures for the traning of new solid-state scientists, the magnitude of the U.S. academic effort lags behind that of other advanced countries and proportionately behind that of other scientific disciplines in the United States. This perception can be documented by the comparisons of publication rates given in Appendix B, even though Appendix B emphasizes solid-state physics. The problem seems to be particularly severe in synthetic solid-state chemistry for which the major academic centers are in Europe.

Preparative solid-state chemistry is a well-recognized and accepted discipline within chemistry departments at many European universities. The French and German university systems have a long history in the training of synthetic solid-state chemists. Unlike the great majority of chemistry departments in the United States, the areas of specialization in many European universities have included emphasis on solids rather than only solutions and gases. Examples of such university research centers can be found at Bordeaux, Nantes, Grenoble, Münster, Göttingen, Freiburg, and Stuttgart. In most cases, these centers receive government support and funding and are, at the same time, an integral part of the chemistry training programs.

In Norway and Sweden, the emphasis has been on crystal chemical problems. However, the synthesis aspect of solid-state science has also been underscored at such institutions as Oslo, Uppsala, Stockholm, and Lund. In the United Kingdom, synthesis and characterization have been noted features in inorganic chemistry at Oxford and are increasingly important in physical chemistry at Cambridge. Such encouragement within chemistry departments and by governments results in sufficient numbers of trained synthesis-oriented scientists to satisfy the industrial, governmental, and university needs of these countries.

III. UNDERGRADUATE EDUCATION

The pattern of chemistry education in the United States generally reflects a broad overview of the physical principles and basic concepts of chemistry. At present, however, this overview understates the importance of solids and the unique chemical and physical properties of condensed phases. As a consequence, our concern here is the development of a stimulating introduction to the basic concepts of solid-state chemistry at the undergraduate level.

At the introductory level, solid-state chemistry has not been integrated into the basic curriculum, even though it is at this stage or earlier that qualified students should be exposed to the field. Few, if any, general chemistry textbooks present an adequate introduction to the chemistry of the solid state. This lack, coupled with the recent decline in the teaching of classical inorganic chemistry in introductory courses, results in the near absence of solid-state chemistry from introductory and subsequent courses. Yet a successful graduate program in solid-state chemistry is predicated on a pool of motivated students aware of the possibilities of the field. The interest in this area is illustrated in Appendix C by a list of pertinent articles from the Journal of Chemical Education during the period 1974-1981. In addition, an analysis of the coverage of solids in four popular general chemistry texts (which are said to have about 70 percent of the market) is given in Appendix D.

We believe that solid-state chemistry should be introduced, at appropriate times, throughout the student's undergraduate experience. It is desirable to introduce this material early, preferably to freshmen, so that students can begin to gain an appreciation of solids at the outset. At the same time, a much-needed introduction to solid-state chemistry can be provided for engineers and other students who may never take another chemistry course. In addition, we recommend that, whenever possible, an introductory or advanced course in solid-state chemistry be offered, with physical chemistry as a prerequisite.

There is also an excellent opportunity to include demonstrations and laboratory experiments in solid-state chemistry in the usual chemistry courses. For example, a suitable freshman chemistry laboratory experiment is to prepare copper sulfide, which is an example of a nonstoichiometric compound. Unfortunately, it is often presented as an example of a stoichiometric compound. At the upper level, a foundation in thermodynamics, phase equilibria, and crystallography is consistent with a sound pedagogical approach to physical chemistry and is essential to understanding solids.

Inorganic chemistry courses are a logical place to extend the presentation of solid-state chemistry, to introduce topics such as nonstoichiometric coumpounds, common structural types, and the reactions of solids, and to give practical laboratory experience. Electronic, magnetic, and optical phenomena can be abundantly illustrated by examples from the solid state. Such illustrations, in addition, provide opportunities to discuss various properties that reflect the three-dimensional nature of solids.

Of paramount concern is the development of laboratory techniques germane to the preparation and characterization of coupled and novel materials. Inorganic and integrated physical inorganic laboratories provide logical opportunities for the introduction of solid-state chemistry experiments, such as the synthesis of ferrites followed by x-ray and magnetic characterization, synthesis of and conductivity measurements on tungsten bronzes and silver halide ionic conductors, and the chemical vapor transport growth of sulfides. Experiments of this general nature require proper equipment, including furnaces, x-ray diffractometers, magnetic balances, and equipment for electrical measurements. Such equipment is generally more expensive than the equipment for traditional experiments, thus the funding of educational developments in this area requires special consideration.

Undergraduate research projects provide an excellent opportunity for the introduction of solid-state chemistry to students. This concept should also be extended to students at the high school level.

Many chemistry instructors do not have the necessary background to incorporate solid-state principles readily into the curriculum. Accordingly, <u>we recommend the establishment of a series of summer workshops to offer in-service courses to college faculty members</u>. These workshops would cover specific topics in detail and indicate ways that solid-state concepts might be integrated into existing courses. If the desirability of including material on solid-state chemistry in the chemistry curriculum can be demonstrated to college instructors, the demand for the inclusion of such material in textbooks surely would follow. Another result of these tutorial workshops would be written source material for teachers wishing to include solid-state chemistry topics in their courses. Some additional suggestions are the following:

1. Inclusion of solid-state articles of a tutorial nature, as well as tested classroom demonstrations, in the Journal of Chemical Education or other generally available sources for teachers.
2. Active participation of solid-state chemists in the ACS Speakers' Bureau.
3. Presentations by industrial speakers in academic institutions to highlight the impact of solid-state chemistry on modern technology.

A noteworthy step relevant to our first suggestion is the "State of the Art Symposium: Solid State Chemistry" in the August 1980 issue of the Journal of Chemical Education (see Appendix C).

Finally, we recommend that a clearinghouse be established to promote interaction among persons in industry and academia and persons in various departments in universities concerned with chemical apsects of condensed materials science and technology. Such a clearinghouse would solicit and publicize opportunities for summer appointments, appointments of longer duration, and joint research and training efforts. In addition, written materials that could be used for training would be exchanged. This clearinghouse might also prepare a brief description of careers in solid-state chemistry to be circulated to advisers of students. We recommend that the Solid State Subdivision of the Inorganic Chemistry Division of the American Chemical Society be requested to consider operating such a clearinghouse. The recently formed "Solid State Information Bank and Clearing House" [see J. Chem. Educ. 57, 530 (1980)] is an encouraging step in this direction, and we strongly urge that this group be supported by the chemistry and materials communities.

IV. GRADUATE EDUCATION

Graduate education of scientists in the synthesis and characterization of advanced materials requires faculty who are knowledgeable in these areas and maintain vigorous graduate research programs. These mentors must communicate their "art" as well as the known science to students who come at present from some traditional division of chemistry. The current shortage in the United States of PhDs trained in SACAM, particularly the chemical aspects, can be traced directly to a scarcity of faculty active in this area at the major research and graduate education universities in the United States. Because of the way in which universities generally are, and probably will continue to be, organized, a research field has the best chance of flourishing if its faculty has a secure departmental home. Solid-state science can be related to a large number of university disciplines, among which are physics, materials science, metallurgy, ceramics, geochemistry, chemistry, and electrical engineering. However, for those portions of solid-state science that embody an emphasis on synthesis and characterization of advanced materials, it seems that the appropriate faculty home is in chemistry or, perhaps, materials science departments. Chemistry departments seem an attractive possibility because (a) many workers already in the field received their training in chemistry departments; (b) chemistry departments tend to be large and often can make room for an additional specialty more easily than other relevant departments; (c) chemistry is usually required of students in the other related fields, so that having solid-state specialists on chemistry faculties might increase the number of students exposed to solid-state concepts early in their careers; and (d) the science of chemistry would be enriched by the development of this important, albeit neglected, part of the discipline--the chemistry of the condensed state.

In our view, the education of people who will contribute to the advancement of solid-state science by synthesizing materials that are novel and significant in their chemical, structural, electronic, morphological, and other properties should be based on a traditional specialization, such as chemistry, physics, or metallurgy. It is the depth of understanding that permits the application of the developing principles to the solid state.

However, effective research in an interdisciplinary area such as solid-state science requires that workers in different aspects of the field and in different academic disciplines communicate closely and work together. High-quality interdisciplinary work requires the collaboration of experts in the pertinent facets of the different disciplines. This interaction is accomplished at a number of institutions through interdisciplinary materials research laboratories. Indeed, a test of the effectiveness of these laboratories might be the degree to which they have established productive interaction among faculty and students from different academic disciplines. Another aspect is ensuring that students from the relevant academic disciplines learn enough of one another's language that they can communicate effectively and efficiently with one another. The synthesizer must be able to talk with the solid-state theoretician and with materials scientists and engineers. The technique usually used to promote this competence at an early stage is to encourage students to take courses in related areas.

Increased numbers of solid-state scientists on chemistry faculties would have a number of positive benefits: (a) training of the manpower needed for SACAM; (b) a more balanced, thus improved, program of teaching and research activities in chemistry departments; (c) increased understanding of the relationship of solid-state science to chemistry; and (d) new, basic research results, both theoretical and experimental.

There are difficulties that result from forces within and outside of chemistry departments. Because a faculty member's career depends on judgments by his professional peers, there is pressure to obtain recognition among others in the same academic field (e.g., chemistry). A young physical chemist's career will be advanced more if he is recognized by other chemists than if he is recognized by, for example, metallurgical engineers. (The same apparently is true in reverse for a young metallurgical engineer.) There is also pressure to obtain significant and stable research funding, which is further complicated by differences in the handling of basic and applied research in funding agencies. These problems can best be dealt with by increasing the awareness within the entire materials community of the challenges and rewards of collaborative research on advanced materials.

V. BEYOND THE UNIVERSITY EXPERIENCE

Most advanced-degree scientists from solid-state chemistry and materials science programs go into industrial or federally financed laboratories. These laboratories typically are organized on a multidisciplinary basis, that is, in terms of projects or programs of several scientists and engineers whose specialties and strengths complement one another. The role of the synthetic solid-state chemist is to design and prepare materials, often materials having new compositions; the ceramist or metallurgist is concerned with mechanical and multiphase aspects; the physical scientist or physicist is primarily responsible for the physical characterization. Generally, one individual is not asked to do creative science across the whole range but rather to deal with one part in depth and to interact with colleagues in the program.

Such multidisciplinary projects require the ability to conduct research in depth, whether it is synthesis, characterization, or theory. An appreciation of those aspects of materials science that are complementary to one's own specialty, together with their basic theory and terminology, is also necessary. A broad familiarity with the range of disciplines encompassed by SACAM is necessary but is inadequate by itself; in-depth training in some one of the SACAM disciplines is an irreplaceable requirement.

Most industrial and other multidisciplinary research and development centers are prepared to continue the training of their staff, broaden their areas of competence, furnish background in new topics, and provide opportunities to gain experience in multidisciplinary efforts. Of course, such on-the-job training represents a substantial investment and generally presupposes an initial capability to do creative work.

A key contribution in the development of many significant and useful solid-state materials has been that of the synthetic solid-state chemist who first envisioned the new material and then succeeded in preparing it. In such efforts art is involved, but, more importantly, so are an understanding of atomic behavior, electronic interactions, geometric relationships, and reaction chemistry and the skill to combine all of these. Of all roles in materials science research, that of the preparative chemist is the least well represented in terms of the numbers of academic faculty and graduating scientists. Solid-state science in general will continue to benefit from the infusion of new concepts that arise from the creation of new materials and structures. We urge the members of university physical science faculties, particularly those in chemistry, to recognize the challenging and pivotal role that solid-state chemistry must play in the future of materials science. The intellectual possibilities, by themselves, are sub-

[redacted]

stantial, and the needs in catalysis, energy technology, electronics, transportation, and chemical processing provide numerous exciting opportunities.

VI. CONCLUSIONS

There are encouraging signs that solid-state chemistry is beginning to receive the recognition and attention that it deserves in academia in the United States. There have been numerous technical symposia on solid-state chemistry at recent ACS meetings. The first and second Gordon Research Conferences on Solid State Chemistry were held in the summers of 1980 and 1982, and a Gordon Research Conference on the Physics and Chemistry of Solids was held in the summer of 1981. The August 1980 issue of the Journal of Chemical Education contains 14 papers from a symposium on Solid State Chemistry in the Undergraduate Curriculum. The Solid State Subdivision of the ACS has created a Solid State Information Bank and Clearing House. While these are noteworthy and substantial steps in the right direction, they are only a start. Solid-state chemistry is only beginning to be recognized as an identifiable discipline in U.S. universities and among the general U.S. scientific community.

PANEL 5. INSTRUMENTATION AND FACILITIES

I. STATUS, SOURCES, AND SPECIAL PROBLEMS OF INSTRUMENTATION FACILITIES COSTING MORE THAN $250,000

A. Background

The group that reviewed these large facilities had detailed knowledge of the status of scanning transmission electron microscopy, synchrotron radiation facilities, high-intensity neutron sources, and the national sub-micrometer research facility. All the funding is from federal sources--the Department of Energy (DOE) and the National Science Foundation (NSF). These large facilities have a great deal of experience and success in providing access and service for a large number of users and have developed suitable procedures for this purpose. These include the review of proposals by an outside committee.

B. Special Problems and Recommendations

All facilities provide users with technical assistance, although there are no formal courses on the use of a given facility. Lack of understanding of the capabilities of a facility often limits its use. Brief courses for potential outside users are the solution to this problem, and <u>we strongly recommend the institution of such courses</u>.

The national submicrometer research facility at Cornell University provides for research and education in technologies important to the electronic and computer industries. There are other important technologies that are not adequately supported by academic research and education centers, for example, photography and heterogeneous catalysis. University centers similar to the submicrometer facility could play important roles in maintaining preeminence in many areas of science and technology that employ advanced materials, and we recommend that the establishment of such centers be given careful consideration.

Until recently there was a serious problem, particularly at the synchrotron radiation facility at Stanford, but also at other DOE laboratories, with DOE patent, technical information, and indemnity policies. These policies infringed on proprietary technologies; consequently, industrial scientists were not using DOE facilities when proprietary technologies were involved, even though in many cases such use would have been of great help. Apparently this problem has been adequately resolved by a change in DOE policies, and the use of DOE facilities by industrial groups is increasing rapidly. This, then, is an example of a problem that was resolved reasonably quickly once it was recognized.

Many of the comments and recommendations that apply to instrumentation in the $50,000 to $250,000 range are also appropriate here.

II. STATUS, SOURCES, AND SPECIAL PROBLEMS OF INSTRUMENTATION IN THE $50,000 TO $250,000 RANGE

A. Typical Equipment under Consideration

Such equipment includes:

- Surface analysis equipment--single- or multiple-use equipment for LEED and ion scattering
- Fourier-transform infrared spectrometers
- Computer-controlled laser Raman spectrometers
- High-resolution gas chromatograph/mass spectrometer combinations
- Transmission electron microscopes
- Low-temperature facilities (for ^{4}He liquefaction, ^{3}He/^{4}He dilution refrigeration, and the like)
- Computerized single-crystal diffractometers, rotating anode x-ray sources, and low-temperature diffraction equipment
- Ion-implantation equipment

B. Sources

The predominant sources for the funding of such equipment are the NSF and DOE. Obtaining funds, even matching funds, from nonfederal sources is becoming increasingly difficult.

C. Special Problems

Frequently, a full-time technician is needed for efficient operation of this type of equipment, especially when the equipment is shared among several users. Funds for the employment and training of such technicians are difficult to obtain as part of the equipment request. Maintenance is a major need, but it is rarely budgeted or anticipated.

Although most prototype equipment in this range was developed in the United States, the commercial versions are often available only from foreign suppliers. For example, most transmission electron microscopes are purchased from Japan or Europe; the same is true of x-ray diffraction equipment. This is situation is undesirable, for replacement parts are often difficult to obtain and maintenance problems are aggravated. It is also undesirable from the viewpoint of the U.S. balance of payments. In addition, the lack of domestic suppliers of high-technology instrumentation precludes the close interaction between the user and the manufacturer that is needed to produce state-of-the-art instrumentation and its associated technology. Many potential users in industry and at universities are not aware of the equipment available at a given institution or are not familiar with the capabilities or operation of the equipment. Dissemination of lists of available equipment and facilities to the solid-state science community and the initiation of short training courses for potential users of state-of-the-art instrumentation would thus be particularly useful.

There are no simple mechanisms by which equipment purchased with federal funds can be used by the industrial community. Yet technological advances depend on the application of state-of-the-art instrumentation in industry. Although industrial scientists would usually be willing to buy time to use such instrumentation, they are frequently unwilling or unable to make the commitment to purchase the expensive instruments and employ the specialists necessary for their operation.

D. Recommendations

Federal agencies that provide funds for the types of equipment discussed in this section should be encouraged to disseminate to the solid-state science community lists of available equipment and facilities including (a) equipment characteristics, (b) probable availability, (c) persons to contact, and (d) charges for use and support.

Research centers where equipment is located should initiate short courses and training programs for potential users. Funds should be provided to support visiting scientists so that they can learn how the instrumentation operates.

The reasons for the poor state of U.S. scientific equipment manufacturing should be investigated. This situation is particularly surprising because many of the prototype instruments were developed by U.S. scientists. A closer interplay of science and technology, leading to the commercialization of new instrumentation for materials characterization, would be highly beneficial.

The part-time use of federally purchased equipment by industrial and other outside scientists should be encouraged. Procedures should be provided to charge equipment time to outside users to aid their part-time access to modern federally funded scientific instruments at universities and national laboratories.

The services of technicians and other support personnel who may be necessary for efficient utilization and maintenance of instruments, especially shared instruments, should be included, whenever possible, in the normal operating procedures and costs.

Many of these special problems and recommendations for dealing with them are also relevant to instrumentation and facilities costing more than $250,000.

III. STATUS, SOURCES, AND SPECIAL PROBLEMS OF INSTRUMENTATION COSTING LESS THAN $50,000

A. Typical Examples of Equipment under Consideration

Such equipment includes:

- Spectrometers
- NMR and ESR equipment
- X-ray diffraction systems
- Mass spectrometers

- Mössbauer systems
- Mechanical testing devices
- Thermoanalytical equipment

B. Sources

The primary sources of funding for new equipment in this range are the NSF and DOE. Some funding is available through the Department of Defense (DOD) agencies [Office of Naval Research (ONR), Air Force Office of Scientific Research (AFOSR), Army Research Office (ARO), and Defense Advanced Research Projects Agency (DARPA)]. The recently announced DOD-University Research Instrumentation Program is particularly noteworthy. In addition, funding is sometimes available through state agencies. University equipment funds are generally limited.

Useful equipment can also be found on federal government excess property lists. Another source for equipment that has served its original purpose but is still usable is private industry. Unfortunately, equipment obtained from these two classes of sources is frequently outmoded and is almost never up to the state of the art. In addition, such equipment is increasingly available for use at national laboratories.

C. Special Problems

Although a great deal of good science is carried out with the aid of older, used equipment, almost all such equipment that is available is from 10 to 15 years behind the state of the art. A great deal of this equipment was acquired in the late 1950s and early 1960s, during the period of expansion of most universities. Much of it is now poorly maintained and deteriorating. Frequently, funds are not available for service contracts or other forms of maintenance. Requests for new models of this "conventional" equipment often are denied because of (a) lack of glamor, (b) the notion that a university should renew its own equipment, and (c) the view that limited equipment funds should be reserved for purchase of new types of instruments.

D. Recommendations

The panel proposes the following steps:

A coordinated systematic program or set of programs should be initiated to support the upgrading of existing equipment and the purchase of new equipment.

Provision should be made for maintenance of instruments and other equipment. For example, funds for the purchase or fabrication of new instruments and equipment could require that additional fund be set aside to cover the cost of their maintenance and could also be accompanied by funds to maintain and upgrade already existing equipment.

Small equipment requests should be supported in such ways as to encourage collaboration within departments, among departments at a given institution, and among departments at neighboring institutions.

Means should be devised to facilitate access to small equipment at larger institutions and centers. Distribution within the solid-state science community of a list of such equipment would be a useful first step.

IV. LEVEL AND SOURCES OF SUPPORT FOR INSTRUMENTATION AND FACILITIES

The major sources of funds for equipment and facilities for materials synthesis and characterization are the NSF Division of Materials Research and the DOE Office of Basic Energy Sciences.

Excluding the major facilities, there were about $20.5 million available for equipment from NSF and $16.3 million from DOE during fiscal year 1981. Of particular significance is the Regional Instrumentation Facilities Program of NSF; this program promises to have a major beneficial impact on equipment needs in selected areas of chemistry, physics, and materials science. The DOE Office of Basic Energy Sciences supports major facilities at the national laboratories. The new synchrotron light source at Brookhaven National Laboratory, the various high-energy electron microscope facilities under construction, and the intense pulsed neutron sources at Argonne National Laboratory and under construction at Los Alamos National Laboratory will all have significant impacts on materials characterization in the near future.

The NSF supports major materials synthesis and characterization facilities through the Materials Research Laboratories and various research centers located at universities. The most recent of these facilities is the National Research and Resource Facility for Submicron Structures at Cornell University.

Another particularly significant program is the new DOD-University Research Instrumentation Program. This program began in fiscal year 1983 and is budgeted at $30 million per year for 5 years. It is estimated that approximately 20 percent of these funds will be spent on instrumentation for advanced materials research.

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APPENDIXES

APPENDIX A. THE SACAM WORKSHOP

I. STEERING COMMITTEE (RESPONSIBLE FOR THE ORGANIZATION OF THE SACAM WORKSHOP)

Murray Robbins, Bell Laboratories, Inc., Murray Hill, New Jersey, <u>Chairman</u>
Neil Bartlett, University of California, Berkeley
Hugo F. Franzen, Iowa State University
Theodore H. Geballe, Stanford University
Frederick Holtzberg, IBM Corporation, Yorktown Heights, New York
Mitchell J. Sienko, Cornell University
M. Stanley Whittingham, Exxon Research and Engineering Company, Linden, New Jersey
Robert E. Hughes, Cornell University, Liaison with Solid State Sciences Committee

II. PANELS

Panel 1: Problems Related to the Character of SACAM Research

Hugo F. Franzen, Iowa State University, <u>Chairman</u>
John D. Corbett, Iowa State University
John B. Goodenough, Oxford University
Larry L. Hench, University of Florida
Frederick Holtzberg, IBM Corporation, Yorktown Heights, New York
Alan G. MacDiarmid, University of Pennsylvania
David A. Shirley, University of California, Berkeley
Fred E. Stafford, National Science Foundation
Michell J. Sienko, Cornell University

Panel 2: Scientific Challenges Arising from Technological Needs

Robert A. Laudise, Bell Laboratories, Murray Hill, New Jersey, Chairman
Harvey K. Bowen, Massachusetts Institute of Technology
John B. Bush, Jr., General Electric Company
Theordore H. Geballe, Stanford University
Merill W. Shafer, IBM Corporation, Yorktown Heights, New York
Arthur W. Sleight, E.I. du Pont de Nemours & Company, Inc.
Allan J. Strauss, Lincoln Laboratory, Massachusetts Institute of Technology
Jack H. Wernick, Bell Laboratories, Murray Hill, New Jersey
M. Stanley Whittingham, Exxon Research and Engineering Company, Linden, New Jersey

Panel 3: Interdependence of Synthesis and Characterization

Neil Bartlett, University of California, Berkeley, Chairman
David Adler, Masschusetts Institute of Technology
Aaron N. Bloch, The John Hopkins University
Warren E. Falconer, Bell Laboratories, Murray Hill, New Jersey
Alan J. Heeger, University of Pennsylvania
Jurgen M. Honig, Purdue University
Leonard V. Interrante, General Electric Company
John M. Longo, Exxon Research and Engineering Company, Linden, New Jersey
Fred Wudl, Bell Laboratories, Murray Hill, New Jersey

Panel 4. Training and Orientation of Personnel for the Advanced Materials Field

Leroy Eyring, Arizona State University, Chairman
F. Jerry Darnell, E.I. du Pont de Nemours & Company, Inc.
Smith L. Holt, University of Georgia
Edward Kostiner, University of Connecticut
Donald S. McClure, Princeton University
Gerd M. Rosenblatt, Pennsylvania State University
Duward F. Shriver, Northwestern University
Arthur H. Thompson, Exxon Research and Engineering Company Linden, New Jersey
Aaron Wold, Brown University

Panel 5: Instrumentation and Facilities

Gabor A. Somorjai, University of California, Berkeley, Chairman
Ephraim Banks, Polytechnic Institute of New York
Arthur I. Bienenstock, Stanford University
Richard C. Brdt, Pennsylvania State University
Rolfe Herber, Rutgers University
Dean L. Mitchell, National Science Foundation
David L. Nelson, Office of Naval Research
Donald K. Stevens, Department of Energy

III. REPORT COMMITTEE (RESPONSIBLE FOR THE PREPARATION OF THE SACAM SUMMARY REPORT)

Robert A. Laudise, Bell Laboratories, Murray Hill, New Jersey, Chairman
Frederick Holtzberg, IBM Corporation, Yorktown Heights, New York
Allan G. MacDiarmid, University of Pennsylvania
Murray Robbins, Bell Laboratories, Murray Hill, New Jersey
M. Stanley Whittingham, Exxon Research and Engineering Company, Linden, New Jersey

IV. PARTICIPANTS (REGISTERED FOR THE SACAM WORKSHOP)

A. F. Armington, U.S. Air Force, RADC/ESM
D. L. Ball, Air Force Office of Scientific Research
L. H. Bennett, National Bureau of Standards
B. Chamberland, University of Connecticut
G. Y. Chin, Bell Laboratories
M. H. Christmann, 3M Company
A. G. Chynoweth, Bell Laboratories
L. E. Conroy, University of Minesota
D. O. Cowan, Johns Hopkins University
M. A. DiGiuseppe, Allied Chemical Company
D. W. Elliot, Air Force Office of Scientific Research
A. J. Epstein, Xerox Corporation
B. J. Evans, University of Michigan
W. P. Evans, Union Carbide Corporation
W. J. Fredericks, Oregon State University
M. Greenblatt, Rutgers University
J. C. Hempel, Swarthmore College
D. J. Hodgson, University of North Carolina

J. A. Kafalas, Lincoln Laboratory, Massachusetts Institute of Technology
W. F. Little, University of North Carolina
J. W. McCauley, Army Materials and Mechanics Research Center
J. S. Miller, Rockwell International
S. Mroczkowski, Yale University
C. E. Myers, State University of New York, Binghamton
A. J. Nozik, Solar Energy Research Institute
N. Palladino, Snamprogetti U.S.A., Inc.
A. H. Reis, Jr., Argonne National Laboratory
R. W. Rice, Naval Research Laboratory
W. M. Risen, Jr., Brown University
H. Robson, Exxon Research and Engineering Company
R. S. Roth, National Bureau of Standards
J. E. Sarneski, Fairfield University
A. E. Schweizer, Airco
A. G. Sigai, Cerox Corporation
H. Steinfink, University of Texas, Austin
G. D. Sturgeon, University of Nebraska, Lincoln
B. I. Swanson, University of Texas, Austin
D. R. Ulrich, Air Force Office of Scientific Research
W. H. Watson, Texas Christian University

V. PLENARY SPEAKERS

The four plenary speakers were asked to present 40-minute talks on specific views of SACAM. The following abstracts contain some of the highlights of the plenary talks.

1. N. B. Hannay - SACAM: A Technological View

In this talk, recognition of the importance of interdisciplinary research was traced to the mid-1950s when the Advanced Research Project Agency (ARPA) and the Atomic Energy Commission (AEC) undertook the creation of interdisciplinary laboratories for materials research. Some of the areas cited as exemplifying the importance of interdisciplinary research were

1. Transistors
2. Dislocations
3. Band structure
4. Single-crystal growth

Some recent, important developments in characterization techniques cited were

1. Neutron activation analysis
2. Scanning transmission electron microscopy
3. X-ray absorption photoelectron spectroscopy
4. Rutherford backscattering

Synthesis of advanced materials was defined as the preparation of novel or new materials with desired properties for a given purpose. Some recent advances in synthesis cited were

1. Intercalation compounds for Li battery electrodes
2. Optical fibers for communications
3. III-V compounds for laser diodes
4. Molecular beam epitaxy

Thoughout, the importance of the interdisciplinary nature of materials research was emphasized.

2. J.B. Goodenough - SACAM: A View from Another Country

As in the first talk, advanced materials were defined as novel or new materials prepared with desired properties to fulfill a specific function. It was noted that materials problems generally originate from an engineering requirement. In order to develop a material to fulfill a desired function, scientists involved in chemistry, characterization, and theory must interact synergistically. The need for maintaining groups large enough so that all the diverse aspects of SACAM research in various disciplines was emphasized.

A comparison of the form of research support maintained by other governments was examined, with emphasis on the Japanese and French systems.

In Japan, universities and industrial institutions carry on research much as in the United States. The basic research effort maintained by the Ministry of Education includes both university and industry research (much along the lines of the Max Planck Institute in Germany). Technological research is supported by the Ministry of International Trade and Industry. The French system is similar to the Japanese system. In France, the Centre National Recherche Scientifique (CNRS) supports industrial scientists in the universities and also maintains a separate research institute (e.g., Grenoble).

The need to strengthen the position of solid-state chemistry within chemistry departments in universities in the United States was emphasized.

3. D. A. Shirley - SACAM: An Academic View

It was argued that synthetic inorganic chemistry is at the heart of the synthesis of advanced materials. The importance of research into the preparation of materials that appear to have no immediate use was discussed. It was asserted that this form of materials research leads to new methods of synthesis and novel properties. Various aspects of basic research in materials synthesis at a number of universities were discussed. Special emphasis was placed on the almost total lack of knowledge of the solid state on the part of many BS and PhD graduating chemists.

4. D. K. Stevens - SACAM: The Government Agency

This talk dealt predominantly with funding. The point was made that other commitments and budgetary constraints indicate that it is not reasonable to expect significant increases in funding in the foreseeable future. Requests for large amounts of additional funding would not be realistic.

APPENDIX B STATUS OF UNITED STATES PUBLICATIONS IN THE SOLID-STATE SCIENCES

Documentation of the status of publications in the solid-state sciences can be obtained by searching the computer-compiled abstracting services. For this survey, a search was made of Physics Abstracts (produced by INSPEC). The objective was to compare the number of publications in the solid-state sciences from the United States and from U.S. universities with the total of such publications. A second objective was to see how many U.S. universities are active in the solid-state sciences.

Tables B.1-B.4 compare the number of publications in the solid-state sciences from the U.S. universities with all publications in the solid-state sciences. In Table B.5, the universities that contributed more than 20 publications to the five selected journals considered in Table B.3 were identified. All of these searches cover 1977-1979.

These data suggest that U.S. universities contribute only a small fraction of the total publications in the solid-state sciences (ranging from about 3 percent in Table B.1 to 9.5 percent in Table B.4 to 27 percent in Table B.3); U.S. contributions in other disciplines are higher (~50% for publications in Physical Review, excluding Section B).

The tabulation of universities in Table B.5 also suggests that much of the U.S. effort in solid-state sciences comes from a few major centers.

It should be noted that these data are biased in favor of U.S. universities since only English language journals are compared.

TABLE B.1 Contributions to the Solid State Sciences Literature[a]

Publications	Number	Normalized
Total publications	32,867	1
United States	7,086	0.22
U.S. universities	1,003	0.03

[a]Publications listed in Sections 60 (Condensed Matter: Structure, Thermal and Mechanical Properties), 70 (Condensed Matter: Electronic Structure, Electrical, Magnetic and Optical Properties), and 81 (Materials Science) of *Physics Abstracts*.

TABLE B.2 Publications in *Physical Review*, excluding Section B

Publications	Number	Normalized
Total Publications	5,580	1
United States	3,754	0.67
U.S. universities	2,551	0.46

TABLE B.3. Contributions to the Publications, *Solid State Communications, Journal of Solid State Chemistry, Materials Research Bulletin, Journal of Physics and Chemistry of Solids, and Physical Review, Section B*

Publications	Number	Normalized
Total Publications	4,756	1
United States	2,133	0.45
U.S. universities	1,268	0.27
United States not corporations	1,600	0.34

TABLE B.4 A Search for the Key Phrase "Solid State" in *Physics Abstracts*

Publications	Number	Normalized
Total Publications	4,432	1
United States	1,191	0.27
U.S. universities	423	0.095

TABLE B.5 The 11 Universities with 20 or More Contributions in the Publications Listed in Table B.3

University	Number
University of California, Berkeley	51
California Institute of Technology	33
University of Chicago	36
Cornell University	41
Harvard University	22
University of Illinois	78
University of California, Los Angeles	40
Massachusetts Institute of Technology	56
Northwestern University	31
University of California, San Diego	31
Stanford University	25
Total	444[a]

[a]These 444 publications are 35 percent of the publications from U.S. universities cited in Table B.3.

APPENDIX C: MATERIALS SCIENCE PUBLICATIONS IN THE JOURNAL OF CHEMICAL EDUCATION, 1974-1981

(A = Articles; N = Notes)

Issue		
Jan. 1974	A	Introduction to the Glassy State in the Undergrate Curriculum, G. P. Johari
	A	Glass Formation and Crystal Structure, J. F. G. Hicks
	A	Sodium Tungsten Bronzes: Oxies with Metallic Character, J. P. Randin
Mar. 1974	A	Single Crystal Diffractometry: An Analogy and An Experiment, W. H. Slabaugh and D. Smith
Apr. 1974	A	Corrosion, W. H. Slabaugh
	A	Intercalation in Layered Compounds, M. B. Dines
	N	A Novel X-Ray Diffraction Experiment, K. G. Shields and C. H. L. Kennard
July 1974	N	The Photoelectric Effect; CAI in the Laboratory, J. R. Garbarino and M. A. Wartell
Sept. 1974	A	Fundamental Theory of Gases, Liquids and Solids by Computer Simulation: Use in the Introductory Course, P. Empedocles
Dec. 1974	N	Definition of a Cubic Crystal Class, G. Smith and C. H. L. Kennard
Jan. 1975	A	Madelung Constants and Other Lattice Sums, E. L. Burrows and S. F. A. Kettle
Apr. 1975	A	Combining Residual Entropy and Diffraction Results to Understand Crystal Structure, J. M. Williams
	A	Reciprocal Vectors in Function Space, P. J. Mjoberg, S. O. Ljunggren, and W. M. Ralowski

	A	The Low Cost Construction of Inorganic Polymer Models Using Polyurethane, M. E. Mrvosh and K. E. Daugherty
June 1975	A	The Failings of the Law of Definite Proportions, L. Suchow
	A	Practical Method of Simulating X-Ray Diffraction, F. Brisse and P. R. Sundararajan
Aug. 1975	N	Construction of a Tetrahedron Packing Model: A Puzzle in Structural Chemistry, W. Schweikert
	N	Unit Cells, R. Olsen and F. Tobiason
Sept. 1975	A	Synthesis and Structure of Magnesium Oxide and Calcium Oxide: An Integrated Inorganic-Physical Experiment, R. Moyer
	A	Raku: A Redox Experiment in Glass, R. Cichowski
Oct. 1975	A	The Chemistry of Color Photography, W. Guida and D. Raber
	N	Construction of Models which Demonstrate Planes, T. J. Clark
Nov. 1975	A	Solid Phase Synthesis, D. C. Neckers
Mar. 1976	A	Thermotropic Crystals: A Use of Chemical Potential-Temperature Phase Diagrams, G. R. Van Hecke
Apr. 1976	A	On the history of Portland Cement after 150 Years, C. Hall
	A	Crystallography - A January Term on the Properties of Crystals, J. C. Howald and G. D. Smith
	A	Other Views of Unit Cells, L. Suchow
June 1976	N	A Computer Program for the Distribution of End-to-End Distances in Polymer Molecules, W. V. Doorne, J. Kuipers, and W. C. Hoekstra
Sept. 1976	A	A Detailed, Simple Crystal-Field Theory Consideration of the Normal Spinel Structure of Co_3O_4, L. Suchow

	A	An Electrochemical Experiment Using an Optically Transparent Thin Layer Electrode, T. P. DeAngelis and W. R. Heineman
Oct. 1976	A	An Electrochemists' Description of Rectification by a pn Junction, D. R. Rosseinsky
Dec. 1976	A	Three Liquid-Crystal Teaching Experiments, J. R. Lalanne and F. Hare
Jan. 1977	A	The Preparation and Characterization of a Sodium Tungsten Bronze, L. E. Conroy
	N	Powder Pattern Program, J.S. Miller and S. Z. Goldberg
Mar. 1977	A	The Silver Halides: A Localized Molecular Orbital Treatment, M. R. V. Sahyun
May 1977	A	Some Structural Principles for Introductory Chemistry, A. F. Wells
	A	Chemical Symbolism and the Solid State: A Proposal, W. B. Jensen
Sept. 1977	N	Organic Macromolecular Chemistry, R. P. Quirk
Dec. 1977	A	Diffracting X-Rays with Photographic Film, T. J. Allen and J. S. Heubner
Mar. 1978	A	Teaching the (Crystallographic) Point Groups, G. O. Brunner
June 1978	A	Chemical Thermodynamics and the Phase Rule, H. F. Franzen and C. E. Myers
July 1978	A	Electrochemistry in the Solid State, J. S. McKechnie et al.
	N	Preparation of a Polysulfide Rubber, G. R. Pettit and G. R. Pettit III
Sept 1978	A	Electronic Structure of Organic Conductors and Semiconductors, Z. G. Soos
Oct. 1978	A	Polymer Experiments: Synthesis of Poly (β-Alanine) and β-Alanine, C. E. Carraher, Jr.

	A	High Pressure Synthetic Chemistry, A. P. Hagen
Nov. 1978	A	High Temperature Chemistry and Rare Earth Compounds: Dramatic Examples of Periodicity, E. D. Cater
	A	Comparision of Ionic and Covalent Iodine Dihalides: An Integrated Experiment, A. A. Woolf
Apr.1979	A	Polymer Photooxidation, N. S. Allen and J. F. Mckellar
June 1979	A	Entropy and Rubbery Elasticity, L. K. Nash
	A	Solving the Phase Problem in Crystal Structure Determination, H. Schenk
	A	Triboluminescence Spectroscopy of Common Candies, R. Angelos et al.
July 1979	A	High Pressure Synthesis of Transition Metal Carbonyls, A. P. Hagen et al.
	A	Solid State Photochemical Isomerization, W. B. Burton
	N	On the Melting Point of Acetanilide, R. S. Lenox and F. J. Haldey
Sept. 1979	A	Preparation and Analysis of Solid Solutions in the Potassium Perchlorate-Permanganate System, G. K. Johnson
	A	Polymer Preparations in the Laboratory, G.M. Lampman et al.
Oct. 1979	A	X-Ray Crystallographic Computations Using a Programmable Calculator, A. E. Attard and H. C. Lee
	A	Corrosion: A Waste of Energy, J. Chem. Educ. Staff
	A	Normal and Inverse Ferrite Spinels: A Set of Solid State Chemistry Related Experiments, C. Chaumont and M. Burgard
	N	Fluorescence Determination of Aspirin in APC Tablets, R. A. Fiigen et al.
	N	A Method for Dispersing Compoinds in Polystyrene Films for Spectroscopic Study, J. T. Wrobleski et al.
	N	A Simple Method of Distringuishing Borosilicate and Soda Lime Glass, W. H. Brown

Nov. 1979	A	The Determination of Entropies of Adsorption by Gas-Solid Chromatography, D. Atkinson and G. Curthoys
Feb. 1980	A	On Thermodynamics of Adsorption Using Gas-Solid Chromatography, E. F. Meyer
	A	Chemistry of Steel Making, N. Sellers
	N	Spectroscopic Cation Analysis Using Metal Salt Pills, M. Barnard
Apr. 1980	A	Corrosion and Preservation of Bronze Artifacts, R. Walker
May 1980	A	Competency Based Modular Experiments in Polymer Science and Technology, E. M. Pearce et al.
	N	The Construction of an Inexpensive Glass Annealing Oven, J. W. Ellis
June 1980	A	Orbital Concepts and the Metal-Metal Bond, W. C. Trogler
	A	Core Curriculum in Introductory Courses of Polymer Chemistry, C. E. Carraher, Jr., and R. D. Deanin
July 1980	A	Surface Chemistry in Heterogeneous Catalysis: An Emerging Discipline, J. M. White and C. T. Campbell
Aug. 1980	A	The Preparation and Characterization of Materials, A. Wold
	A	Needs and Opportunities in Crystal Growth, S. Mroczkowski
	A	An Introduction to Luminescence in Inorganic Solids, J. A. DeLuca
	A	Electron Spin Resonance of Tetrahedral Transition Metal Oxyanions (MO_4^{n-}) in Solids, M. Greenblatt
	A	Common Misconceptions about Crystal Lattices and Crystal Symmetry, C. P. Brock and E. C. Lingafelter
	A	The Introduction of Crystallographic Concepts Using Lap-Dissolve Slide Techniques, G. M. Bodner, T. J. Greenbowe, and W. R. Robinson
	A	Concepts of Order-Disorder Theory in the Undergraduate Curriculum, J. M. Honig

	A	Chemistry and Physics of Amorphous Semiconductors, D. Adler
	A	The Application of High-Resolution Electron Microscopy to Problems in Solid State Chemistry: The Exploits of a Peeping TEM, L. Eyring
	A	Layered Compounds and Intercalation Chemistry: An Example of Chemistry and Diffusion in Solids, M. S. Whittingham and R. R. Chinelli
	A	Optical Fibers and Solid State Chemistry, C. M. Melliar-Smith
	A	Preparation and Physical Properties of One-Dimensional Structures: $Ba_p(Fe_2S_4)_q$, J. S. Swinnea and H. Steinfink
Aug. 1980	A	Some Lower Valence Vanadium Fluorides: Their Crystal Distortions, Domain Structures, Ferrimagnetism, and Composition Dependence, Y. S. Hong, R. F. Williamson,and W. O. J. Boo
	A	On the Structural and Luminescent Properties of the $ScTa_{1-x}Nb_xO_4$ System, L. H. Brixner
Oct. 1980	A	Crystals and X-Rays: A Demonstration, M. M. Julian
May 1981	A	Structural Information from Liquid- and Solid-Phase ESR: The Example of Triphenyl-Substituted Radicals $(C_6H_5)_3A$ of Group IVB Elements, M. Geoffrey and J. H. Hammods
	A	Chemical Principles Revisited: Solar Photovoltaic Cells, C. D. Mickey
Aug. 1981	N	Brain Tinglers: "Holey Crystals," H. I. Feinstein
Nov. 1981	A	Introduction to Polymer Chemistry, F. W. Harris
	A	Chain Reaction Polymerization, J. E. McGrath
	A	Step-Growth Polymerization, J. K. Stile
	A	Molecular Weight and Molecular Weight Distributions in Synthetic Polymers, T. C. Ward

A The Morphology of Crystalline Polymers, P. H. Geil

A An Overview of the Basic Rheological Behavior of Polymer Fluids with an Emphasis on Polymer Melts, G. L. Wilkes

A Mechanical Properties of Polymers, J. J. Aklonis

A Rubber Elasticity, J. E. Mark

A Field Test Evaluation Report on Introduction to Polymer Chemistry, K. Chapman and J. Fleming

A EMMSE: Education Modules for Materials Science and Engineering, P. H. Geil and S. H. Carr

A Macromolecules in Undergraduate Physical Chemistry, W. L. Mattice

A Block and Graft Copolymers, J. E. McGrath

A Organometallic Polymers, C. E. Carraher, Jr.

A High-Strength/High-Modulus Fibers from Aromatic Polymers, J. Preston

A Ion-Containing Polymers; Ionomers, C. G. Bazuin and A. Eisenberg

A Interpretations of Polymer-Polymer Miscibility, O. Olabisi

A Polymers for Extreme Service Conditions, P. E. Cassidy

The 14 articles appearing in the August 1980 issue are, in effect, the major part of the proceedings of the first State of the Art Symposium, Solid State Chemistry in the Undergraduate Curriculum, which was conducted at the ACS National Meeting held in Houston, Texas, March 24-28, 1980.

The papers appearing in the November 1981 issue were presented in the symposium on State of the Art for Chemical Educators III: Polymer Chemistry, held at the Atlanta ACS meeting in March 1981.

We apologize to the authors of any pertinent contributions that were inadvertently overlooked.

APPENDIX D: COVERAGE OF "SOLIDS" TOPICS IN FOUR GENERAL CHEMISTRY TEXTS

General Chemistry, 6th ed., by William H. Hebergall, Frederic C. Schmidt, and Henry F. Holtzclaw, Jr. (Heath, Lexington, MA, 1980)

Crystalline solids, unit cells, packing	6 pages
Amorphous solids and glasses	1 paragraph
Crystal defects	1 paragraph

General Chemistry: Principles and Structure, 2nd ed., by James Brady and Gerard E. Humiston (Wiley, New York, 1980)

Solids	1 chapter, 22 pages

- X-ray diffraction
- Lattices, ionic radii, packing
- Band structure
- Defects

Chemical Principles, 4th ed., by William L. Masterton and Emil J. Slowinskii (Holt, Rinehart and Winston, New York, 1977)

X-ray diffraction, cubic lattices	4 pages
Defects	3 pages
Metallic bonding	3 pages

Chemistry: The Central Science, 2nd ed., by Theodore L. Brown and H. Eugene LeMay (Prentice-Hall, Englewood Cliffs, NJ, 1981)

X-ray diffraction	3 pages
Lattice, unit cells, packing	4 pages
Defects	1 paragraph
Bonding	2 pages
Amorphous solids, liquid crystals	4 pages

, 2nd ed., by Theodore L.
tice-Hall, Englewood

	3 pages
	4 pages
	1 paragraph
	2 pages
stals	4 pages

APPRENDIX E: INTRODUCTORY COURSE IN SOLID-STATE CHEMISTRY

The Massachusetts Institute of Technology (MIT) has recognized the importance of familiarizing undergraduates with the principles of solid-state chemistry. Accordingly, the Department of Materials Science and Engineering at MIT has instituted an optional course, primarily for freshmen, entitled "Introduction to Solid State Chemistry." Introduction to Materials Sciences and Engineering, by K. M. Ralls, T. H. Courtney, and J. Wuff (Wiley, New York, 1976) is the primary text used in the course. The syllabus includes the following topics:

1. Atomic spectra and electronic structure
2. The Periodic Table
3. Bonding in solids
4. Crystal structure
5. X-ray crystallography
6. Band structure of solids
7. Defects in solids
8. Nucleation and growth
9. Mechanical properties of solids
10. Fracture
11. Phase transformations
12. Electrochemistry
13. Reaction rates and catalysis
14. Diffusion and oxidation
15. Organic materials, polymers, and ceramics
16. Applications

The enrollment data since the initiation of the course show a generally steady increase in the number of students taking the course:

1976-1977	303	
1977-1978	337	
1978-1979	434	
1979-1980	533	
1980-1981	550	
1981-1982	525	
1982-1083	640	(This is an estimate, based on a Fall 1982 enrollment.)

This course provides an introduction to the chemistry of the solid state, with special emphasis on structure-property relationships. After an intensive review of the atomic and electronic structure of the elements, the concepts of chemical bonding, crystal strucuture, thermodynamics, and kinetics are treated in the context of the reactivity of materials. In the second part of the course, the developed relationships are applied to the study of single-phase and multiphase systems and their behavior in different environments. The systems discussed include metals, glasses, polymers, and electronic materials. Three lectures per week outline the fundamental principles of solid-state chemistry, and in two recitations per week these principles are amplified in more detail and applied to real systems. The recitations, conducted in a seminar style, also provide an opportunity to discuss homework problems. Laboratory visits are organized for the students to obtain an insight into advanced graduate and postgraduate research in chemistry and physics of the solid state.

This course has proven particularly attractive and helpful to students interested in engineering subjects such as electrical, mechanical, and aeronautical engineering. It satisfies the premedical inorganic chemistry requirement. The intensive review of atomic and electronic structure during the first two weeks is intended to bring students with an inadequate chemistry background to a level where they will be able to understand the remainder of the course.