REPORT OF THE BASIC ENERGY SCIENCES ADVISORY COMMITTEE PANEL ON D.O.E. SYNCHROTRON RADIATION SOURCES AND SCIENCE

NOVEMBER 1997

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January 14th, 1998

Dr. Martha A. Krebs, Director
Office of Energy Research
United States Department of Energy
Washington, DC 20585

Dear Martha,

The purpose of this letter is to summarize the discussions of the Basic Energy Sciences Advisory Committee at its meeting on October 8 - 9, 1997 at the Holiday Inn in Gaithersburg as they related to the report from our Panel on Synchrotron Radiation Sources and Science.

This Panel was assembled in response to the Charge presented to BESAC in your letter of October 9th, 1996 to reassess the need for and the opportunities presented by each of the four synchrotron light sources operated by the Office of Basic Energy Sciences. You suggested that an expert panel should be assembled that, as part of its deliberations, should visit each of the four light sources to meet with members of the management staff and the user communities. You also requested that the panel should be asked to address the following issues and questions:

1. What has been the scientific impact of synchrotron radiation based research during the past decade, and what is it expected to be during the next decade?
2. What is the scientific and technological demand for synchrotron radiation? From what fields and sectors? Who are the newcomers? How has the demand changed since the 1984 Seitz-Eastman report, and how might it change in the future? Please provide quantitative information whenever possible, e.g., how has structural biology, geosciences, environmental sciences, or x-ray microscopy changed during the past decade at the various light sources?
3. What is the user demand at each of the Department of Energy (DOE) synchrotron light sources? What is the distribution of users? Are there special needs served (e.g. scientific, industrial, geographical) at the different light sources, and if so, are these needs growing or declining?
4. What is the expected future capability of each synchrotron light source over time? How do the capabilities complement one another?
5. What does each light source see as its own vision of the future? How do the visions complement each other? How well do the visions accommodate potential changes found in item 2?
6. In a constant budget scenario, what is the appropriate level of research and development (R&D) funding for efforts related to continuously improving current facility operations such as accelerator R&D, the design of insertion devices, the design of advanced instrumentation, etc.? How should these funds

Headquarters: 3412 Hillview Avenue, Post Office Box 10412, Palo Alto, CA 94303, USA • (415)855-2000 • SR&D Fax: (415)855-2287
Washington *Office:* 2000 L Street, NW, Suite 805, Washington, DC 20036, USA • (202) 872-9222 • Fax: (202) 293-2697

be apportioned between the facilities themselves and the user community, including the broader accelerator R&D community? What is the priority between support for such R&D and direct support for users?

7. In a constant budget scenario, what level of investment should DOE/Basic Energy Sciences (BES) make in R&D for 4th generation synchrotron sources and how should this effort be distributed among the facilities and other research sectors?
8. In a constant budget scenario, is the level of DOE/BES *support* of synchrotron radiation related research for users and user-controlled beamlines appropriate and, if not, how should it be changed?
9. If additional funds were available to DOE/BES should they be invested in items 6, 7. and 8 and, if so, what should the priority be among them?
10. What would be the consequences of the shutdown of one or more of the four DOE/BES synchrotron light sources?

We were very fortunate to be able to secure the services of Dr. Birgeneau to act as Chairman for the Panel, and he assembled a very distinguished group of people, representing all aspects of the synchrotron light source community; their names and affiliations are listed in their report. In addition, each of the four synchrotron radiation source facilities had a representative who was invited to attend the visits and meetings (they were excluded only from those parts of the meetings that discussed matters deemed to be sensitive). I attended all the meetings and visits also as an ex officio member, but I did not participate in the deliberations apart from clarifying the requirements of BESAC. On the basis of my observations, I believe that the caliber of the Panel members, and of its Chairman and Vice-Chairman, was of the highest order; and they have prepared what we believe to be an excellent report.

The BESAC meeting review was based on an executive summary of their report, containing their recommendations. The final complete report, reflecting input from our discussions, was received subsequent to the meeting, and has been reviewed by all the Committee members, who have indicated their acceptance of it.

The meeting began with an introduction from Dr. Dehmer outlining the need for the guidance on the issue, and discussing the significance of the Charge. This was followed by an excellent introduction to synchrotron radiation from Dr. Martin Blume. Dr. Keith Hodgson presented an outline of the Stanford Synchrotron Radiation Light Source (SSRL), emphasizing their more recent activities. Dr. Michael Hart presented an overview of the Brookhaven National Synchrotron Light Source (NSLS). Dr. Neville *Smith described the* Lawrence *Berkeley* Advanced Light Source (ALS), pointing out the difference between this and the other three sources in its provision of extreme brightness in the longer wavelength region. Finally, Dr. David Moncton described the Argonne Advanced Photon Source (APS), describing the management structure as well as the functions of the beam lines currently in place.

Dr. Herman Winick briefly reviewed the capabilities of the facilities in the U.S. that are not funded by DOE, and then spent rather more time describing the situation in the rest of the world. Outside the U.S. there are currently 35 light sources in operation in 13 countries; 11 sources are under construction, and a further 15 are in the design phase.

Following this general introduction, Dr. Birgeneau began the presentation of the Panel's report. Twelve members of the Panel presented reviews of different aspects of the scientific nature of the research to which the light sources are contributing, and Dr. John Rush summarized the current budgets for the four DOE synchrotron light sources, and the reactions of the staffs to different possible funding scenarios over the next five years.

Finally, Dr. Birgeneau described the nature of the Panel's deliberations, and of their overall views on the extent and quality of the research being conducted at the facilities. He reported that the Panel had learned about the breadth of the research being done, the tremendous impact it has had in various fields, and how each of these fields has grown as a result. He also said that the Panel was impressed by the evolution of the community, and concluded unanimously that the facilities are phenomenally cost-effective.

Dr. Birgenau then outlined the Panel's recommendations and conclusions, listing them in order of priority. These were discussed in considerable detail by the Committee, and the listing below is from the form in which they appear in the Panel's final report.

Panel Recommendations and Conclusions

The Panel prefaced their recommendations by reemphasizing that they concluded unanimously that shutdown of any one of the four DOE/BES synchrotron light sources over the next decade would do significant harm to the Nation's science research programs and would weaken our international competitive position in this field.

Priority 1

The Panel recognizes the extreme importance of operating effectively the three hard x-ray sources for their very large user communities as well as the importance of a modest investment in research and development of a fourth generation x-ray source. The recommended funding levels for FY98 are as follows:

A.	SSRL	$21.0M
B.	NSLS	$33.8M ($3M increase)
C.	APS	$84.7M
D.	4th Generation X-ray Source R&D	$3.0M

The SSRL and APS figures are the FY98 DOE requests. The NSLS figure is increased by $3.0M above the FY98 DOE request figure. The Panel recognizes the dire need for increased general user support at the NSLS PRT beam lines. The $3.0M is to be used by NSLS to fund user support personnel for the PRT beamlines to facilitate their use by general users. Items A., B., and C. must increase at at least the rate of inflation for these facilities to remain viable. For item D., we recommend that the actual distribution of the 4th generation x-ray source research funds be determined by another panel made up of potential users, accelerator and FEL physicists. The present panel suggests a focused approach to this development given the limited funding available. This funding should extend over five years.

Priority 2

The second set of priorities concerns the development of CAT beamlines at the APS and the modernization of PRT and facility beamlines at the NSLS.

A.	APS front ends	$4.0M
B.	APS facility beam lines	$4.0M
C.	NSLS PRT and facility beamlines	$3.0M

The APS should be provided with $4.0M per annum to develop the insertion devices and front ends for the remaining sectors. In addition, the APS should be provided with $4.0M per year to develop facility CAT beamlines; this should make possible the development of one facility sector every two or three years. Funding for outside user APS CAT beamlines should be raised through the normal peer review process. $3.0M per annum should be provided to modernize and upgrade facility and PRT beamlines at the NSLS. These $3.0M should be distributed both through the facility and directly to the PRT community itself via a competitive peer review process in consultation with the facility.

Priority 3

The ALS as a third generation source provides the highest brightness in the UV/soft x-ray range. The panel recommends funding at the DOE's requested FY98 level.

A.	ALS	$35.0M

2nd Generation Facility Upgrades

Both SSRL and NSLS have proposed upgrades which, in the view of the Panel, would be very cost effective. The Panel recommends:

A.	NSLS	$12M per annum for 3 years
B.	SSRL	$15M per annum for 3 years

It is recommended, however, that the funding for these upgrades should be carried out under a special initiative which is separate from the routine budgeting process. For example, BES might seek partnerships with other divisions within DOE and with other agencies such as NIH for these upgrades. Alternatively, the funding for these upgrades could appear as a 3 year add-on or "spike" analogous to the peak in the overall BES synchrotron budget in 1994 due to the construction of the APS.

In the above prioritization scheme, the priority of this recommendation is 2.5, that is, intermediate between priority 2 and priority 3, for funding beyond 1998.

Funding of priorities 1, 2, and 3 requires a total of $188.5M per annum in FY98 dollars. This represents an increase of 11% over the requested FY98 budget; the Panel note that the budget in FY94 was $224.2M. They believe that funding at the level of $188.5M per year for the four DOE synchrotron facilities is fully justified and indeed is required for the U.S. to retain its leadership role in this important field. At the same time, upgrade and modernization of the second generation facilities are essential. In the event of inadequate funding levels, the facilities should be funded in the priority order given above.

Priority 1, 2, & 3 are recommendations for the equilibrium budgets for the next decade, year-by-year, increasing at the rate of inflation and they total $180.5 million per annum. The FY98 Presidential request is $17 1 million. The Panel concluded the investment in synchrotron radiation was cost effective. In the event of inadequate funding levels, the facilities should be funded in the priority order given.

Following this presentation, BESAC discussed the recommendations, paying particular attention to what the consequences of budget shortfall in the next few years might be, since it appeared to some that under these circumstances the ALS might have inadequate resources to remain in operation.

Dr. Birgeneau repeated the Panel's strong recommendation that, come what may, closure of any one of the four light sources would have a very serious negative effect and must be avoided. He also pointed out some of the Panel's suggestions for alternative funding paths.

BESAC Conclusions and Recommendations

The Committee unanimously welcomed the Panel's report, and complimented both Dr. Birgeneau and the Panel on the outstanding quality of their work.

We recommend that the Report should be published as soon as possible, since it will be of great value to the research community: considerable interest in it has already been expressed.

We accept and support the Panel's recommendations and their priority rankings, while recognizing that the additional funding required may present problems. We repeat the recommendation that we have made earlier that we do not wish to see the investigator-initiated part of Basic Energy Science's budget to be adversely affected by increases in user facility expenditures.

I will, of course, be happy to discuss with you in more detail any of the points made above, at your convenience.

With best wishes,

Sincerely,

John Stringer
Chair, Basic Energy Sciences Advisory Committee

Synchrotron Radiation Sources and Science

Report of a Review held at

Massachusetts Institute of Technology
Cambridge, MA

National Synchrotron Light Source
Brookhaven National Laboratory
Upton, NY

Advanced Photon Source
Argonne National Laboratory
Argonne, IL

Stanford Synchrotron Radiation Laboratory
Stanford University
Stanford, CA

Advanced Light Source
Lawrence Berkeley National Laboratory
Berkeley, CA

May - August, 1997

Robert J. Birgeneau (Chair)
Massachusetts Institute of Technology
Cambridge, MA 02 139

Zhi-Xun Shen (Vice-Chair)
Stanford University
Stanford, CA 94305

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1.0 EXECUTIVE SUMMARY

Executive Summary

Up until 1990, the Department of Energy - Basic Energy Sciences acted as steward for two "second generation" synchrotron radiation facilities, the Stanford Synchrotron Radiation Laboratory (SSRL) at Stanford-SLAC and the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory. Since 1990 two "third generation" sources, the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory and the Advanced Photon Source (APS) at Argonne National Laboratory have been designed, constructed and commissioned. The ALS is a 1.5 to 1.9 GeV UV-soft x-ray facility while the APS is a 7 GeV x-ray facility; both of these are based on undulator insertion devices.

With the commissioning of these two new sources it is now important to assess the current state of synchrotron radiation-based research including the facilities themselves, the science and technology carried out at such facilities, the size and nature of the user community, and finally, the costs associated with such research. As expected, concomitant with the construction and commissioning of the ALS and the APS has been a significant increase in the total cost of operations and research at the four Department of Energy synchrotron radiation facilities. Indeed, synchrotron radiation research now accounts for more than 25% of the D.O.E. Office of Basic Energy Sciences budget. It is therefore of paramount importance to assess the cost effectiveness of this research.

Based on these considerations in the spring of 1997 the Basic Energy Sciences Advisory Committee established a panel "to help in the reassessment for the need for and the opportunities presented by each of the four synchrotron light sources operated by the Office of Basic Energy Sciences". This panel was chaired by Prof. Robert J. Birgeneau of the Massachusetts Institute of Technology and the vice-chair was Prof. Zhi-Xun Shen of Stanford University. Sixteen additional members who were leading scientists and technologists working in academia, industry, and the national laboratories were appointed. These scientists represented a wide range of fields and were broadly distributed geographically. The majority had themselves carried out research at one or more of the four D.O.E. facilities; however, a significant number of panelists had no direct synchrotron radiation research experience. Two members of the panel also served on BESAC. Finally, the chair of BESAC, Dr. John Stringer, as well as representatives from each of the four facilities served as ex officio members. (Note that other U.S. synchrotron sources such as CHESS and SRC which are supported by the NSF rather than DOE were not evaluated in this study and are not discussed at all in this report.)

In brief, the committee was charged to assess the nature and scientific importance of synchrotron radiation research, past present and future, with a time horizon of ten years, the size and nature of the user community both globally and facility by facility, and the facilities themselves including especially their plans and vision for the future. The committee was asked to make detailed budget recommendations under various budget scenarios. Finally, the committee was asked to consider the consequences of the shutdown of one or more of the D.O.E./BES synchrotron light sources. We will anticipate the most important of our recommendations at this point by stating emphatically that the committee concludes unanimously that shutdown of any one of the four D.O.E./BES synchrotron light sources over the next decade would do significant harm to the nation's science research capabilities and would considerably weaken our international competitive position in this field.

In order to gather information the committee sent a list of 12 questions to each of the facilities. These questions were answered in detail by each facility. A general introductory meeting was held at MIT on May 9 and 10. At this meeting the four D.O.E. facilities as well as international VUV and x-ray facilities were reviewed. In addition, experts in a broad range of disciplines discussed the role of synchrotron radiation research in their fields. Over the summer the panel carried out site visits of 1 1/2 days duration each to the four D.O.E. synchrotron facilities. The panel met on August 25 and 26 to review the information it had received and to formulate its recommendations. These recommendations were presented to BESAC on October 9 and 10, 1997.

The most straightforward and most important conclusion of this study is that over the past 20 years in the United States synchrotron radiation research has evolved from an esoteric endeavor practiced by a small number of scientists primarily from the fields of solid state physics and surface science to a mainstream activity which provides essential information in the materials and chemical sciences, the life sciences, molecular environmental science, the geosciences, nascent technology and defense-related research among other fields. The user community at U.S. synchrotron facilities continues to grow exponentially, having reached more than 4000 on-site users annually in FY97. The research carried out at the four D.O.E. synchrotron sources is both very broad and often exceptionally deep.

We believe that the growth in the number of participants in the synchrotron field and, most especially, its increasing diversification will continue for at least the next decade and accordingly facilities must be provided to accommodate these users. One of the side-effects of this growth is that there has been a marked increase in the number of novice, non-specialist users who require significant technical support in order to carry out their experiments This development is reflected in our funding recommendations.

The synchrotron radiation facilities play a central role in education, especially at the graduate level. Since 1990, approximately 100 PhD's per year have been obtained based on research performed at SSRL and the NSLS. With the initiation of research at ALS (1993) and APS (1996) this number is expected to grow considerably.

Each of the four D.O.E. synchrotron research centers is a national facility which serves both the nation as a whole and a significant number of international users. Nevertheless, the facilities have a surprising “regional” character. For example, about one half of the APS CAT members reside in the state of Illinois while more than 40 per cent of NSLS users are from the New York - New Jersey - New England area. Thus NSLS is in good measure an East Coast facility, the APS serves predominately the Mid-West and similarly SSRL and the ALS serve primarily West Coast synchrotron radiation users. This character is likely to persist over the next decade.

It is self-evident that research which requires very high brightness will be carried out overwhelmingly at the third generation sources. Nevertheless, most current synchrotron research requires high flux as opposed to high brightness and therefore can be carried out equally well at second and third generation sources. Finally, the third generation sources could not possibly accommodate the more than 3000 users currently carrying out research at the second generation sources (SSRL and NSLS) especially since the overall community is expected to continue to grow in size.

There are various models for allocation of beamline resources, that is, for deciding who specifies, builds, owns, operates, maintains and uses the beamlines. Beamline allocation models cover the spectrum from facility beamlines which are fully built, owned and operated by the facility (FOOB's) to PRT's and CAT's in which consortia of outside users build, own and operate the beamlines. Each facility has a mixture of FOOB's and PRT/CAT's although, for example SSRL is overwhelmingly FOOB's while the APS is exclusively CAT's albeit with some of these entirely facility owned. This diversity seems to serve the community well provided that the PRT/CAT beamlines are properly maintained and operated and that appropriate support is provided to outside users. This turns out to be an emerging problem at the NSLS and one of our funding recommendations is aimed at ameliorating this situation. Otherwise, we do not recommend any significant changes in the current FOOB-PRT/CAT system.

As noted above, the panel believes that all four D.O.E. synchrotrons are essential to the national scientific and technological enterprise. The panel was very impressed by the outstanding performance of the second generation facilities (SSRL and NSLS), by the number of users they serve well, by their ability to renew and improve themselves, by their ability to continue cutting-edge research even though the storage rings themselves are not the most advanced, by their commitment to education, and by their abilities to engage new users and address new problems. Given the outstanding track record and clear vision demonstrated by these facilities, the panel expects these facilities to continue to thrive scientifically in a cost-effective manner. These centers are national resources and they should be adequately funded, upgraded and modernized in a timely fashion to serve better the national needs.

The APS is newly commissioned and therefore it is difficult to evaluate at this time the full impact of the research which will be carried out there. It is clear, nevertheless, that it will be the premier hard x-ray facility in the U.S. and indeed the world for the foreseeable future. The panel was impressed by the APS's ability to build the facility and achieve the design capability on-time and on budget. The CAT system has attracted of order 1000 participants from 85 U.S. universities, 32 industries and 25 research laboratories. The CATs will operate 40 of the 68 available beamlines. Continual development and implementation of the remaining 28 beamlines will occur over the next five to ten years given adequate funding. It is essential that these beamlines be properly funded by D.O.E. and other sources. We believe that a number of the open sectors should remain undeveloped until at least the first generation of experiments are completed so that one can assess any new and unexpected scientific and technological opportunities.

The ALS is a third generation synchrotron radiation user facility of very high brightness optimized for the UV and soft x-ray regions. It will be the U.S.'s premier UV and soft x-ray source for the foreseeable future. Again the ring was built on-time and on-budget. In contrast to the APS which has only two international competing facilities (ESRF in France and Spring-8 in Japan), the ALS will have at least 7 international competitors. Currently 16 out of a total of 80 possible beamlines have been instrumented. To-date the ALS user community is relatively small, 7% of the U.S. total, and more than one-third of the users come from Lawrence Berkeley National Laboratory itself. There seems to be limited participation in ALS research by U.C. Berkeley faculty. It appears that since the time of the Seitz-Eastman report, important scientific issues which require UV radiation have decreased in number compared to those which require hard x-rays; the UV community has correspondingly decreased in relative size now representing only about 15% of the total community. The ALS must therefore be very aggressive in seeking out new scientific opportunities and it must cooperate more effectively with its existing user community in this endeavor. On the other hand, the ALS has an impressive industrial research program centered on the needs of the semiconductor-microelectronics, magnetic storage and bio-technology companies in Silicon Valley and the San Francisco Bay Area.

We have also considered “fourth generation” x-ray sources which will in all likelihood be based on the free electron laser concept. If successful, this technology could yield improvements in brightness by many orders of magnitude. It is our strong view that exploratory research on fourth generation x-ray sources must be carried out and we give this item very high priority.

One of the most impressive features of current synchrotron radiation research is its remarkable diversity. Nevertheless, stewardship of the SSRL, NSLS, ALS and APS rests exclusively with Basic Energy Sciences. We, therefore considered the question of broadening the base for support of operations of these four facilities. After extensive discussions, we concluded that this is not practicable. D.O.E has considerable expertise and experience in the management of large national facilities that is not found in other agencies. The stewardship role played by D.O.E. of its synchrotron facilities has been outstandingly effective and ensures that only one agency has responsibility for the efficient operation of these facilities. D.O.E./BES should take political advantage of the broad and successful impact of its facilities, especially in health-related fields, to increase its own base budget. We do, however, recommend diversification of the funding sources for special initiatives such as the proposed SSRL and NSLS upgrades.

We now present our explicit recommended funding priorities. We preface this by re-emphasizing that the committee concludes unanimously that shutdown of any one of the four D.O.E./BES synchrotron light sources over the next decade would do significant harm to the nation's science research programs and would weaken our international competitive position in this field.

Recommended Funding Priorities

The committee has divided its recommendations for on-going funding of the facilities into three sections. The three sections are in priority order, but all items within each section have the same priority. We have separately evaluated the requests for upgrades by SSRL and NSLS. Since the requisite funding for these upgrades need extend only over three years, we treat this recommendation on a different basis.

Priority 1

The panel recognizes the extreme importance of operating effectively the three hard x-ray sources for their very large user communities as well as the importance of a modest investment in research and development of a fourth generation x-ray source. The recommended funding levels for FY98 are as follows:

A.	SSRL	\$21.0M
B.	NSLS	\$33.8M (\$3M increase)
C.	APS	\$84.7M
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The second set of priorities concerns the development of CAT beamlines at the APS and the modernization of PRT and facility beamlines at the NSLS.

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A.	ALS	$35.0M

2nd Generation Facility Upgrades

Both SSRL and NSLS have proposed upgrades which, in the view of the panel, would be very cost effective. The panel recommends:

A.	NSLS	$12M per annum for 3 years
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It is recommended, however, that the funding for these upgrades should be carried out under a special initiative which is separate from the routine budgeting process. For example, BES might seek partnerships with other divisions within DOE and with other agencies such as NIH for these upgrades. Alternatively, the funding for the upgrades could appear as a 3 year add-on or "spike" analogous to the peak in the overall BES synchrotron budget in 1994 due to the construction of the APS.

In the above prioritization scheme, the priority of this recommendation is 2.5, that is, intermediate between priority 2 and priority 3, for funding beyond 1998.

Funding of priorities 1, 2, and 3 requires a total of $188.5M per annum in FY98 dollars. This represents an increase of 11% over the requested FY98 budget; we note that the budget in FY94 was $224.2M. We believe that funding at the level of $188.5M per year for the four DOE synchrotron facilities is fully justified and indeed is required for the U.S. to retain its leadership role in this most important field. At the same time, upgrade and modernization of the second generation facilities are essential. In the event of inadequate funding levels, the facilities should be funded in the priority order given above.

2.0 INTRODUCTION

Introduction

Since the beginning of human scientific inquiry, photons have been the primary tool for the investigation of the microscopic and macroscopic properties of matter. The sources of light for such scientific investigations have evolved continuously over time beginning with the sun and culminating with the laser. Although many beautiful and important experiments have been performed using laboratory sources such as lasers, arc lamps and water-cooled rotating copper anodes for x-rays, a range of important problems had been inaccessible because of limitations in the source brightness and, therefore, ultimately in the intensity and collimation of the photon beam.

This situation has changed dramatically, however, because of the advent of synchrotron radiation sources over the past three decades; this has led to a genuine scientific revolution. Synchrotron radiation is a unique source of photons, by virtue of its high intensity, brightness, stability, and broad energy range, extending from the far infrared to the x-ray region and beyond. The radiation is created when relativistic charged particles within an electron accelerator are deflected by a magnetic field. The intensity of the synchrotron light can be further increased with the use of insertion devices. The simplest of these is the wiggler magnet that puts a series of sharp bends in the electron trajectory of the synchrotron, thus increasing the net radiation from that region. A more sophisticated device called an undulator in effect puts in a periodic array of kinks so arranged that the light from each adds up in phase, giving an enormous increase in brightness. Although synchrotron radiation represents a drain of energy in an accelerator, it was eventually recognized to be a source of intense radiation for new classes of experiments, first in solid state and surface physics and then in other sciences.

The modern era in U.S. synchrotron radiation research, especially in the x-ray region, began in the late 70’s and early 80’s with the transition of SPEAR at the Stanford Synchrotron Radiation Laboratory (SSRL) from parasitic to partially dedicated operation and the construction of the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory. These are referred to as “second generation” facilities. These were followed by the construction of the Advanced Light Source (ALS) at Lawrence Berkeley Laboratory in the early 1990’s and the Advanced Photon Source (APS) at Argonne National Laboratory in the mid 90’s. These are so-called “third generation” sources which are optimized for the VUV and x-ray spectral ranges, respectively. “Third generation” here means that the facilities are based on undulator insertion devices. As will be discussed in great detail, these four D.O.E. synchrotron radiation sources have made and are making possible a remarkable range of scientific research which simply would not be possible otherwise. A “fourth generation” source which will be discussed briefly in this report would in all likelihood be a true laser device operating in the UV and/or x-ray range.

As stated above, synchrotron radiation research began primarily as a subfield of solid state physics and surface science. This tool now plays an essential role in a broad range of fields including biology and medicine, chemistry and polymer science, solid state physics and materials science, molecular environmental science, geoscience, surface and interface science, atomic and molecular science, agriculture and forestry, and other fields. Synchrotron radiation has also been used to address issues important to industry such as micro-analysis, surface properties of industrial materials, thin film growth, lithography, rational drug design, catalysis, and polymer processing.

The last major review of synchrotron radiation science and technology occurred in 1984. This was the renowned “Seitz-Eastman” report entitled “Major Facilities for Materials Research and Related Disciplines” which was carried out under the auspices of the National Research Council - National Academy of Sciences. This prescient study reviewed the field of synchrotron radiation research among others and concluded that synchrotron facilities offered “incomparable scientific and technical opportunities; they will enable scientists and engineers to pursue otherwise inaccessible areas of science and technology”. The Seitz-Eastman Committee, among its varied recommendations, called for the timely construction of both a 6 GeV Synchrotron Radiation

Facility and a 1 to 2 GeV Synchrotron Radiation Facility both of which would be based on state-of-the-art insertion devices. These "third generation" synchrotron radiation sources have indeed been designed, constructed and commissioned. They are the Advanced Photon Source, a 7 GeV x-ray facility, at the Argonne National Laboratory and the Advanced Light Source, a 1.5 to 1.9 GeV VUV facility at Lawrence Berkeley Laboratory.

The Seitz-Eastman Committee also reviewed the science and technology that could be carried out at such light sources. They were careful to emphasize that such sources would provide "both identifiable and as yet unforeseen opportunities for research not possible at present facilities". Indeed, as we shall discuss in detail in this report, the depth and breath of synchrotron radiation research at both the second and third generation sources was barely anticipated in 1984.

With the commissioning of these two new sources it is now important to assess the current state of synchrotron radiation-based research including the facilities themselves, the science and technology carried out at such facilities, the size and nature of the user community, and finally, the costs associated with such research. As expected, concomitant with the construction and commissioning of the ALS and the APS has been a significant increase in the total cost of operations and research at the four Department of Energy synchrotron radiation facilities. Indeed, synchrotron radiation research now accounts for more than 25% of the D.O.E. Office of Basic Energy Sciences budget. It is therefore of paramount importance to assess the cost effectiveness of this research.

Based on these considerations in the spring of 1997 the Basic Energy Sciences Advisory Committee established a panel "to help in the reassessment for the need for and the opportunities presented by each of the four synchrotron light sources operated by the Office of Basic Energy Sciences". This panel was chaired by Prof. Robert J. Birgeneau of the Massachusetts Institute of Technology and the vice-chair was Prof. Zhi-Xun Shen of Stanford University. Sixteen additional members who were leading scientists and technologists working in academia, industry, and the national laboratories were appointed. These scientists represented a wide range of fields and were broadly distributed geographically. The majority had themselves carried out research at one or more of the four D.O.E. facilities; however, a significant number of panelists had no direct synchrotron radiation research experience. Two members of the panel also served on BESAC. Finally, the chair of BESAC, Dr. John Stringer, as well as representatives from each of the four facilities served as ex officio members. The panel members are listed at the end of this section.

The charge to the committee is given in Appendix A. In essence, the committee was to assess the nature and scientific importance of synchrotron radiation research, past, present and future, with a time horizon of ten years, the size and nature of the user community both globally and facility by facility, and the facilities themselves including especially their plans and vision for the future. The committee was asked to make detailed budget recommendations under various budget scenarios. Finally, the committee was asked to consider the consequences of the shutdown of one or more of the D.O.E./BES synchrotron light sources. We will anticipate the most important of our recommendations at this point by stating emphatically that the committee concludes unanimously that shutdown of any one of the four D.O.E./BES synchrotron light sources over the next decade would do significant harm to the nation's science research capabilities and would considerably weaken our international competitive position in this field.

In order to gather information the committee sent a list of 12 questions to each of the facilities. The explicit questions are given in Appendix B. These questions were answered in detail by each facility. A general introductory meeting was held at MIT on May 9 and 10. The program for this meeting is given in Appendix C. At this meeting the four D.O.E. facilities as well as international VUV and x-ray facilities were reviewed. In addition experts in a broad range of disciplines discussed the role of synchrotron radiation research in their fields. Over the summer the panel carried out site visits of 1 1/2 days duration each to the four D.O.E. synchrotron facilities. The panel met on August 25 and 26 to review the information it had received and to formulate its recommendations. The recommendations were presented to BESAC on October 9 and 10, 1997. This report summarizes the committee's conclusions about the scientific and technological case for synchrotron radiation, the nature of the facilities and their individual roles in the overall U.S. program in this field, beamline instrumentation, methods of organizing research at these facilities, and the user community, both general and members of Participating Research Teams/Collaborative Access Teams (PRT/CAT). Finally, of course, the panel's recommendations in response to the D.O.E. - BESAC charge are presented.

The format of this report is as follows. In section 3 the essential concepts of bending magnets and insertion devices are introduced and basic quantities such as flux and brightness are defined. Section 4 contains descriptions of the four D.O.E. facilities with the order determined by the chronology of commissioning. The scientific and technological case is given in nine separate subsections in section 5. Machine and instrumentation issues are discussed in section 6. User data and user issues, publications and education data are presented in section 7. The facility budgets including the FY98 D.O.E. requested budgets are reviewed in section 8. Consequences of shutdown of any one of the four facilities are presented in section 9. Finally our conclusions and recommendations are given in section 10. A series of appendices provide ancillary information. These include the charge letter (A), the information requested from the facilities (B), the program for the May 9- 10 general information meeting (C), data on international synchrotron radiation facilities (D) and environment safety and health procedures at each of the four synchrotron facilities (E).

BESAC PANEL ON SYNCHROTRON RADIATION SOURCES AND SCIENCE

Robert J. Birgeneau (MIT), Chair
Zhi-Xun Shen (Stanford), Vice Chair
David Bishop (Lucent)
Gordon Brown (Stanford)
William Colson (Naval Postgraduate School)
Jonathan Greer (Abbott Labs)
Sol M. Gruner (Cornell)
Linda Horton (ORNL)
Janos Kirz (SUNY Stonybrook)
Raymond Jeanloz (UC Berkeley)
Donald Levy (Univ. of Chicago)
Ewan Patterson (SLAC)
Douglas Rees (CalTech)
John Rush (NIST)
Thomas Russell (Univ. of Mass.)
Kenneth Schweizer (Univ. of IL)
Joachim Stohr (IBM)
Ruud Tromp (IBM)

Keith Hodgson (SSRL delegate)
Samuel Krinsky (NSLS delegate)
Neville Smith (ALS delegate)
Gopal Shenoy (APS delegate)
John Stringer (EPRI) ex-officio (Chair of BESAC)

Debra L. Martin, Administrative Assistant

3.0 BASIC CONCEPTS

Basic Concepts

Properties of Synchrotron Radiation

3.1 Bending Magnet Source

The needs of high energy physics research led to the construction of storage rings capable of storing electron and positron beams at high energy (many GeV) for durations up to many hours. The centripetal acceleration of relativistic electrons or positrons through the dipole magnets of a storage ring produces intense electromagnetic radiation called synchrotron radiation. The vertical opening angle 2ψ of this radiation sheet emitted in the orbital plane of the charged particle is approximately $1/\gamma$, where γ is the relativistic enhancement of the particle rest energy. This fan of radiation has a horizontal opening angle θ, which is approximately equal to $2\pi/N_B$, where N_B is the number of bending magnets in the storage ring. Typical values for ψ and θ are a fraction of a milliradian and a few radians, respectively.

Synchrotron radiation has several properties that make it a suitable source for research. The radiation from a bending magnet (see Fig. 3.1.1A) of a storage ring has a spectral distribution over a wide range of energy. The radiation is distributed over the electromagnetic spectrum from infra-red, through optical, UV, soft x-rays, and into hard x-rays and is determined by the energy of stored particle beam and the magnetic field of the bending magnets. The spectrum of radiation from a source is characterized by the critical energy $\varepsilon_c(\mathrm{keV}) = 0.665\,1\ BE^{2}$, where $\boldsymbol{B}$ is the magnetic field (in T) of the bending magnet, and the particle beam energy E is in GeV. For example, the critical energies of bending magnet radiation from the ALS operated at 1.9 GeV is about 340 eV and from the 7-GeV APS is about 19.5 keV. In most experiments, only a narrow energy bandwidth is selected by the use of monochromatizing optics.

The other important property of synchrotron radiation is its extremely high intensity. Traditionally the photon "intensity" is measured in units of photons per second in a defined energy bandwidth. The measure of the intensity of the synchrotron radiation from a bending magnet source is usually called the photon "flux" and is defined as

$$\text{Flux} = \frac{\text{number of photons}}{\text{milliradian }(\theta)\sec\ (0.1\%\ \text{bandwidth})}, \text{ for all } \psi.$$

The photon flux from the horizontal radiation fan from a bending magnet can be collected over large values of θ using appropriate optics in specific cases and focused at a sample.

There are two other qualities that are generally used to define the quality of synchrotron radiation. They are "spectral brilliance" and "spectral brightness". The spectral brilliance is the spectral intensity divided by the phase-space volume into which the radiation is emitted from the particle beam. Thus

$$\text{Spectral brilliance} = \frac{\text{number of photons}}{(\text{mm})'\ (\text{milliradian})^{2}\sec\ (0.1\%\ \text{bandwidth}).}$$

Here the phase-space volume is obtained by convoluting the Gaussian distribution describing the particle beam in the storage ring and the radiation field. (Some authors prefer to call this quantity ‘brightness’ in analogy with classical optics.) Indeed, when the brilliance is integrated over the particle beam width and height, and over the vertical opening cone angle ψ of radiation, one obtains the photon flux. There are numerous experiments that require the highest x-ray density on the sample. This is realized from the high spectral brilliance of the synchrotron radiation originating from a small phase-space volume. For these, the third-generation synchrotron facilities (ALS and APS) provide the required particle beam characteristics with very small natural emittance of the particle beam (typically 5-10 nmrad). On the other hand, there are also a large number of experiments that are flux intensive which can also be performed at the second-generation synchrotron facilities (NSLS and SSRL) with somewhat larger values for the particle beam emittance.

The “spectral brightness” defines the intensity of the synchrotron radiation in a unit solid angle and is fully governed by the electromagnetic theory.

$$\text{Spectral brightness} = \frac{\text{number of photons}}{(\text{milliradian})^2\ \text{sec}\ (0.1\%\ \text{bandwidth})}$$

The spectral brilliance can now obtained by dividing the spectral brightness by an effective source area, which is a Gaussian convolution of the particle and radiation beam source sizes.

The bending magnet radiation is naturally polarized, with the electric field parallel to the plane of the particle orbit in the storage ring. Such energy distribution and linear polarization make a wide range of measurements possible. Experiments have also been performed using the circularly polarized radiation available above and below the plane of particle orbit (with opposite helicity) from the bending magnet in a storage ring. However, the flux of circularly polarized radiation from a bending magnet source is considerably lower than the on-axis linearly polarized radiation. Special insertion devices (described below) have been designed and built to meet this need.

Another important characteristic of synchrotron radiation that has recently been exploited is the coherence. Simply put, this represents the ability of radiation to exhibit interference patterns. The coherence can be separated into two types. Transverse coherence refers to the coherence of the electromagnetic response at two points in the transverse plane of the radiation at a given time. If the response is measured at different times, it is referred to as temporal coherence. Temporal coherence is determined by the bandwidth of radiation, and the spatial coherence is governed more by the phase-space area of the source. While coherent photons can be realized at a bending magnet sources, the undulator sources at third-generation facilities provide more efficient capability.

3.2 **Wiggler and Undulator Sources**

The primary purpose of the bending magnets in a storage ring is to maintain the circulating electron or positron bunches by bending the particles into a closed orbit. New magnetic structures called wigglers and undulators (see Fig. 3.1.1A and B respectively), which are inserted along a straight section in a storage ring, are more efficient radiation sources than are bending magnet sources. Such magnetic devices are sometimes called “insertion devices.” An insertion device is a magnetic structure made up of a periodic array of either permanent magnets or electro-magnets. The device does not produce a net displacement or deflection of the stored beam in the closed orbit.

The angular deflection of the particle beam in an undulator is less than or comparable to the natural vertical emission angle of synchrotron radiation ψ and is defined by the dimensionless deflection parameter $K = 0.934\ B\lambda_0$. Here, B is the peak magnetic field (in T) produced by the undulator magnets, and λ_0 is the magnetic period (in cm) of the trajectory in the undulator.

Oscillating relativistic charges produce synchrotron radiation at each of the poles as they move through the periodic fields in an undulator. These wave packets constructively interfere to produce spectrally compressed harmonics of pseudo-monochromatic radiation. To a first approximation, the wavelength of first harmonic of this radiation is λ_0/γ^2. An undulator with a 3-cm period will generate first harmonic radiation of about 44Å at the ALS and 1.58, at the APS. The photon energy (in keV) of the n-th harmonic along the undulator axis is given by

$$E_n = \frac{0.949\ n\ E^2}{\lambda_0\ (\ 1 + K^2/2)} \qquad (n = 1,\ 3,\ 5\ ,..........).$$

Varying the magnetic field B (and hence K) by opening the gap of the undulator provides the energy tunability of the radiation from each of the radiation harmonics. The radiation harmonics from an ideal undulator will have an energy spread of about 1/(nN), where N is the number of magnetic periods in the undulator. Because of the low phase-space volume of the particle beam in the third-generation facilities (ALS and APS), these tunable radiation harmonics have very large brilliance ($\approx 10^{19}$ units).

For an undulator of N magnetic periods and a particle beam with small phase-space volume or beam emittance (available at the ALS and APS), the half-angle of the central radiation cone of useful photons is approximately $1/(\gamma\sqrt{N})$. A typical undulator with 100 periods will contain most useful radiation in a cone with an approximate half-angle of 38 μrad at the ALS and 7 μrad at the APS. The small beam divergence of the undulator radiation in both the x- and y-directions enhances both the spectral brightness and the spectral brilliance

The physics of the undulator performance was tested on the second-generation synchrotron radiation facilities. However, the third-generation facilities have been optimally designed to obtain the best performance from the undulator sources. The most prominent feature of the third-generation sources is the large number of straight sections for such undulators (12 at the ALS and 35 at the APS). The magnetic period of the undulators, the minimum undulator gap, and the energy of the stored particles have been optimized to realize maximum radiation energy tunability using various harmonics. Finally, the particle beam emittance and the energy spread have been minimized, and the values of p-functions and x-y coupling in the storage ring orbit are readily optimized to provide the highest on-axis spectral brilliance and optics-matched performance.

The low emittance of the third-generation synchrotron radiation facilities permits one to generate coherent radiation using the undulators. For example, at the ALS an undulator beam with full transverse coherence can be realized in the vertical (y) direction for wavelengths longer than about 90Å. On the other hand, such beams are realized even in a shorter wavelength range (both at the ALS and APS) either by reducing the x-y coupling in the stored beam or by using apertures in the photon beam. The experiments carried out on these coherent beams of radiation will build the user base for the possible fourth-generation radiation facility based on a free-electron laser (FEL), which will generate fully coherent radiation in both the x- and y-directions.

An insertion device called a wiggler is used on both the second- and third-generation storage rings to produce a very intense beam of synchrotron radiation. These devices are similar to undulators but have large values for the deflection parameter K (2 10). This makes the interference effects of the radiation from different magnets of the wiggler small, making the device behave like a series of bending magnets sources whose synchrotron radiation is combined to produce an intense beam. Wigglers particularly enhance the photon flux. Generally, the fields of the magnets used in a wiggler are stronger than the fields of the bending magnets, thus increasing (e.g., using superconducting magnets) the critical energy of the spectral distribution from the device in comparison to that of the bending magnet spectrum. The radiation opening angle from a wiggler in the plane of the orbit (0) is about K/γ. There are many wigglers operating on the ALS, NSLS, and SSRL that extend the energy spectrum of the radiation beams to higher photon energies and increase their flux.

The wigglers and undulators have minimal effect on the operation of the storage rings, and they provide a unique way of tailoring the radiation characteristics to meet the needs of a new class of experimental programs. This capability is build into the design of the third-generation synchrotron radiation facilities where the newly conceived devices can be introduced in a storage ring straight section without reconfiguring the facility. Such demands for radiation sources are now being met both at the ALS and the APS where a need for circularly polarized photons has been realized by new user groups. Both the facilities will operate undulators and wigglers that will produce intense beams of circularly polarized photons with variable helicity in different energy spectral ranges.

The undulator brilliance discussed here is the time-averaged value because particle bunches travel many times through an undulator every second. The FELs on the other hand have small duty cycles and generate much higher peak brilliance of coherent photons, at the present time, in the long wavelength range. Thus the FELs and undulator sources at the third-generation synchrotron facilities play a complementary role in the long wavelength range where both sources are operable with regards to peak vs. average brilliance, tunability, and coherency of photons. Extending the FEL capabilities to a lower wavelength range is hence very desirable but challenging. Both the FELs and undulator sources require low-emittance particle beams, as well as long periodic magnetic structures. Undulator radiation can become stimulated in the self-amplified spontaneous emission (SASE) mode as it experiences the periodic magnetic field from a long undulator. This naturally leads from a simple undulator source (at a third-generation synchrotron radiation facility) to a high gain SASE FEL operation in the future (as a possible fourth-generation radiation source).

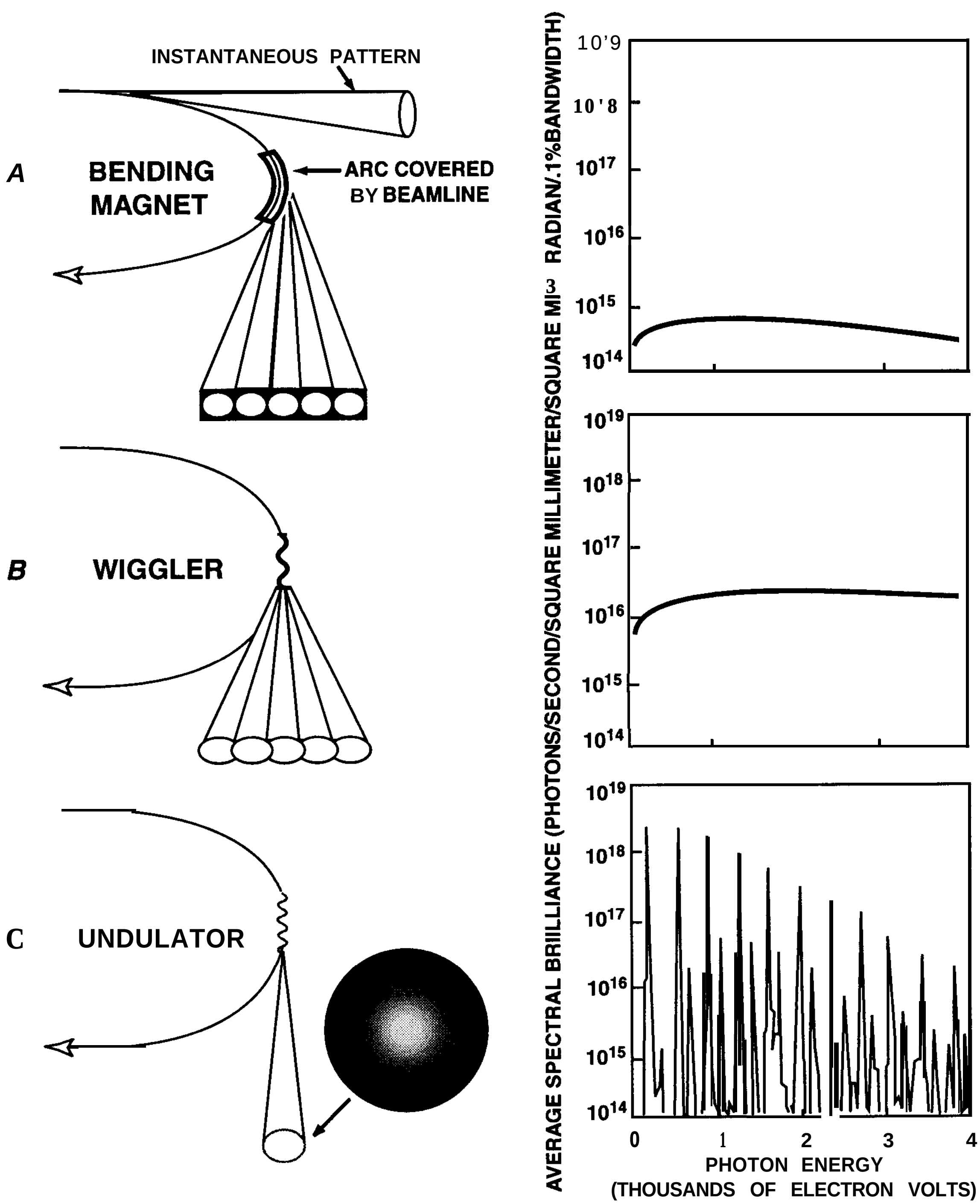

INSTANTANEOUS PATTERN
A
BENDING MAGNET
ARC COVERED BY BEAMLINE
B
WIGGLER
C
UNDULATOR
AVERAGE SPECTRAL BRIILLIANCE (PHOTONS/SECOND/SQUARE MILLIMETER/SQUARE MI³ RADIAN/.1%BANDWIDTH)
10’9
10'8
10¹⁷
10¹⁶
10¹⁵
10¹⁴
10¹⁹
10¹⁸
10¹⁷
10¹⁶
10¹⁵
10¹⁴
10¹⁹
10¹⁸
10¹⁷
10¹⁶
10¹⁵
10¹⁴
0
1
2
3
4
PHOTON ENERGY
(THOUSANDS OF ELECTRON VOLTS)

Figure 3.3.1

4.0 FACILITY DESCRIPTIONS

Note that the following subsections in the 4.0 Facility Descriptions section were provided by the individual facilities and were incorporated as received into the report.

4.1 Stanford Synchrotron Radiation Laboratory

BACKGROUND

SSRL's SPEAR storage ring has been a source for synchrotron radiation research for twenty-three years. Preliminary experiments were carried out in 1973, and the first beam line went into operation in 1974. SPEAR ran in a parasitic mode until 1979 when the storage ring was committed to dedicated synchrotron radiation production for 50% of its operating time. By 1986, it became clear that more running time and an independent injector were needed if SSRL was to meet its increasing user demands. The injector, the most recent major upgrade to the accelerator complex, was completed in the fall of 1990. In the next year, SPEAR became a fully dedicated synchrotron radiation light source. Since then, SSRL has made, and continues to make, improvements to the injector, storage ring and beam lines as well as constructing new beam lines and developing new instrumentation.

RESEARCH PROGRAMS

SSRL is focused on the application of synchrotron radiation to research that embraces, but is not limited to, biology, chemistry, engineering, environmental science and physics. SSRL has been, and continues to be, a leader in many scientific fields, and has made notable contributions in the areas of:

- High-Resolution Angle-Resolved Photoemission Study of High-T, Superconductors
- Protein Crystallography
- Structure of Non-Crystalline Materials
- Applied Interface and Surface Structure
- Applications of X-ray Absorption Spectroscopy to the Study of Biological Systems and Molecular Environmental Science

SSRL has an especially rapidly growing program in the field of molecular environmental science, and is conducting research in toxic waste storage, decontamination, and remediation. The Laboratory is engaged in a continuing collaboration with Silicon Valley companies in experiments that have resulted in a number of industrial applications which push well beyond the current state-of-the-art in trace impurity analysis techniques. SSRL has developed a world class program in the application of synchrotron radiation to structural molecular biology research. In addition to basic scientific research, the Laboratory has a commitment to research in accelerator physics and the development of advanced technologies for enhancing the intensity, brightness, stability and reliability of synchrotron photon beams.

OPERATIONS

The SSRL facility continues to operate with consistent reliability. During the November 1996 to July 1997 run, over 95% of the scheduled user shifts were delivered during approximately 9 months of running time. Beam time was used by 266 different proposals in a total of 553 experimental starts involving 1134 researchers. Users came from 169 different institutions including 36 private companies, 16 U.S. laboratories, 64 U. S. universities, 14 foreign laboratories, and 38 foreign universities. Publication data are still being collected for 1997; however, to date users have reported over 208 publications. In some measure, the increased productivity and user beam time (up by about 40% from 1995) are attributable to the DOE Scientific Facilities Initiative, which, for the first time, provided SSRL with the funding to run "full time".

In FY 1998, SSRL will be providing user beam from November 3, 1997 to July 3 1, 1998 (nearly 9 calendar months). In spite of the increased running time, the facility remains considerably oversubscribed. In FY 1997, the users requested 44.7% more time than the facility was able to provide. On the high-intensity multipole wiggler and undulator beam lines the over demand exceeded 100%. It is likely that the demand for beam time will increase substantially in the future as the result of fast-growing areas such as structural molecular biology, molecular environmental sciences, and trace impurity analysis.

FACILITIES

Presently, SSRL has 26 experimental stations on 22 beam ports with 4 more stations under construction or commissioning. Recent facility improvements are resulting in increased stability and reliability of the ring and the beam lines. The stations on the SPEAR storage ring cover the spectrum from 5 to 45,000 eV. The basic parameters of the SPEAR ring, under typical operating conditions, are:

Energy	3.0 GeV
Current	100 mA (top of fill)
Lifetime	30 hr (I*tau=3.0 Amp-hr)
Emittance	130 nm-rad (natural); ~ 160 nm-rad with present high field wigglers
Circumference	234 m

The complement of beam lines includes 10 bending magnet stations and 16 insertion device stations. SSRL provides its users with long lifetime VUV/soft X-ray radiation and with hard X-rays for those not requiring high brightness. SSRL's facilities are especially valuable to the very large number of users located on the West Coast. The Laboratory provides its users with training, with high quality service and support, and with a wide variety of advanced instrumentation and specialized experimental equipment.

INDUSTRIAL COLLABORATIONS

There has been a strong industrial presence at SSRL since the facility became operational. At present, approximately 30% of SSRL's users come from private industry. The companies working at SSRL range from major corporations such as Xerox, Exxon and AT&T Bell Laboratories to small businesses supported by SBIR grants. There are currently 41 projects (approximately 1/3 of the active proposals) which involve collaborations between industry and university and/or government laboratory researchers. Areas receiving a great deal of attention are biotechnology and advanced materials characterization.

EDUCATIONAL ACTIVITIES

SSRL is strongly tied to Stanford University and graduate education has been an integral part of SSRL's program since the Laboratory's beginning. SSRL, together with the Stanford Applied Physics Department has offered a graduate program in accelerator physics for the past ten years. A number of graduate students trained at SSRL are now in key positions at corporations such as Hewlett-Packard and IBM, while others have gone on to make significant contributions to other synchrotron facilities and in academia. To date, about 350 Ph.D. theses have been awarded on work partially or fully performed at the Laboratory. SSRL also hosts undergraduates from across the country in a summer research program sponsored by SLAC. Additionally, SSRL sponsors workshops, which train users and promote the development of new fields. For example, the Laboratory has recently organized workshops in cryocrystallography and molecular environmental science.

FUTURE PLANS

SSRL has a continuously evolving plan for facilities and operational upgrades with the following goals:

(Maximizing scientific opportunities by implementing beam line improvements.

(Maintaining SPEAR reliability, efficiency and stability.

(Planning and implementing a major upgrade of the SPEAR ring.

(Designing and developing a fourth generation Linac Coherent Light Source (LCLS) research facility.

(Improving user support and throughput, more efficient integration of staff, and more effective long and short range planning.

Beam Line and Facilities Improvements

Consistent with these goals, SSRL has adopted an integrated program of improvements to SPEAR, to the experimental stations, and to laboratory infrastructure. 1997-98 will see the completion of the commissioning of the new Beam Line 9 for structural molecular biology, and progress will continue on the construction of Beam Line 11, the molecular environmental science beam line. A Laboratory-wide 100MB network will soon be completed. Examples of other future improvements include: increasing beam stability by improvements to the SPEAR orbit feedback system, improvements to the beam line computer systems, implementing significant instrumentation and optics upgrades on selected experimental stations, installing an improved system for accelerator beam dynamics studies, and completing the expansion of buildings housing experimental facilities.

Major SPEAR Upgrade

The SPEAR storage ring has undergone, and is continually undergoing, incremental ‘improvement to enhance its reliability and performance. In 1996, SSRL initiated a design study for a major upgrade of SPEAR and its beam lines to 3rd generation light source standards. The phase one design goals for SPEAR3 are for 3 GeV, 200 mA operation with at-energy injection and with a beam emittance of about 15 nm-rad. Phase two would increase the current to 500 mA and enable higher-energy operation. The first phase upgrade involves lattice magnets, vacuum chamber, booster, and some beam line components. Beam line source point locations for insertion devices would remain essentially unchanged; and source point locations for bending magnets would change minimally. A magnet lattice is being developed that provides much improved beam parameters. The bulk of the first phase conversion would take place during a shutdown of approximately six months, with other work being done during earlier short shutdown periods. A preliminary design study will be completed in 1997, with more detailed studies continuing in FY 1998. If the SPEAR3 upgrade project is approved, detailed design and fabrication will be conducted in FY 1999 and FY2000, with the first phase accelerator conversion taking place in FY2001 or FY2002 depending on funding profile.

Fourth Generation Source Development

SSRL is engaged in a design study that will form the basis of a formal proposal for the development of a 4th generation light source, the Linac Coherent Light Source (LCLS). The study is a collaboration that involves several divisions of SLAC and a number of other scientific institutions. The remarkable characteristics of LCLS radiation have the potential for opening up a number of important new scientific frontiers. The LCLS would utilize the last one-third of the SLAC linac to accelerate electrons to a range of energies between 5 and 15 GeV. This source would create a photon beam of unprecedented brightness, coherence and peak power, far surpassing anything available in 3rd generation sources today. Design goals are a peak brightness of 5×10^{33} photons $/(\text{s-mm}^2\text{-mrad}^2\text{-.01\%}$ bandwidth) (13 orders of magnitude greater than any existing radiation sources) and a peak power of 10 GW in the wavelength region 1 .5- 15 Å. The design team has the goal of producing a design, complete with cost estimate and construction schedule, by late 1997. In parallel with the LCLS Design Study, a BNL/SLAC/UCLA collaboration to develop and test high performance rf photocathode guns for the LCLS is making considerable progress. The first of 4 guns has been completed, initial testing began at BNL in early October, and a dedicated Gun Test Facility (GTF) has been set up in the SSRL injector linac vault. The ultimate goal is to develop a gun, which will meet the LCLS requirement to produce a charge of 1 nC, or more with a normalized emittance of 1 mm-mrad or less in a pulse with duration of 10 picoseconds or less.

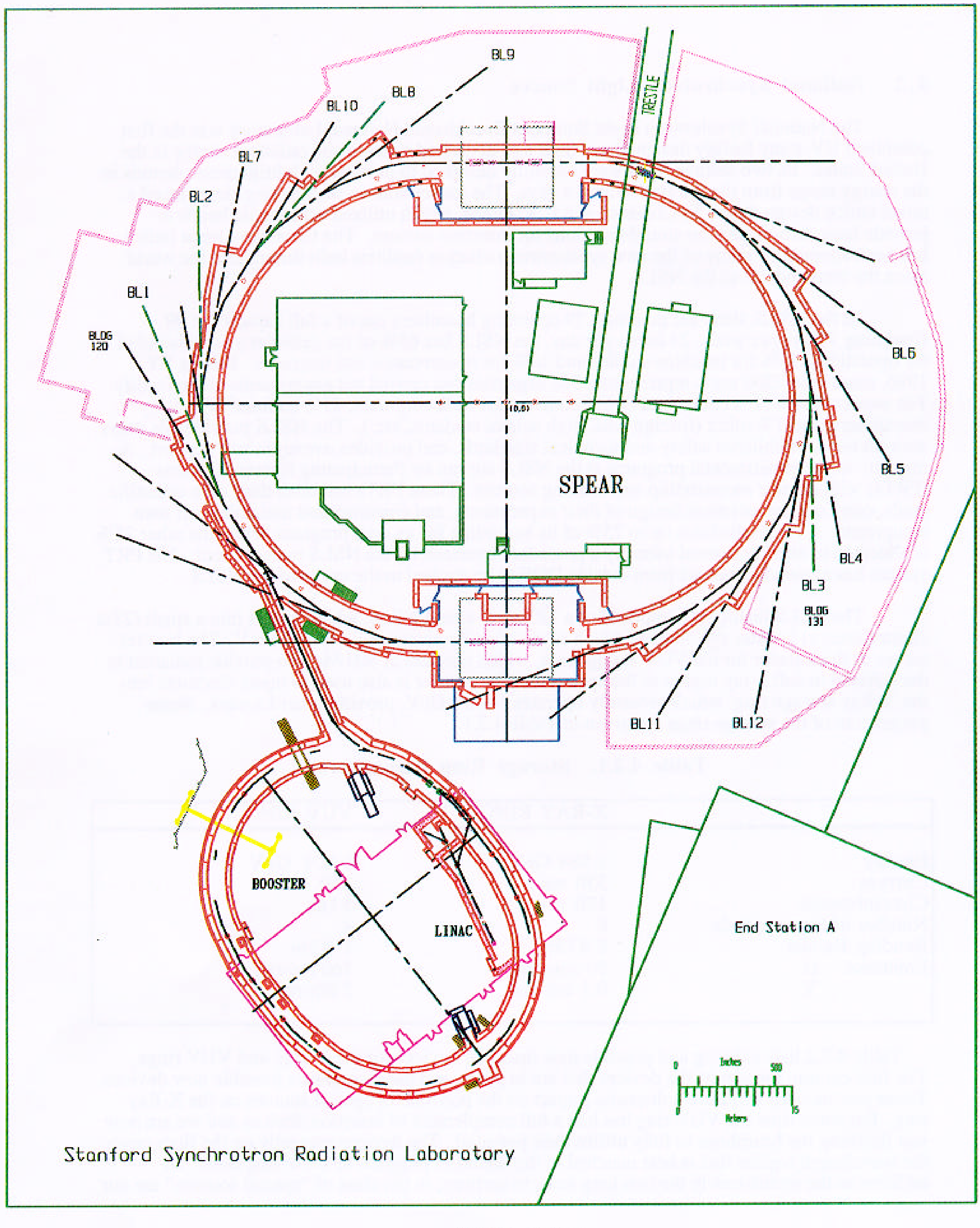

BL9
BL8
BL10
BL7
BL2
BL1
BLDG 120
TRESTLE
(0,0)
SPEAR
BL6
BL5
BL4
BL3
BLDG 131
BL11
BL12
BOOSTER
LINAC
End Station A
0
Inches
500
0
Meters
15
Stanford Synchrotron Radiation Laboratory

Figure 4.1.1

4.2 National Synchrotron Light Source

The National Synchrotron Light Source at Brookhaven National Laboratory was the first combined UV-x-ray facility designed and built as a dedicated synchrotron radiation source in the United States. Its two storage rings were carefully designed to provide high brightness photons in the energy range from the infrared to hard x-rays. The low emittance storage rings introduced a novel lattice design due to R. Chasman and C.K. Green, which utilized achromatic bends to provide long zero-dispersion straight sections for insertion devices. The Chasman-Green lattice has been adopted by many of the new synchrotron radiation facilities built throughout the world since the construction of the NSLS.

At the NSLS, there are presently 79 operating beamlines out of a full capacity of 99. Operating 7 days per week, 24 hours per day, the NSLS has 65% of the calendar year scheduled for operations, 15% for machine studies and 20% for maintenance and upgrades. During FY 1996, more than 2200 users representing 365 organizations carried out experiments at the facility. The user community is comprised of 61% university, 11% corporate, 21% national laboratory researchers, and 7% other (foreign labs, high school students, etc.). The NSLS provides its users with photons, establishes safety and technical standards, and provides oversight and support. A majority of the experimental programs at the NSLS are run by Participating Research Teams (PRTs) with diverse membership and funding sources. These PRTs establish their own scientific goals, carry out the technical design of their experiments, and construct and maintain their own equipment. A PRT schedules up to 75% of its beamtime for its own program, while the other 25% is allocated to outside general users by a procedure overseen by the NSLS management. The PRT system has allowed resources from outside DOE to be applied to the usage of the NSLS.

The NSLS facility is comprised of a 120 MeV electron linac which injects into a small (28m circumference) booster synchrotron which accelerates the electrons up to 750 MeV. The booster serves as the injector for the VUV storage ring, which operates at 800 MeV to provide radiation in the infrared to soft x-ray region of the spectrum. The booster is also used to inject electrons into the X-Ray storage ring, which presently operates at 2.58 GeV, providing hard x-rays. Some parameters of the storage rings are given in Table 4.2.1.

Table 4.2.1. Storage Ring Parameters

		X-RAY RING	VUV RING
Energy		2.584 GeV	0.808 GeV
Current		350 ma	850 ma
Circumference		170 m	51m
Number of Superperiods		8	4
Bending Radius		6.875m	1.91m
Emittance	H	90 nm-rad	160 nm-rad
	V	0.1 nm-rad	3 nm-rad

Table 4.2.2 lists existing and possible new insertion devices for the X-Ray and VUV rings. The first column represents the devices that are in place, and the second lists possible new devices. These new devices will have a dramatic impact on the portfolio of special sources on the X-Ray ring. For some time the VUV ring has had a full complement of insertion devices and we are now just finishing the beamlines to fully utilize their potential. The devices presently on the floor cover the wavelength regime that is best matched to the scientific program of VUV ring users. In addition to the undulators in the two long straight sections, in the class of “special sources” are our

infrared ports that fall into two types: very large aperture for far-IR (100 mrad x 100 mrad) and medium aperture for mid-IR (100 mrad x 50 mrad). We now have infrared ports on U2, U 10 and U12 in addition to the original infrared port on U4.

Table 4.2.2. Insertion Devices: Existing and Proposed

	Existing	Possible Future Devices
X1	Soft X-ray undulator	Same
x 9	RF	In-vacuum small gap undulator
x13	R&D straight section Small gap undulator, Time varying polarized wiggler	Next generation prototypes
x17	Superconducting wiggler	New superconducting wiggler (1997)
x21	Hybrid wiggler	Hybrid wiggler with reduced gap and period.
X25	Hybrid wiggler	Hybrid wiggler with reduced gap and period.
X29	RF	In-vacuum small gap undulator
u 5	UV undulator	Same
U13	UV undulator	Same

Facility Development

Users are the core of the present and future research at the NSLS. The PRT system was a critical ingredient. However, the scientific climate has changed and so must NSLS's approach to the user market. We will continue to improve access to the facility for the breadth of users whose research depend on synchrotron radiation, and will work to inform those scientists whose laboratory based programs could benefit greatly from using synchrotron radiation. But to do this, we foresee that the makeup of some PRTs will change over time, and this change may require varying degrees of NSLS participation. We anticipate an increase in the need for user support and also in new forms of user demand. We expect greater participation by less experienced users who are not synchrotron radiation experts, for example, in engineering, environmental sciences and biology. An increase in NSLS staff will be required to meet these needs.

The present complement of experimental beamlines was designed in the early 1980's. The PRT system under which they were designed and built provided a substantial investment and quickly created a thriving research community and a large-scale science program. These beamlines still serve the community extremely well but, in many cases, superior performance could be achieved by upgrading optical elements. Better mirrors, monochromators and detectors are now available that can yield orders-of-magnitude improvements in experimental data rates at very modest cost, as outlined in the NSLS Phase III proposal.

The area that is the most exciting and, after long neglect, is now showing the most progress, is detector development. Parallelism in detection is still little exploited in the synchrotron radiation community worldwide, but is high on everyone's agenda. There have been significant advances in charged coupled device [CCD]-based two dimensional detectors and image plates for crystallographic applications. The NSLS has developed a 12%element energy resolving detector for X-ray spectroscopy which was demonstrated to users at this years annual Users Meeting. We would like to carry forward an aggressive R&D program in detector development.

The accelerator systems at the NSLS are approaching a high level of maturity, but there are important areas where significant improvements are possible. A high degree of reliability has been achieved through an intensive program of hardware upgrades and preventive maintenance; however, the facility still requires work on the power distribution and water systems to reduce downtime. Increased reliability at the highest currents also requires an additional RF drive system, and the replacement of old RF cavities with design flaws, by new cavities of improved design.

The NSLS has been a leader in the development of advanced insertion devices. R&D in the Xl3 straight section has led to the successful development of a time-varying elliptically polarized wiggler (with APS and BINP Novosibirsk), and of an in-vacuum small gap undulator (with Spring-8). When replacing the old RF cavities by ones of improved design, we plan to leave room between the two cavities in each RF straight for the installation of small gap undulators, thus increasing the contingent of magnetic insertion devices by two.

At the NSLS, global orbit feedback systems were developed and implemented for the first time. These have provided the NSLS with a level of orbit stability unsurpassed even at the newest facilities. Through improvements in orbit monitoring and feedback algorithms, the stability can be even further improved. Improvement in beam position monitoring together with digital feedback technology presently under development at the NSLS, will provide a significant advance in the state-of-the-art in orbit stability.

In the X-Ray ring , we are in the midst of a program to increase the source brightness by more than an order of magnitude. Thus far, we reduced the vertical emittance from 2 nm-rad down to 0.1 nm-rad. After replacing half of the beryllium windows with a more robust design, the electron current was increased from 250 ma to 350 ma this year. Once the remaining beryllium windows are replaced (in December 1997 shutdown) we plan to increase the operating current towards a likely maximum of 440 ma. Operation of the X-Ray ring at 2.8 GeV has been achieved and is possible up to currents of 250 ma with existing RF power systems. During September and November 1997, the X-Ray ring will run for one week at 2.8 GeV so users can assess the value of the higher energy. Finally, machine physics studies have recently demonstrated operation of the X-Ray ring at a higher tune that decreases the horizontal emittance from 90 nm-rad down to 45 nm-rad. With continued work, this could be the preferred mode of operation a year from now. Replacing the hybrid wigglers on X21 and X25 by devices with one-half the gap and one-half the period could provide a further doubling of the brightness of these sources.

The funding required for the NSLS to meet its goal of increasing user support and upgrading beamline optics and accelerator hardware is: (1) a 20% increase in the operating and capital budgets, i.e. an increment of $5 M/year operating and $1 M/year capital/ARAM; (2) the Phase III construction project with a cost of $33.7 M.

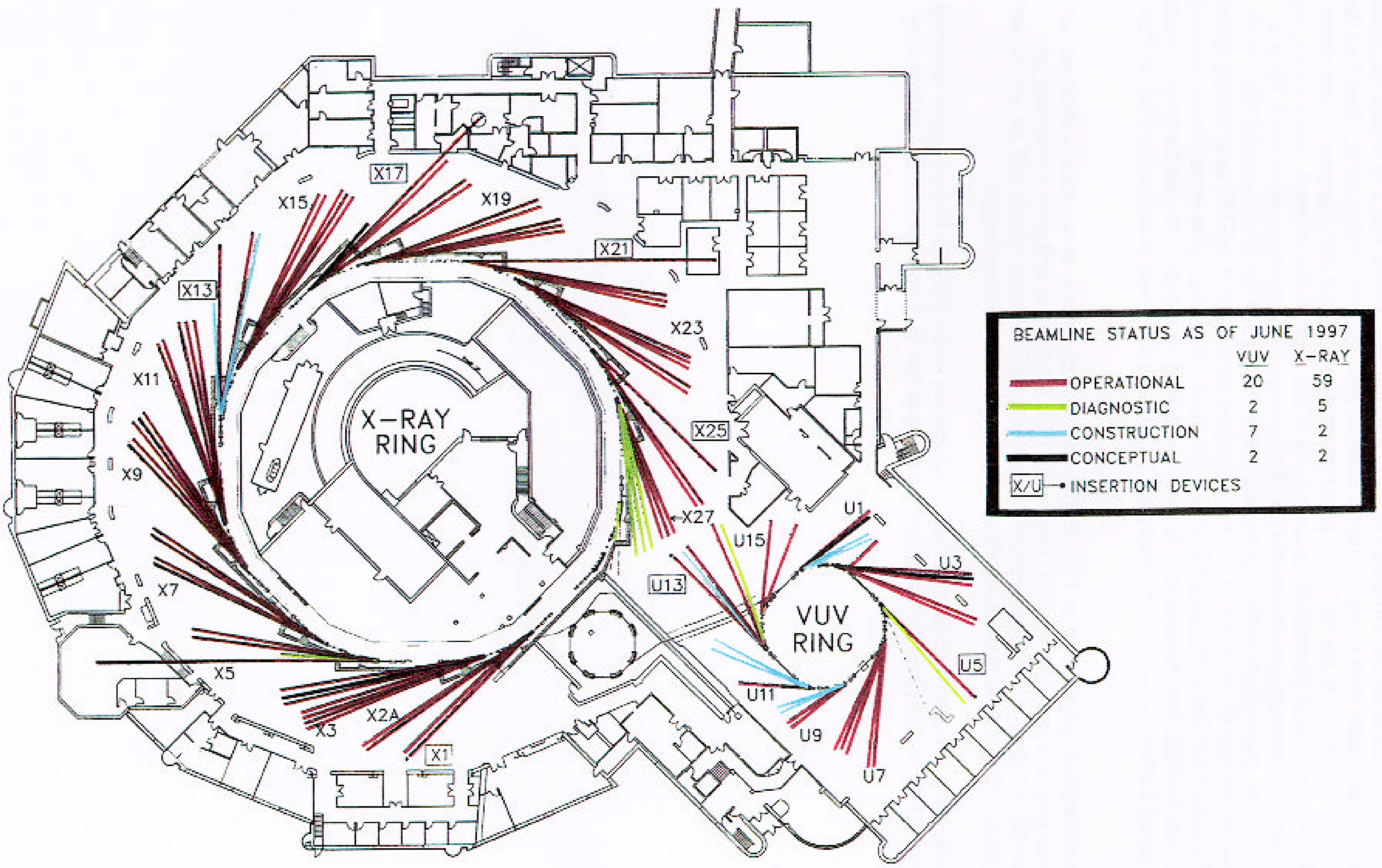
Fourth Generation Source Development

The NSLS has been actively pursuing free electron laser (FEL) sources, and aims to provide its users with access to these powerful new tools. Key initiatives are our participation in the Accelerator Test Facility (ATF) and the establishment of the Source Development Laboratory (SDL). The ATF is operated jointly by the NSLS and the BNL Center for Accelerator Physics as a user's facility for accelerator and beam physicists. The ATF program in RF photocathode guns is recognized internationally as cutting-edge R&D, as exemplified by its recent measurement of slice emittance in a 10 ps electron bunch. The SDL was established to pursue the science outlined in the NSLS Deep Ultra-Violet Free Electron Laser (DUV-FEL) conceptual design report. The cost of the SDL facility has been minimized by using an existing 2 10 MeV linac and the 10m long NISUS wiggler, originally built by STI Optronics for Boeing Aerospace.

Key to our plans is the development of sub-harmonically seeded FELs in which harmonic generation converts a laser seed to much shorter wavelength radiation. Much of the theory of these devices has been developed at the NSLS. A proof-of-principle High-Gain Harmonic-Generation (HGHG) FEL experiment is planned to be carried out at the ATF in the infrared, using a CO, laser seed. Self-amplified spontaneous emission (SASE) has already been observed at the ATF at 1 micron wavelength, and further work is planned for this fall. Both the SASE and HGHG work will be extended into the VUV at the SDL. An important advantage of HGHG over SASE is that HGHG will produce a beam with much higher longitudinal coherence. The experiments planned for the ATF and the SDL are milestones, not just for the BNL program, but also for other projects like the proposed Linear Coherent Light Source at SLAC and the Tesla Test Facility FEL at DESY, Hamburg.

The successful operation of an FEL facility in the ultraviolet is an essential milestone, and the experience gained in running the SDL ultraviolet FEL for science will give accelerator and beamline scientists a preview of the important system integration issues which will be critical for the success of science programs utilizing short wavelength free electron lasers.

To carry out a demonstration of SASE to saturation in the NISUS 10 m wiggler will cost $2.5 M. To produce useful photons and a user program at the SDL to exploit them will cost an additional $10 M.



BEAMLINE STATUS AS OF JUNE 1997

	VUV	X-RAY
🟥 OPERATIONAL	20	59
🟩 DIAGNOSTIC	2	5
🟦 CONSTRUCTION	7	2
⬛ CONCEPTUAL	2	2

X/U → INSERTION DEVICES

Fig. 4.2.1

4.3 Advanced Light Source

The Advanced Light Source is a third-generation synchrotron radiation user facility of very high brightness optimized for the ultraviolet and soft x-ray regions. This is the range that includes the K-edges of the first row elements (C, N, 0) of the periodic table. The ALS came into operation in late 1993 with a single beamline and has since been adding beamlines at a steady rate. At present there are 16 operating beamlines out of an ultimate capacity of about 80 beamlines. The salient parameters of the ALS are summarized as follows:

Energy	1.0 -1.9 GeV
Current	400mA
Horizontal emittance (@ 1.5 GeV)	4 nm-rad
Vertical emittance (@ 1.5 GeV)	0.12 nm-rad
Horizontal beam size	200 pm
Vertical beam size	20 pm
Pulse length	35 ps

The ALS has 12 long straight sections of which ten are available for insertion devices. At present there are four undulators and one wiggler installed. Two more undulators are under construction, so seven of the ten available straight sections will be operational by the end of 1998. In addition, there are ten bend-magnet beamlines in operation and four under construction. The beamline status is summarized in the Fig. 4.3.1.

Scientific Program

Of the four DOE-operated facilities, the ALS is the odd-one-out in that it has been optimized for performance in the VUV/soft x-ray region. The other three facilities service primarily the hard x-ray region. There is a different flavor to the kind of research done in the two regions. In the hard x-ray region, the research question is mostly “where are the atoms?’ with much emphasis on molecular structure and crystal structure using techniques such as diffraction and EXAFS. In the lower energy region, the question tends to be “what are the electrons doing?’ with emphasis on chemical bonding and valence bands using techniques such as spectroscopy and photoemission. The two kinds of information are of course complementary and both are required for a complete understanding.

The diversity of the scientific program at the ALS can be seen by inspection of the figure. The program ranges over the physical and life sciences and has both basic and applied research aspects. The word “microscopy” recurs frequently. High brightness translates into high spatial resolution at the sample. X-ray microscopies, spectromicroscopies, and “micro” and "nano" techniques in general therefore represent a mainstream activity at the ALS, a development foreseen in the 1984 Eisenberger-Knotek report. The high spatial resolution can be achieved through photon optics (zone plates and demagnifying mirrors) or electron optics (photoemission electron microscopy). Efforts are proceeding on all fronts. Present resolutions are in the 50-1000 nm range, and theoretical estimates indicate that resolution below 10 nm should be possible.

High brightness translates also into high resolving power, and this feature drives basic research at the ALS. Programs in chemical dynamics, atomic and molecular physics, and condensed matter physics are benefiting from the unprecedented energy resolution available at the ALS. The high resolution promises to be of special importance in the elucidation of the electronic properties of highly correlated materials, such as the high-temperature cuprate superconductors.

A development ***not*** foreseen in the Eisenberger-Knotek report is the resurgence of soft x-ray emission (SXE) spectroscopy. Since x-ray emission has an inherently low cross section, it benefits greatly from the high brightness of the ALS. And since it is a photon-in/photon out technique, it is immune from the short-sampling-depth limitation of conventional photoemission and is applicable to buried interfaces and wet samples of relevance to environmental science.

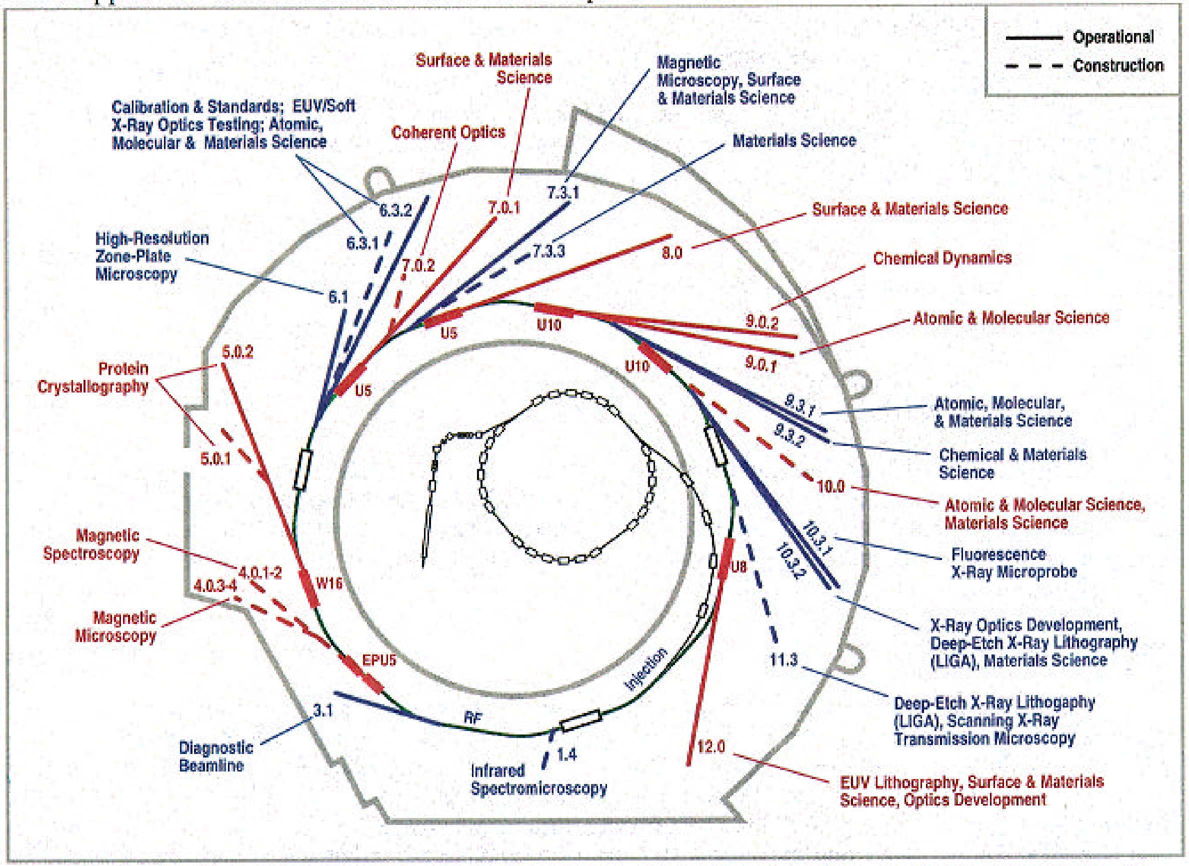


Fig. 4.3.1 Current and planned beamlines at the ALS through 1998. Beamline designations X.Y.Z refer to storage ring sector number X, port number Y, and branch number Z. A fourth digit is used for additional branching. There are 12 sectors. Ports 0 are insertion-device ports, ten of which are available for insertion devices; ports 1, 2, 3, and 4 are bend-magnet ports. Each branch may service multiple experimental stations.

The industrial research program at the ALS is centered on the needs of the semiconductor-microelectronics, magnetic-storage, and biotechnology companies in Silicon Valley and the San Francisco Bay Area. Intel and Applied Materials have established a micro-XPS facility for the characterization of large wafers. Amgen and Hoffman-LaRoche have already invested in the protein crystallography beamline, and other biotech companies are expected to follow. Local magnetic-recording and storage companies (IBM and Read-Rite) are showing strong interest in both lithography and spectromicroscopy.

User Access

There are two principal means of access to the ALS: (1) through membership of a Participating Research Team (PRT), or (2) as an independent investigator (II). A PRT is a consortium that brings in resources towards the construction, operation and maintenance of a beamline, in recognition for which the PRT receives some percentage of guaranteed beam time. The remaining beam time (25% or more depending on the beamline) is allocated to IIs on the basis of a proposal review mechanism. Peer review is an integral part of the process. Proposals for

PRTs must have approval of the ALS Program Advisory Committee (PAC), and proposals from IIs are ranked by the ALS Proposal Study Panel (PSP). Strong preference is given to those proposals that truly need the high brightness of the ALS.

Future Plans

The ALS management has developed a "Roadmap" for the full utilization of the ALS. Its main feature is an orderly build-out of the remaining straight-section and bend-magnet beamlines. This program (estimated cost $64M) will proceed as fast as funding rates allow. There is a pending $10-15M initiative to build out a sector dedicated to molecular environmental science.

In addition to its Roadmap, the ALS management envisions a major "infrastructure" expansion (estimated cost $60M) involving the construction of buildings adjacent to the ALS to house laboratories, offices, and auxiliary facilities for users.

In its strategic planning, the ALS management adheres to the view that science in the 21st century will be dominated by four main areas: (1) nanoscience, (2) life science, (3) environmental science, and (4) information science. These areas are responsive to societal needs, an important consideration in the post-Cold War funding climate. In **nanoscience,** the length scale of the of soft x-ray microscopes at the ALS match very well to the analytical needs of the microelectronic and magnetic-storage industries. In **environmental science,** speciation spectroscopy and biomicroscopy on wet materials in the soft x-ray region will complement the vigorous efforts already under way in the hard x-ray region. In **life science,** the ALS offers a very competitive protein crystallography facility, as well as programs in biomicroscopy and spectroscopy on metallo-organic systems. ALS contributions to **information science,** largely a software activity, will be through the hardware relevance of its nanoscience work. Basic research at the ALS will advance through the higher resolving power offered by high brightness.

4.4 Advanced Photon Source

In October of 1983, an ad hoc committee was convened by the Department of Energy, Office of Basic Energy Sciences, with the charter to solicit and evaluate ideas from synchrotron-radiation providers and users as to the future opportunities and technical needs for synchrotron-radiation-based research. The committee, co-chaired by Peter Eisenberger and Michael Knotek, found that current research and development programs in materials science, physics, biology, chemistry, geosciences, and other fields that use synchrotron radiation could greatly benefit from the availability of high-brilliance x-ray beams. The committee named as its highest priority the development of a 6-7 GeV storage ring facility utilizing undulators to deliver these unprecedented x-ray beams. Later, this recommendation was endorsed by the Major Materials Facilities Committee of the National Academy of Sciences, chaired by Frederick Seitz and Dean Eastman. These events led to the construction of the 7-GeV Advanced Photon Source storage ring at Argonne National Laboratory. Construction of the facility started in 1990. Users began commissioning beamlines and performing early scientific research in late 1996.

The APS facility (Fig.4.4.1) is situated on an SO-acre site and comprises a particle-beam injection and storage system (450-MeV linac; positron accumulator ring; 7-GeV booster synchrotron; 7-GeV storage ring); undulators; beamline front ends; undulator test line; a circular experiment hall to accommodate experiment beamlines; user laboratory/office modules adjacent to the experiment hall; a central laboratory and office building for operations staff; a support building to provide utilities; and a residence facility for APS users.

Synchrotron radiation produced by 35 bending magnet sources and 35 insertion device (undulators, special wigglers) sources are made available, so that in all, 70 beamlines can be used for experimental research. In the current phase of the construction, funds were made available to develop 40 (20 bending magnet, 18 undulator and 2 wiggler) of the 70 radiation sources.

All the planned technical facilities are now operational and have met design specifications. The storage ring performs with the designed positron beam emittance of 8.2 x 10-9 nm-rad at 100 mA of stored current and with beam lifetimes of 15 to 40 hours, depending on the positron fill pattern. The x-ray beam brilliance of nearly 10_{19} photons s-lmm-, mrad-, (0.1% Bandwidth) and the undulator performance on energy tunability have exceeded the design goal. Extensive R&D has produced the engineering and optical technology required to handle the extreme powers and power densities produced by the undulator x-ray radiation. Beam stability and reproducibility have exceeded specifications.

The first compliment of 40 beamlines have been assigned to user groups, whose proposals were reviewed and approved based on their scientific program and the criticality of high-brilliance APS x-rays to their work. These Collaborative Access Teams (CAT s) have obtained approximately $160M to fund construction of 40 beamlines. Funding has come from the DOE, the National Science Foundation, the National Institutes of Health, industry, private foundations, and state governments. Construction of CAT beamlines is well under way. In fact, nearly half of the beamlines are being used for scientific research. An additional two beamlines utilize x-ray beams to monitor the performance of the storage ring facility.

The CAT membership comprises the principal investigators at the APS. These groups will bring both students and postdocs to support their planned research. In addition, each of the CATs will provide at least 25% of their total available beam time to Independent Investigators, who are generally not CAT members, but whose research programs can be performed on beamlines already constructed by a CAT. Currently, CAT member institutions include 85 U.S. universities; 32 industries; and 25 federal and other research laboratories. The principal investigators from the U.S. universities, industry, and research labs number 465; 225; and 291, respectively. Foreign representation in the CATs numbers 52, with a major contribution of over $3 million coming from Australia to support its research programs.

Science at the APS centers on using the unique properties of the radiation produced by the undulator, wiggler, and bending magnet sources. The radiation provides very high brilliance in the hard x-ray range from under 1 keV to few hundred keV. The high brilliance allows traditional x-ray techniques to be used for measurements performed with a time window of tens of picoseconds, thus providing a unique capability to observe the time evolution of various systems, such as catalysts, biomolecules and human cells. The radiation from APS undulators is partially coherent, which supports unique experimentation in many fields, particularly condensed matter physics. The ability to produce circularly polarized x-rays using specialized undulators or wigglers greatly enhances the importance of synchrotron radiation studies of magnetic materials.

The ability to use appropriate x-ray optics to focus undulator radiation on a submicron-sized area leads to a new capability “x-ray microscopy” which will advance our knowledge of materials with importance in technology, bioscience, environmental science, and chemical science.

The scientific research proposed by members of the CATs will probe areas such as atomic physics, condensed matter physics, materials science, geoscience, biophysics, chemistry of complex materials, structural biology, and environmental science. These studies will have technological applications in numerous fields, such as environmental remediation, industrial enzymes, liquid crystals, solid state lasers, polymers, synthetic membranes, microfabrication, electrode position, corrosion prevention, fibers, high-technology products, ceramics, new drugs, and catalysts. While early experimentation at APS beamlines is already leading to discoveries in the areas of science and technology mentioned above, demand for additional radiation sources is growing. This interest will result in the implementation of the remaining 28 x-ray beamlines at the

APS. At the time of this writing, six new beamlines have been committed to the study of magnetic materials, structural genomics, and x-ray analytical service work for small industries. Additional beamlines are being requested for x-ray imaging of materials, human tissue, and archeological samples. It is anticipated that such interest will lead to full implementation of the research capabilities of the APS within the next five years or so, depending on funding availability.

In the process of developing the APS, many excellent teams with unique scientific and technological capabilities have been established within the APS organization. They have achieved advances in accelerator technologies, insertion device technologies, high-heat-load engineering, x-ray optics fabrication, and metrology. In addition to being the driving force for new synchrotron radiation technology, both at the APS and nationwide, this expertise has become an international resource supporting (with full cost recovery) many new synchrotron facilities under construction, including BESSY II in Berlin and Spring-8 in Japan. These APS teams also help form the backbone for R&D on fourth-generation radiation sources now being performed in the U.S. and at HASY Lab. in Hamburg.

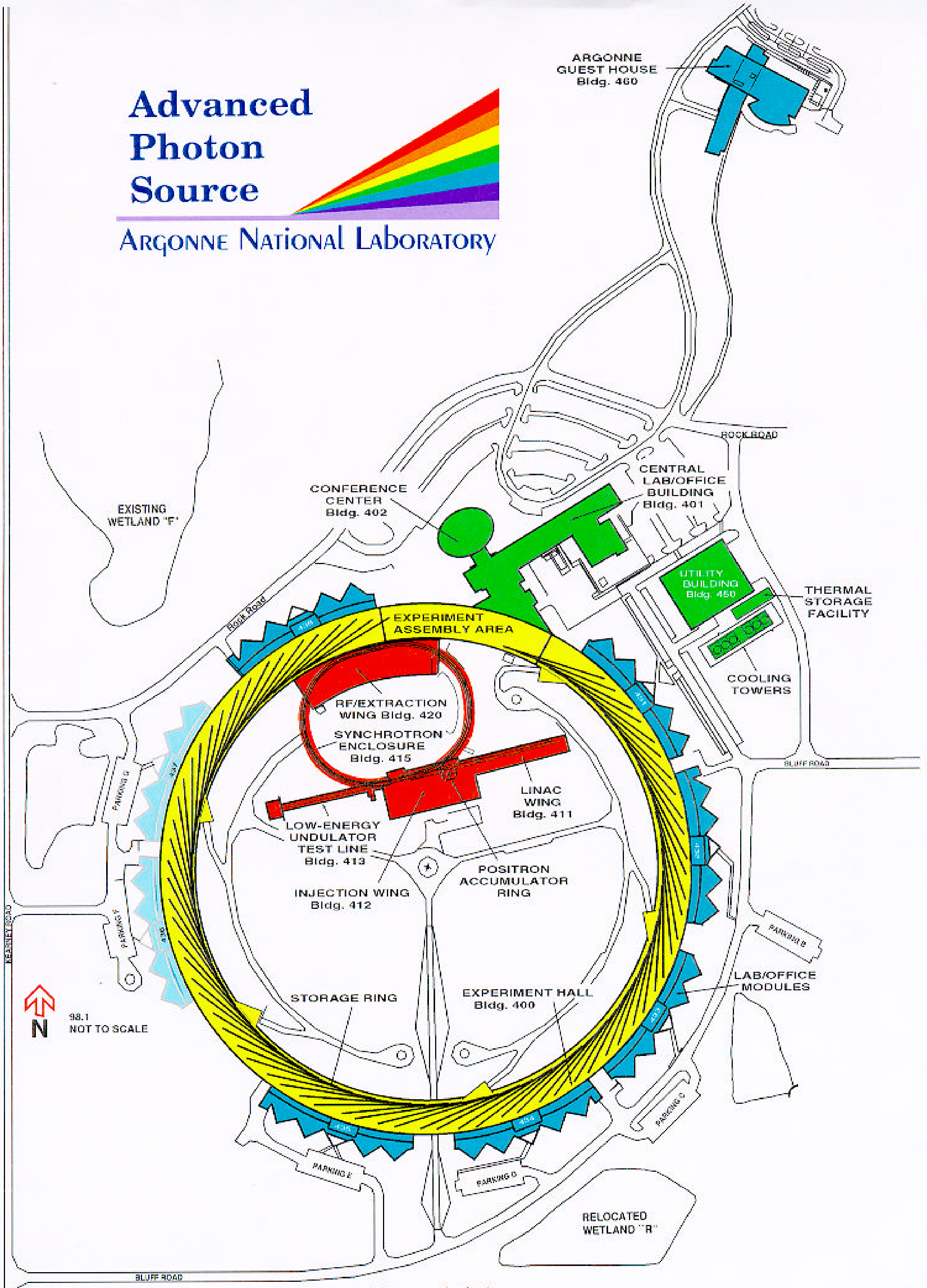

Advanced
Photon
Source
ARGONNE NATIONAL LABORATORY
ARGONNE
GUEST HOUSE
Bldg. 460
EXISTING
WETLAND "F"
CONFERENCE
CENTER
Bldg. 402
ROCK ROAD
CENTRAL
LAB/OFFICE
BUILDING
Bldg. 401
UTILITY
BUILDING
Bldg. 450
THERMAL
STORAGE
FACILITY
COOLING
TOWERS
Rock Road
438
EXPERIMENT
ASSEMBLY AREA
RF/EXTRACTION
WING Bldg. 420
SYNCHROTRON
ENCLOSURE
Bldg. 415
LINAC
WING
Bldg. 411
BLUFF ROAD
PARKING G
437
LOW-ENERGY
UNDULATOR
TEST LINE
Bldg. 413
POSITRON
ACCUMULATOR
RING
INJECTION WING
Bldg. 412
KEARNEY ROAD
PARKING F
436
PARKING B
LAB/OFFICE
MODULES
N
98.1
NOT TO SCALE
STORAGE RING
EXPERIMENT HALL
Bldg. 400
PARKING C
435
434
PARKING E
PARKING D
RELOCATED
WETLAND "R"
BLUFF ROAD

Figure 4.4.1

5 .O THE SCIENTIFIC & TECHNOLOGICAL CASE

5.0 Scientific and Technological Case

This section summarizes the scientific and technological impact of synchrotron radiation based research. Unlike the Seitz-Eastman of 1984 where the emphasis was on evaluating and projecting the merit of building future facilities, this report focuses more on what has been accomplished in synchrotron science since that report. The evolution of the field over the last decade also indicates the obvious future trends in the areas where extrapolation is possible. Of course, there are areas where a simple extrapolation may not be possible. An example of this is development of 4th generation light sources.

The most straightforward and most important conclusion of this study is that over the past 15 years in the United States synchrotron radiation research has evolved from an esoteric endeavor practiced by a small number of scientists primarily from the fields of solid state physics and surface science to a mainstream activity which provides essential information in the materials and chemical sciences, the life sciences, molecular environmental science, the geosciences, nascent technology and defense-related research among other fields. The research carried out at the four D.O.E. synchrotron sources is both very broad and often exceptionally deep. The breadth of the research is well indicated by NSLS data which show that research results obtained at NSLS have been published in more than 250 journals. The high quality of synchrotron-based research is illustrated by the large number of publications in premier journals such as Science, Nature and Physical Review Letters. This is especially true in the life sciences where in recent years more than 60% of the biological crystal structures published in that field’s leading journals were obtained using synchrotron techniques.

Given the remarkable success of synchrotron radiation-based science, it is impossible to do justice to this vast body of research. What will be discussed in this section is a very small fraction of total number of works carried out using synchrotron radiation. We divide this section into the following topical areas: materials research, surface science, polymers, atomic, optical, molecular physics and chemistry, molecular environmental science, geosciences, structural biology, microscopy, and technological impact.

5.1 Materials Research

Synchrotron-based research has had a profound and extraordinarily broad impact on condensed matter physics and materials science. The synchrotron experiments contribute ubiquitously to materials research, ranging from fundamental issues to important practical problems. For example, the users of NSLS have published papers in more than 250 journals, with a significant fraction of these in materials science. The combination of intense, bright sources, tunability and high photon energies has allowed vastly improved resolution with many orders of magnitude increases in signal enabling the study of weak scattering from small samples and surfaces, novel spectroscopies such as magnetic and inelastic scattering, real-time studies and studies using the coherent properties of the beam. These experiments have had the effect of forcing us to rethink our basic understanding of semiconductors, metals, superconductors, alloys, composite materials, liquid crystals, surfaces and interfaces, magnetism, dynamic processes, elementary excitations, electronic structure, and factors controlling phase equilibrium. The impact on science in the last quarter century of these new techniques after the previous 75 years of research with tube-based X-ray sources may be compared to the impact of the electron microscope after hundreds of years of work with the optical microscope. In both cases, whole new worlds have been opened up and in both cases it is difficult to think of an area which has not been significantly impacted as a result. As an investment in science, synchrotron-based materials research has been extraordinarily cost effective and productive for the United States. In this section we will present a selected set of highlights of the accomplishments and potential of synchrotron-based materials research in this country. It is, of course, completely impossible to do justice to this vast body of work and what we discuss is but a small fraction of the broad range of accomplishments and opportunities.

One of the most important scientific successes spawned by synchrotron sources has been in the area of photoelectron spectroscopy. Synchrotron based photoemission spectroscopy experiments at the Wisconsin Synchrotron Radiation Center (SRC), SSRL and NSLS have profoundly impacted our understanding of a wide range of materials, especially those of semiconductors, their surfaces and interfaces. These experiments have played a critical role in advancing theoretical understanding and calculational capabilities that form the essential scientific foundation for the electronics industry. More recently, synchrotron based experiments at NSLS, SSRL and ALS have contributed significantly to our understanding of C_{60} and other novel forms of carbon. Issues ranging from crystal structure, phase transitions, electronic structure and superconductivity have been addressed using the power of synchrotron radiation. The experiments on C_{60} and related materials provide good examples showing how effectively the synchrotron community can respond to problems in material science.

Synchrotron based photoemission experiments have also made fundamental contributions to our understanding of the basic physics of strongly correlated electron systems. These studies have elucidated the electronic structure of high-Tc superconductors and have shown most clearly the d-wave structure in the energy gap in the superconducting state and in the pseudo-gap in the normal state. Angle-resolved photoemission experiments done at SSRL and SRC in particular have been crucial in leading this effort. Fig.5.1.1 reproduces the original observation of the superconducting gap anisotropy. The figure presents photoemission spectra above and below T_c for overdoped Bi2212 at two different locations in k-space. As expected in a d-wave pairing state, while the spectra taken at A clearly show the effects of a gap opening, the spectra taken at B hardly change above and below T_c, suggesting that the gap is undetectable within the experimental uncertainty. The experiment shown in Fig.5.1.1 has contributed significantly towards the current consensus of d-wave pairing symmetry in the high-T, superconductors. This higher order pairing state, which is different from the s-wave pairing symmetry of conventional superconductors, is a key step towards a comprehensive understanding of the remarkable phenomenon of high-temperature superconductivity. In a similar fashion, the recent observation of a d-wave-like normal state pseudo-gap shows that the superconducting transition is very different from the traditional paradigm of BCS-Eliashberg mean-field theory which describes the transition in conventional superconductors.

Angle-resolved photoemission data from oxide materials with strong antiferromagnetic interactions have also evinced the important role of magnetism in a clear way. Recently, an angle-resolved photoemission experiment at SSRL has provided so far the only experimental indication of the separation of spin and charge degrees of freedoms of electrons in one-dimensional solids - an important theoretical concept that was first envisaged about thirty years ago. Combined photoemission, spin-polarized photoemission and x-ray absorption experiments at NSLS have contributed significantly to our understanding of the colossal magnetoresistance behavior in $La_{1-x}Sr_xMnO_3$. In particular, spin-polarized photoemission experiments provide possible evidence for half-metallic behavior with conduction electrons of a single spin.

X-ray absorption, core level x-ray photoemission spectroscopy (including the pioneering work in Europe using conventional ESCA lab) as well as resonant photoemission spectroscopies have been used to understand the electronic structure of both occupied and empty states of a wide range of materials: metals, semiconductors, insulators, as well as materials exhibiting various magnetic behaviors, metal-insulator transitions, charge-density wave, spin-density wave and superconducting instabilities. Significant efforts have been devoted to strongly correlated materials such as Ce and U intermetallic compounds and transition metal oxides. This is particularly true for the transition metal oxides where a combined experimental and theoretical effort has led to a new classification of these materials and the introduction and verification of the important concept of charge-transfer insulators. Early x-ray photoemission spectroscopy and resonance photoemission experiments at NSLS and SSRL have provided important information on the orbital character of the conduction electrons as well as important parameters such as the Coulomb interaction U, the charge transfer energy A and the hybridization t. Spin-resolved photoemission, mainly carried out at NSLS in this country, has shown some interesting results from magnetic materials. X-ray magnetic circular dichroism experiments, pioneered at NSLS, and used at SSRL and ALS have also impacted our understanding of the role magnetism on electronic structure.

Another important phenomenon exhibited by certain low dimensional transition metal compounds with nested Fermi surfaces is that of a charge density wave (CDW) instability. Here high resolution synchrotron x-ray diffraction has changed our picture of the charge density wave state. Although it had been well known for quite some time that x-rays were nearly ideal as a probe of the structure of the charge-density wave state, neither conventional laboratory x-ray sources nor even the first generation of synchrotron x-ray sources were capable of realizing that potential. The highest quality samples of a CDW material available to-date are single crystal whiskers of $NbSe_3$. Further, the best $NbSe_3$ whiskers are very small with cross sectional dimensions on the order of 2 microns by 10 microns. Early on, this small sample size, coupled with the high q resolution required to resolve these long-range ordered structures, conspired to keep experimental counting rates too low for high quality experiments. However, the high brilliance of modern insertion device beam lines has enabled workers at CHESS to study very small samples at high resolution while still obtaining sufficient count rates to obtain signal to noise ratios between 10^4 and 10”. These high quality data sets have revealed entirely new physics, which was inaccessible just a few years ago. For example, the tremendous signal to noise ratio revealed that two length scales are required to describe the phase-phase correlation function providing a direct measurement of the amplitude coherence length.

As noted above and as will be discussed in the next section, synchrotron radiation has played an important role in investigations of magnetic materials. One of the most surprising applications is that of magnetic x-ray scattering. In the absence of resonant enhancement, the magnetic scattering crossection is typically between 10^{-5} and 10^{-6} of the charge scattering crossection. In spite of this weak crossection, a number of important investigations have been carried out and undoubtedly this area of research will continue to expand in the future especially if reactor-based neutron scattering facilities in the United States are allowed to diminish. Synchrotron magnetic x-ray scattering is complementary to neutron scattering with several important strengths. First, the small cross section results in extinction-free scattering, so that the order parameter itself and any associated large length scale fluctuations may be reliably determined. This is of particular importance in studies of phase transitions. Second, the small penetration depth of x-rays, typically on the order of 2 μm, may reduce the effect of concentration gradients in alloys and mixed magnetic materials. Third, the high reciprocal space resolution allows large length scales to be probed. Fourth, the relatively poor energy resolution (- 10eV) ensures integration over all relevant thermal fluctuations. Fifth, the contributions due to the orbital and spin magnetic moments may be distinguished through polarization analysis.

A recent example has been the studies of the magnetic ordering processes in diluted magnets such as $Fe_{0.5}Zn_{0.5}F_2$ in an applied magnetic field. This represents a model realization of a generic disordered system - the random field Ising model (RFIM). Because of extinction effects, neutron scattering was unable to provide reliable measurements of the order parameter as a function of field and temperature. Figure 5.1.2 shows the results of such measurements in $Fe_{0.5}Zn_{0.5}F_2$ carried out at NSLS. These data have led to a new model for the RFIM which in turn has enabled researchers to produce a consistent picture of all existing data - thermodynamic, magnetic, optical and scattering. We expect that studies of such disordered magnetic materials especially in thin film geometries will evolve into a major activity at both the second and third generation light sources.

Another area of research made possible by synchrotron x-ray sources is that of inelastic x-ray scattering. Inelastic x-ray scattering (IXS) has developed rapidly in the last five to ten years into an important new tool for the study of condensed matter systems. The technique measures the dynamic structure factor, $S(q,\omega)$ the Fourier transform in time and space of the charge density-density correlation function. IXS thus provides information on the dynamic properties of the system. Recent activities in two energy regimes highlight the potential of the technique to contribute in diverse areas of condensed matter physics.

At moderate energy resolutions (-1 eV) IXS is sensitive to electronic excitations. In this regime, the method provides advantages over, for example, electron scattering through the ability to measure out to large momentum transfers. As a result, the field has made important contributions to the study of the electron gas in metallic systems, revealing the relative roles of many-body interactions and band structure effects in determining the electron dynamics. The experimental work, performed in part at the NSLS, provides data in the relevant regimes for the first time, and has sparked renewed theoretical efforts on this important, and unsolved, many-body problem.

At ultra-high resolution (- 1meV) the dynamics of the ion cores (phonons) may be probed. In this regime, the key strength of the technique exploited to-date is the ability to study small momentum transfers, which are not accessible at these energy transfers in neutron scattering experiments because of kinematic constraints. This is of particular utility in amorphous systems. Experiments performed at the ESRF have elucidated the dynamics of liquids and glasses. In particular, this work has demonstrated the existence of so-called “fast” sound in water and ice. Ultra-high resolution scattering is an area that benefits directly from the high brightness of third generation sources, and this field should grow rapidly in the U.S. over the next five years.

As the new sources come on-line, and beamlines continue to improve at second generation sources, the applications of the technique will further diversify. Possibilities include the study of electron dynamics in nano-particles to investigate quantum finite size effects, and work performed at very high pressures, as achieved in diamond anvil cells, which exploit the small beam size. In addition, the very recent discovery of resonant enhancements in the inelastic cross-section, in the hard x-ray regime, allow for the possibility of studying electronic excitations in high-i! materials not previously accessible with IXS due to limitations imposed by absorption. Resonant IXS will provide the ability to measure such energies as the charge transfer gap in high-T, superconductors, and other strongly correlated electron systems, and therefore will yield important experimental input to models of electronic structure in systems of intense current interest to the materials science community.

As a complement to IXS, studies of the dynamics at extraordinarily low energies, corresponding to time scales of milliseconds to seconds are now being pursued at third generation sources. These are based on fluctuation spectroscopy which explicitly uses the coherence of the beam. Such studies are at their earliest stage, but they promise to give new insights into the low energy dynamics of many systems including especially those under the rubric of “soft condensed matter.”

Synchrotron radiation is naturally matched to studies of structures and ordering processes in “soft condensed matter.” Specific applications in polymers will be discussed in section 5.3. The subfield, “soft condensed matter” includes a wide variety of materials such as thermotropic liquid crystals, complex fluid mixtures exhibiting micellar, lamellar and more exotic phases, lipid bilayer systems, stacked membranes and many materials derived from biology. A schematic picture of one such structure - a DNA cationic liposome complex is shown in Figure 5.1.3. Workers at Santa Barbara have probed the solution structures of such DNA-liposome complexes on length scales from subnanometers to micrometers using synchrotron x-ray diffraction (at SSRL) and optical microscopy.

Many liquid crystal materials can be prepared as freestanding films with thicknesses varying from nanometers (2 molecules) to microns (that is, macroscopic). Synchrotron radiation experiments in such free standing films have revolutionized our picture of the phases and phase transitions in thermotropic liquid crystals. Specifically, they have elucidated the interplay between orientational and positional order and they have shown how such order evolves from two to three dimensions. Again, we expect that synchrotron x-ray diffraction studies of soft-condensed matter systems, especially in thin film geometries, will be an ever-expanding area of research at both second and third generation light sources.

Chemical crystallography is another sub-area of materials research where synchrotron radiation has contributed important advances. In particular, a major impact of synchrotron x-rays on structural chemistry and crystallography is the development of very high resolution powder diffraction using a crystal analyzer in the diffracted beam. This advance has been pioneered at the NSLS and has created a leap forward in the powder method over the past decade, analogous to the impact of profile refinement on neutron powder diffraction a decade earlier. Thus, it is now possible with powder methods to determine by ab initio solution or refinement structures containing up to 30 independent atoms, and groups throughout the world are working to extend the complexity of structures addressed. This development has made major contributions in many areas, including structure studies for the understanding and tailoring of new zeolites widely used by the chemical industry as catalysts and molecular sieves, and studies of new compounds and alloys based on C,,. This new tool has also provided critical information on the structure and properties of many complex oxide systems, including high T_c superconductors and magnetic and magnetostrictive materials. Studies of phase equilibria in inorganic solids vs. temperature and pressure and even of solid state reaction kinetics have also been enabled. Also, in a growing trend, totally new materials' structure results are now being achieved by the combination of high resolution synchrotron x-ray and neutron powder diffraction.

We now turn from applications which traditionally fall under the rubric of "condensed matter science" to ones which are described as "materials science." Three questions begin the characterization of materials: what is the elemental composition? what is the structure? and what are the defects? Synchrotron radiation provides powerful new tools with which to answer these questions. A good example is the emergence of resonance (anomalous) x-ray scattering. Although it was recognized quite early that resonance x-ray scattering offered a revolutionary means of studying materials, early attempts were often frustrated by instabilities in the x-ray energy. As synchrotrons have matured however, resonance (anomalous) x-ray scattering has emerged as a powerful tool for the characterization of materials. By tuning near an x-ray absorption edge, it is now possible to control precisely the scattering contrast between the sample elements. This allows measurements with both low and high contrast between elements. In pioneering experiments at SSRL and at the NSLS, the local structure of amorphous and crystalline solid solution alloys have been determined with unprecedented precision. For example, both short-range chemical and displacive correlations have been determined for crystalline solid solution alloys with atoms nearby in the periodic table. Static atomic displacements of less than 0.0001 nm are now routinely measured. These measurements, which were unimaginable before the availability of synchrotron radiation, contradict our existing phenomenological picture of solid solution alloy structure and challenge existing theoretical calculations of phase stability; theorists are now challenged to include both static and dynamic displacements in their calculations and have an experimental basis by which to judge their theoretical progress.

The ability to alter the scattering contrast between elements in materials is now widely exploited. Resonance (anomalous) x-ray scattering has been used to help determine crystal structure in practically all conceivable x-ray diffraction experiments including powder diffraction, surface diffraction and truncation rod scattering and standard Bragg scattering. In some cases, the information obtain can go well beyond the identification of structure. For example, in the 80's investigators began studying diffraction anomalous fine structure (DAFS) from Bragg reflections to determine the chemical state of atoms at a particular co-ordination site. With DAFS they were able to determine the chemical state of an element at different lattice sites. This new information cannot be obtained by alternative methods. Similarly, researchers combined DAFS with truncation rod to determine both the structure and chemistry of buried interfaces. Again this new information cannot be obtained by other methods.

Ultra-fast dynamics in phase transitions represent another class of experiments which are made possible by intense synchrotron radiation. Pioneering work was carried out at CHESS with measurements of laser melting in Si. By using the time structure of synchrotron radiation sources, it was possible to demonstrate unambiguously that pulsed laser melting on a nanosecond time scale was a thermal melting process rather than a plasma excitation of the electronic system; the transition from plasma excitation to thermal melting was found to take place on the order of 10 picoseconds which is 100 times faster than originally predicted. Synchrotron radiation was also used to study the phase evolution during pyrolitic reactions. Recent work at CHESS and the ESRF illustrates a continued need to improve both spatial resolution and measurement speed to detect intermediate phases during complicated reactions.

As will be discussed in detail in section 5.8 the availability of intense and tunable synchrotron radiation, coupled with the emergence of efficient CCD sensors has also revolutionized our ability to image materials. Efforts by scientists in industry and national laboratories have resulted in the ability to image materials in 2 and 3 dimensions with micron resolution. X-ray microscopy and x-ray tomography can now provide pictures of mesoscopic structures of materials even when the structure lies deep within the sample. This information can include both the chemistry and crystallography of the observed structures.

X-ray microdiffraction is a rapidly emerging field with great promise for the characterization of materials. X-rays complement electron microprobes which can study the phase and orientation of nm scale grains at the surface of a sample. With x-ray microdiffraction, it is possible to determine the phase, texture and strain of grains both at the surface of a sample and deep within the sample with -0.1-10 μm^3 resolution. Because x-ray microdiffraction is non-destructive, it will soon be possible to characterize the three dimensional crystallographic structure of a test sample and follow the structure during processing. The observed microstructure can then be compared to theoretical predictions to validate mesoscopic-dynamics codes.

Another growth area possible with third generation x-ray sources is measurement of -process characteristics in "real time." Experiments are already planned at the APS to study thin film growth during laser and plasma deposition. Expansion of these studies to solidification and other non-equilibrium systems may provide new understanding of the dynamics of technologically important processes such as welding, corrosion, sintering and casting.

Of all the areas of materials science that have been studied and will be studied, perhaps the most important to the DOE will be study of actinide chemistry. The country faces a cleanup of the legacy of the cold war of Herculean proportions. Many of the most elementary essential questions remain open such as the valence of the various actinide elements in the presence of a witch's brew of other chemicals. Such knowledge is crucial to the development of optimal strategies for containing the actinides in inert environments. Synchrotron studies of this type, pioneered at SSRL, will be seen as having played a vital role in providing this basic underpinning of scientific knowledge. The intense sources and tunability of the X-rays allows one to do element specific measurements of very small quantities of these materials which is beneficial for many reasons. Large quantities of these compounds would require certification of the laboratories for work on radioactive materials which would be enormously costly. Large quantity samples are difficult to transport safely and also expose the researchers to added risk. Many of the important questions involve the study of intrinsically dilute concentrations such as the uptake of these elements by plants as a way of collecting and concentrating them from ground water. Manifestly, this is a crucially important area for research and an example of work that synchrotron based X-ray sources are uniquely capable of doing.

One of the most interesting aspects of the large body of materials research done at US synchrotron facilities is the fact that much of it is done by industry. The impact of these tools in many areas such as semiconductor manufacturing, polymer growth, magnetic materials, glasses and displays has been significant and continues to grow. Techniques for looking at amorphous magnetic alloys, low concentrations of impurities on semiconductor surfaces and in optical fibers, real-time CVD growth of compound semiconductors, doping and local structure of optical glasses, electromigration in VLSI interconnects, oxide growth and roughness in IC's, plastic flow in metals and many others are examples of experiments that US industry cares about enough to pay to do them at these facilities. This kind of materials science allowed by these sources represents an important competitive technological edge provided by our past investment in this type of research; manifestly, this will be enabled in the future by a healthy and active synchrotron radiation research community in this country. This will be discussed in great detail in section 5.9.

The breadth of materials based research which has been impacted by synchrotrons is truly impressive. It ranges from the most interesting fundamental question in solid state science, why high T_c superconductors exist, to understanding the microscopic behavior of the most important man-made material used on the planet-Portland cement. Our understanding of a vast range of technologically important materials has been significantly improved by synchrotron radiation research. Because of our substantial investments in the past we are the leaders in this type of research in the world. This investment has paid off handsomely in both science and technology. A continued commitment is required if we are to maintain this leadership position.

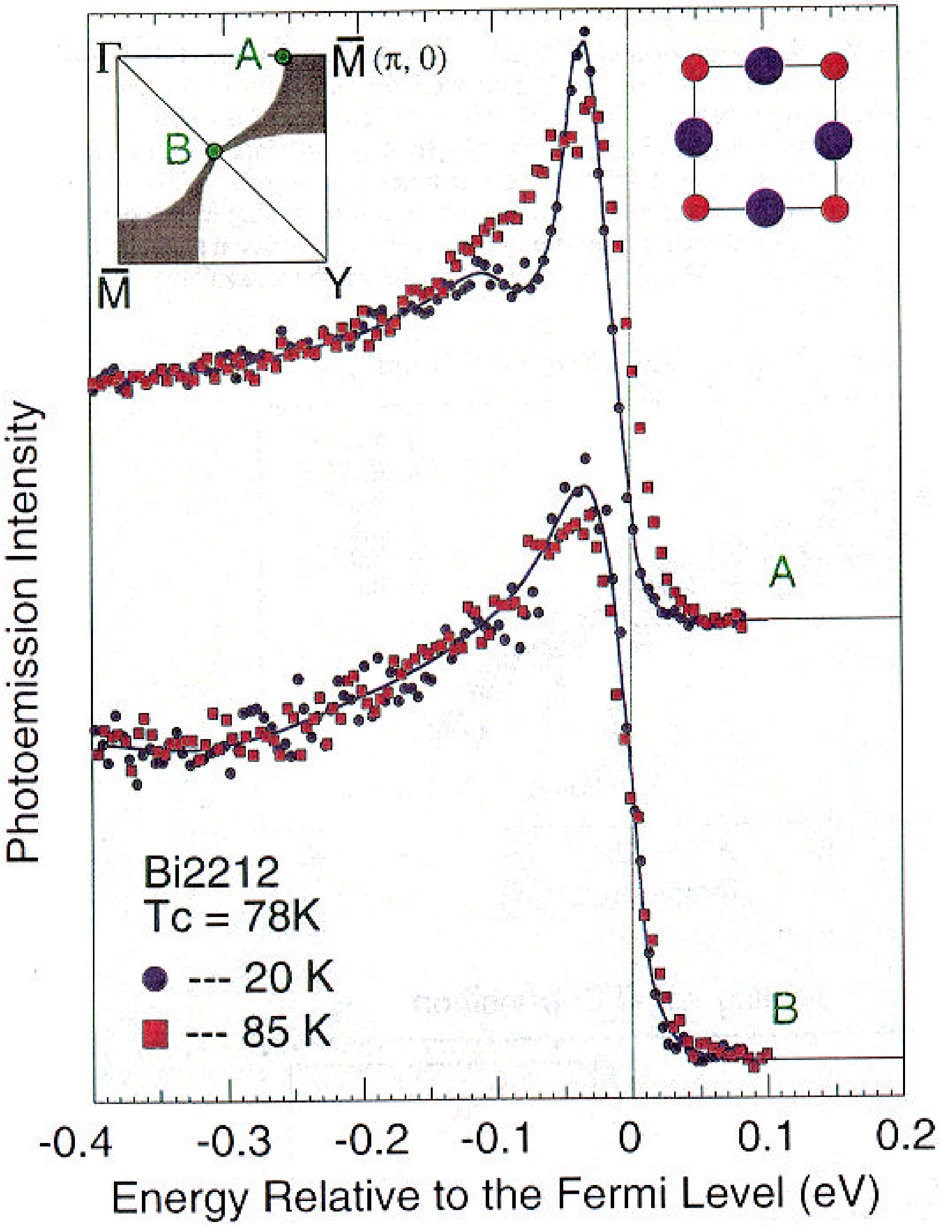


Fig.5.1.1 reproduces the original observation of the superconducting gap anisotropy. It presents photoemission spectra above and below T_c for overdoped Bi2212 at two different locations in **k**-space. As expected in a d-wave pairing state, while the spectra taken at A clearly show the effects of gap opening, the spectra taken at B hardly change above and below T_c, suggesting that the gap is undetectable within our experimental uncertainty.

Fig. 5.1.2 (a) The ZFC order parameter squared in $Fe_{0.5}Zn_{0.5}F_2$ as measured at the (100) position with x-rays for five fields and H=OT. For $H\neq 0$, the data are well described by a power-law-like behavior with a broadened transition region. The broadening is modeled by a Gaussian distribution of transition temperatures of width $\sigma_{ZFC}(H)\alpha AH^2$. (b) The $H\neq 0$ data of (a) replotted as a function of the temperature interval away from T,(H) as measured in units of H^2. This illustrates the rounding of the transition which is attributed to nonequilibrium effects arising from extreme critical slowing down and the univeral scaling behavior of the *trompe l'oeil critical* phenomena. The inset shows the phase boundary of $Fe_{0.5}Zn_{0.5}F_2$

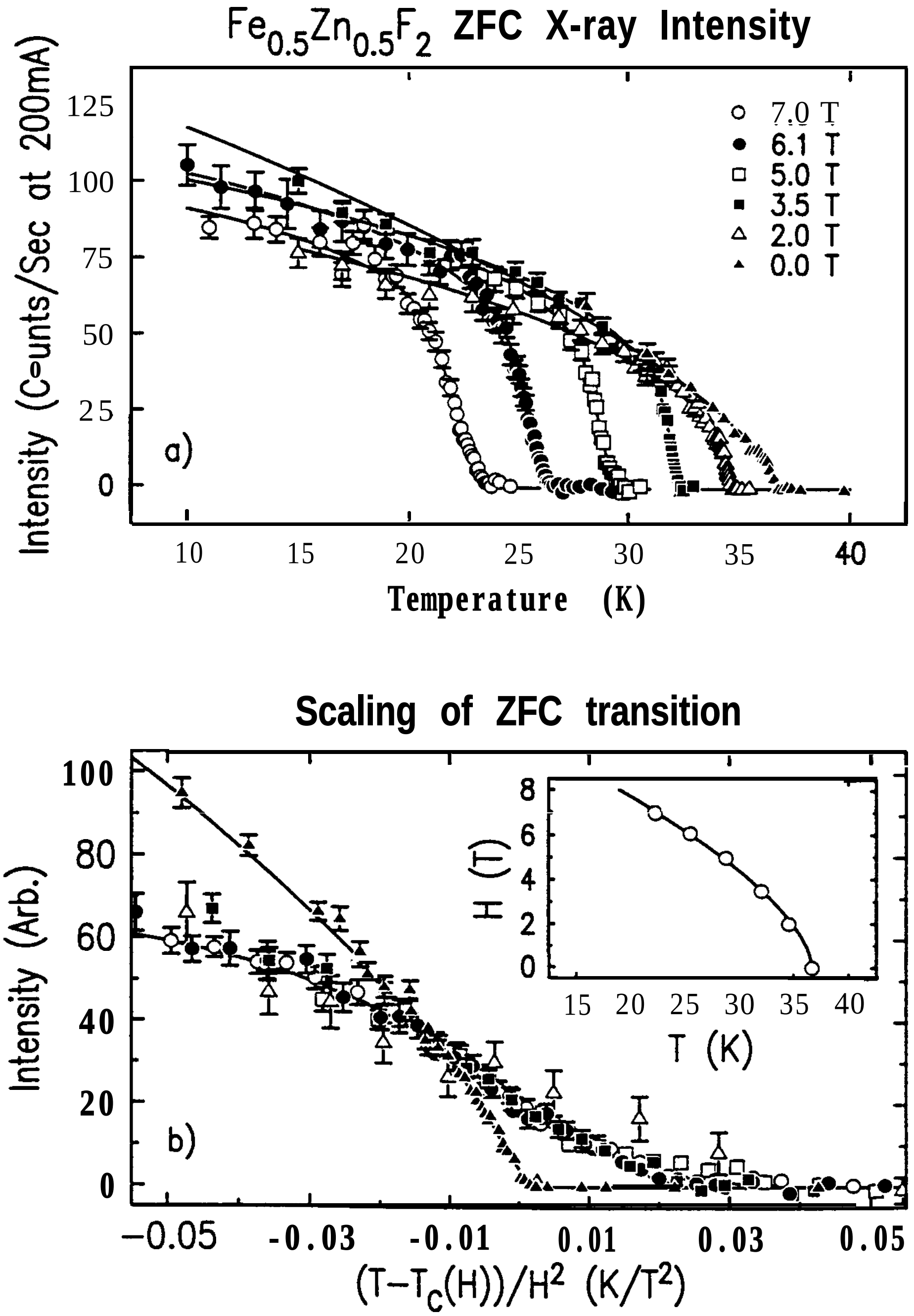


Fig. 5.1.2

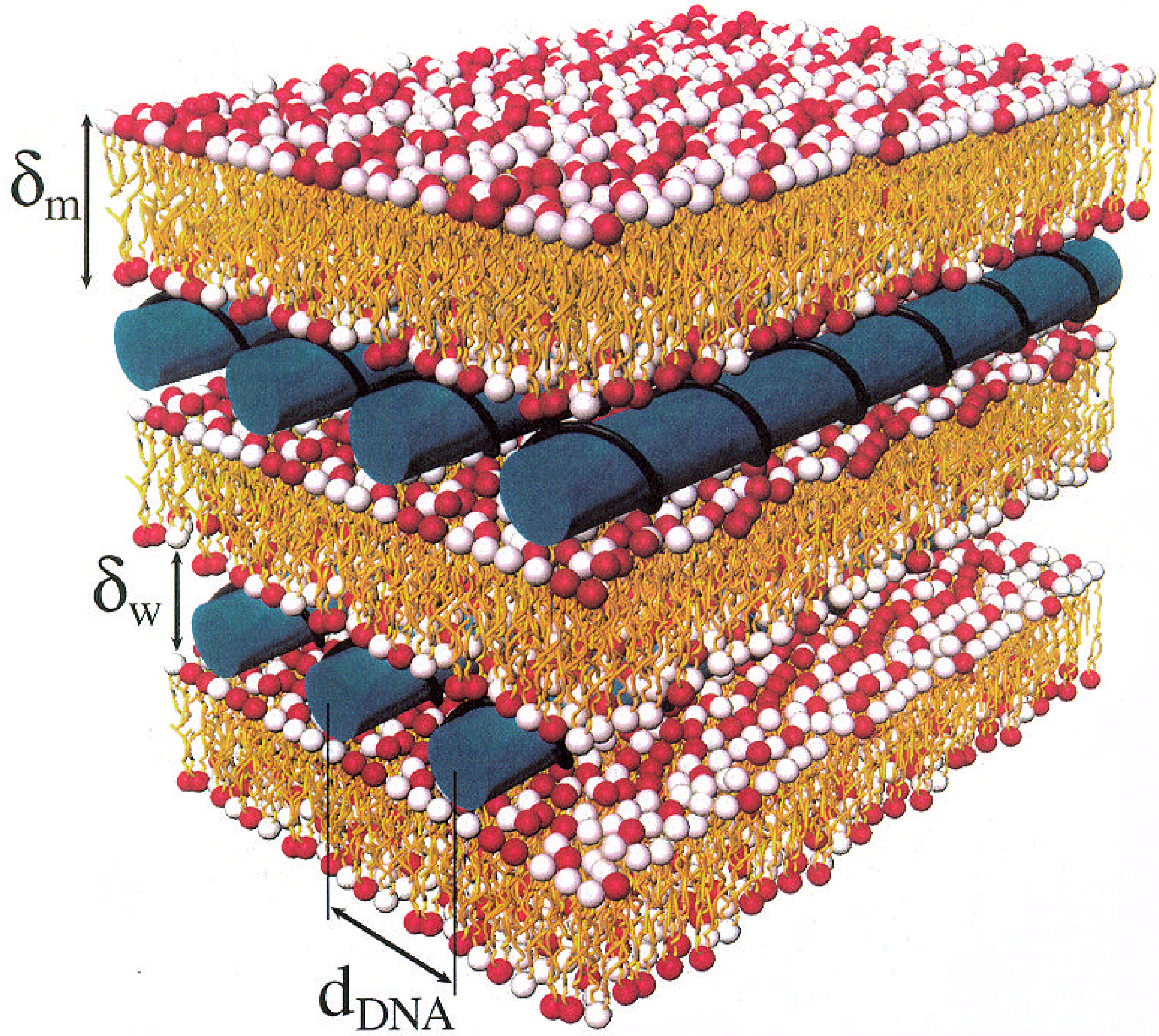


Fig. 5.1.3 Schedmatic picture of the local arrangement in the interior of lipid-DNA complexes. The semiflexible DNA molecules are represented by rods on this molecular scale. The neutral and cationic lipids comprising the membrane are expected to locally demix with the cationic lipds (red) more concentrated near the DNA.

Stewardship of Nuclear Weapons Stockpile

Research at synchrotron facilities will potentially make significant contributions to the DOE's Science-Based Stewardship Program. In particular, synchrotron-based x-ray diffraction and spectroscopic methods can provide detailed information about aging processes in metallic, polymeric and other organic components of the enduring stockpile. While monitoring the degree of aging is necessary in its own right, such studies can also help to reveal the microscopic mechanisms involved. For example, recent work using x-ray absorption spectroscopy has documented variations of near-neighbor atomic coordinations in plutonium alloys, comparing the effects of aging versus composition. Similarly, spatially variable changes in polymer crystallinity can be quantified using x-ray diffraction. Detailed information of this kind is essential for the reliable prediction of aging phenomena needed for enhanced surveillance.

In addition, synchrotron radiation makes it possible to characterize materials under conditions of very high pressures and temperatures. Thus, the effects of aging on the yielding strengths, equations of state and other thermomechanical properties of materials can now be precisely documented at relevant pressures and temperatures. Though static in nature, such experiments provide an important complement to dynamic measurements, especially when the latter require the use of difficult subcritical underground experiments. Specifically, synchrotron-based high-pressure research can provide essential data both for planning the most effective dynamic measurements and to aid in their interpretation. More generally, the high pressure-temperature experiments carried out at synchrotrons offer some of the most stringent tests of existing materials theories, whether atomistic (e.g., based on quantum mechanics) or more macroscopic and phenomenological in character. Testing and improving such theoretical models of material properties plays a central role in the long-term stewardship program.

5.2 Surface Science

Overview

The field of modern "surface science" was created and defined in the 1960's by the pursuit to understand the fundamentals underlying two important technologies: semiconductor devices and heterogeneous catalysis. The continuing importance of the two areas is reflected by the 1997 world wide annual revenues of the associated industries: $150 billion and $1300 billion, respectively. The initial emphasis in this work was on the development of quantitative analytical techniques and on studying "model systems" consisting of well-prepared, well-controlled and reasonably well defined surfaces, mostly single crystal substrates that were studied under ultrahigh vacuum (UHV) conditions. In addition to studies associated with the two main technologies, work has been aimed at understanding the general principles of chemisorptive and physisorptive bonding; the oxidation and corrosion of surfaces, the magnetic properties of surfaces and interfaces, the structure of liquid surfaces and electrolytic interfaces and the nature of phase transitions in two dimensional systems.

As a result of this work, during the 30 year period from the mid 1960's to the mid 90's our understanding of surfaces has undergone a revolution. At the beginning of this period we could not determine any of the important characteristics of a surface, as for example the chemical identity of surface species, their atomic geometries (structure), their electronic charge distributions (bonding), their magnetic properties and the dynamics of their atomic motions. Improvements in UHV technology and the development of sophisticated experimental and theoretical techniques laid the foundation for the revolution in our knowledge. Most of the important surface properties of "model systems" can now be determined accurately and quantitatively. In parallel with this development, surface analysis (e.g. x-ray photoemission and Auger spectroscopy) has found a routine use in industrial settings for studying more complex technologically relevant systems. The development of new surface tools appears to be reaching saturation, although refinements and extensions of them will no doubt occur, for example at third generation synchrotron radiation sources.

From a synchrotron radiation perspective it is important to recognize that the formative years of surface science overlapped with those of synchrotron radiation research. Because of the emphasis of traditional surface science on model surfaces and UHV techniques, surface science research has had a strong historical link with VUV/soft x-ray science. The growth of the surface science community in the 70's therefore paralleled the growth in the VUV/soft x-ray synchrotron radiation community, in particular, the increased utilization and development of photoemission spectroscopy. Up to the early 80's, at the time of the Eisenberger-Knotek and Seitz-Eastman reports, surface science research with synchrotron radiation predominantly involved the use of VUV/soft x-ray radiation. In fact, it is interesting to note that at that time, because of the strong surface science effort, the VUV/soft x-ray synchrotron community produced a comparable number of scientific publications as the entire hard x-ray synchrotron community. Over the last 10-15 years a significant shift has occurred. The overall scientific productivity of the hard x-ray community is now considerably larger and the two energy regimes are contributing about equally to surface science studies, largely due to increased use of various x-ray scattering techniques.

What has been accomplished?

To a large degree, the early scientific goals of understanding the basic properties of "model" surfaces have been accomplished. The structure of clean surfaces, ultra thin films and of chemisorption complexes can now be determined routinely. We have obtained a fundamental understanding of semiconductor surfaces and interfacial junctions, like Schottky barriers, through observation of bulk and surface electronic states. We understand many of the dynamic and kinetic properties of surfaces and the fundamental growth modes of thin films. Through sophisticated imaging techniques we can directly observe the growth of materials down to atomic dimensions. We understand the connection between chemical viewpoints of surfaces, emphasizing the local bonding, and physical viewpoints based on two or three dimensional band structure. Surface science has also established a framework of mechanistic concepts, principles, and insights of surface chemical reactions and of the surface chemical bond which form the basis of heterogeneous catalysis. We have even mastered the ability to move atoms on a surface, one at a time.

Contributions of Synchrotron Radiation Techniques

The revolution in our understanding of surfaces has come from an interplay of many approaches and the application of many techniques. Synchrotron radiation techniques have made many significant contributions. Ultraviolet photoemission spectroscopy (UPS) of solids, pioneered with laboratory sources in the 60's has been used by many groups in conjunction with VUV/soft x-ray synchrotron radiation since the 70's and it has been extensively applied to many kinds of problems. It has directly revealed the electronic "surface states" postulated in conjunction with the invention of the transistor and allowed the observation of molecular orbitals associated with the surface chemical bond. Synchrotron radiation based UPS, especially in its angular resolved mode developed in the 70's, has emerged as the technique-of-choice for the study of the electronic structure of surfaces (and solids) and together with theory has provided the basis of our present understanding of such structure. During the last ten years spin resolved UPS studies have revealed the spin-dependent electronic structure of surfaces. Through observation of spin dependent quantum well states in transition metal multilayers such studies have provided an explanation of the oscillatory exchange coupling in such systems.

Building on the concepts of laboratory based ESCA spectroscopy developed in the 60's, synchrotron radiation based x-ray photoemission spectroscopy (XPS) in the 50-1000eV range has provided valuable element and chemical state specific information of surfaces. It has led to the identification of reaction intermediates at surfaces and at interfaces which could be identified only because of the increased spectral resolution and the enhancement in surface sensitivity afforded by tunable synchrotron radiation. Magnetic dichroism in core level photoemission is presently being used as a surface and element specific probe of magnetism.

Other important contributions have come from the photoelectron diffraction (PD) technique. In contrast to LEED this technique offers elemental and chemical state specificity, a significant advantage in the study of heterogeneous systems. Photoelectron diffraction has revealed detailed information on the structure of chemisorbed atoms and molecules and is now one of the three most used methods (together with LEED and SEXAFS) for studying surface structures. The closely related photoelectron holography technique has been shown capable of providing three-dimensional images of surface structure with atomic resolution. This technique is being further developed at the ALS.

Surface x-ray diffraction has been used to determine the structure of clean surfaces and ultra thin films with unprecedented accuracy and precision. Presently, it is replacing LEED as the technique of choice for structure determinations of ordered surfaces when it is available. It has also been applied for in situ studies of thin film growth. Application of this technique to the study of phase transitions and correlations in two dimensional inert gas layers has had an important impact on soft matter physics. Owing to the large x-ray penetration depth in matter, this technique has also given us unprecedented insight into the structure of electrolytic metal surfaces buried under a liquid, and together with STM and AFM has revolutionized our understanding of these technologically important interfaces. Furthermore, this technique has revealed the structure of liquids above such interfaces. We have greatly improved our understanding of polymer surfaces and the structure of liquid surfaces by application of x-ray diffraction and reflectivity measurements.

Surface sensitive x-ray absorption spectroscopy in the extended fine structure regime (SEXAFS) pioneered in the late 70's at SSRL was the first technique to challenge surface structure determinations by LEED. Owing to the high precision of the technique for bond length determinations we have learned that bond lengths at surfaces are similar to those expected from chemical rules established for the bulk. Over the last ten years the technique has provided detailed information on the local dynamics of atomic motions at surfaces and the links between static and dynamic structure. To-date, only LEED has determined more surface structures than SEXAFS, with SEXAFS and PD contributing about equally.

The related NEXAFS technique developed in the early 80's at SSRL has given us detailed information on the structure of molecular chemisorption systems. From detailed studies of the molecular orientation at surfaces in more than one hundred systems we have learned how to link the molecular chemisorption geometry to the geometry and molecular orbital structure of the free molecule. More recently, NEXAFS has revealed the orientation of large organic molecules on surfaces and the orientation and relaxation of molecular groups at polymer surfaces, disordered systems that cannot be studied with diffraction techniques. Owing to its elemental and chemical specificity, its sensitivity to local bonding anisotropies through its polarization dependence, and its applicability to disordered systems, the technique is increasingly being applied for technological surface analysis, often in conjunction with photoelectron emission microscopy (PEEM).

Absorption measurements with circularly polarized x-rays, so-called x-ray magnetic circular dichroism (XMCD) spectroscopy, pioneered at HASYLAB in the late 80's, have significantly impacted our understanding of surface and interface magnetism. A related technique is based on the absorption of linearly polarized light and it can be used for the study of antiferromagnets. The development period of the XMCD technique around 1990 overlapped with a renaissance in magnetics research caused by the discovery of the giant magnetoresistance effect and oscillatory exchange coupling in thin transition metal multilayers. Such systems are presently being introduced into magnetic storage devices. Especially soft x-ray measurements at the transition metal L edges, first carried out at NSLS, have provided unique information relevant for such systems, in particular, the absolute size of magnetic moments for each element can be determined. Measurements at various synchrotron laboratories have revealed the existence of enhanced and reduced moments in ultra thin magnetic films and their dependence on crystallographic structure, as well as the existence of induced interfacial moments in non-magnetic metals. Through a unique separation of spin and orbital moments, XMCD has provided an unprecedented clear picture of the origin of the magnetocrystalline anisotropy in thin film multilayers. The technique has also been used in conjunction with a PEEM microscope for magnetic imaging.

Use of infrared synchrotron radiation pioneered at NSLS, has made possible absolute reflectivity measurements of adsorbate covered surfaces. Such spectra showed broadband reflectance changes and the appearance of dipole forbidden modes as anti-resonances. The data imply that electrons excited in the near surface region scatter inelastically from the adsorbates and that even the DC conductivity of thin films can be strongly affected by adsorbates on th surface. A program has been initiated to simultaneous study thin film resistivity and infrared reflectivity.

Finally, the advent of third generation sources has allowed the practical application of x-ray emission spectroscopy to the study of surfaces. Such studies, pioneered by researchers at Max-Lab in Sweden in the early 90's were developed into a practical tool at the ALS. The results have allowed an unprecedented atom-specific look at the surface chemical bond, challenging prevailing frontier molecular orbital models in favor of chemical models which use the individual atoms in the molecule and substrate as a starting point.

The Future

Surface science has thus made enormous progress in the past 30 years, and in some sense might be considered a mature field. But in an era where nanoscale technologies are becoming increasingly important, where the future of whole industries depends on devising new methods of packing more objects or information into smaller areas and volumes, it is apparent from simple geometrical arguments that the effects of surfaces and interfaces are becoming increasingly more important. This alone guarantees the future vitality and importance of this scientific area. In addition, certain experimental techniques to be discussed below will take on new dimensions in view of third generation synchrotron radiation facilities. On the other hand, general scientific and technological trends are expected to change the direction and emphasis of surface science. Over the next ten years new impulses and directions are anticipated from three areas: nanoscale and thin film technologies, environmental molecular science, and life sciences.

While the era of "classical" surface science, characterized by a revolution in fundamental knowledge obtained from model systems and by the development of surface science techniques, may be coming to an end, the importance of surface and interface phenomena will remain, most likely increase. Driven by the need to understand "real" rather than "model" systems the field is bound to change. The study of homogenized, well-defined surfaces will be increasingly supplemented (possibly replaced) by the study of "real" surfaces and interfaces which are inhomogeneous on the smallest possible scale. Studies in UHV environments will be extended to studies in gaseous or liquid environments. It will also be necessary to address the surface properties of materials of increased complexity, e.g. non-crystalline materials such as polymers. It will no longer suffice to understand atomic and charge distributions at solid surfaces and interfaces but the spin distribution as well. Owing to an increasing number of devices based upon spin dependent transport across interfaces the understanding of interfacial magnetism is becoming of increasing importance. Overall, there will be increased technological applications of surface science techniques, with emphasis on techniques which offer lateral resolution down to atomic dimensions coupled with elemental, chemical and magnetic specificity.

In general, the study of buried "surfaces", i.e. interfaces, will become of increased importance. This requires the development of new techniques with enhanced depth capabilities and depth resolution. This transition is driven by the need to understand the properties of solid-solid interfaces in hi-tech devices, the reactions at solid-liquid interfaces in heterogeneous catalysis and in the environment. The latter is driven by increased societal concern with the impact of hazardous waste, which is reflected by the rapid growth of the field of environmental molecular science. In the future we also anticipate increased emphasis on interfacial problems in the life sciences, especially in biology where interactions at both solid-liquid and liquid-liquid interfaces are of fundamental interest and great practical importance.

Synchrotron radiation research will have an especially important role in this development. While electron and ion based techniques are typically limited to the study of vacuum terminated surfaces, x-rays offer the advantage of increased depth capabilities. X-rays have been demonstrated to be effective probes of buried interfaces, e.g.in electrochemistry. Fluorescence holography or standing wave techniques which place the maximum wavefield amplitude at a selected distance below the surface are new techniques on the horizon. The desire to study systems which are heterogeneous on the smallest scale naturally requires techniques with elemental, chemical and magnetic specificity. Again, x-rays have this capability. It is anticipated that in the near future these capabilities will be available at a spatial resolution near 20nm in the scanning and imaging mode as discussed in the microscopy section of this report. This resolution is about a factor of 10 better than the line width of electronic devices or the magnetic bit size in storage media and it is therefore useful for many technological applications. Photoemission electron microscopy (PEEM), in principle, has the capability of even better resolution down to 2nm. This would enable the study of phenomena associated with the grain size or magnetic domain size in polycrystalline materials, typically used in technological manufacturing.

5.3 **Polymers**

Polymers are ubiquitous. Their applications range from the microscopic (dielectric insulators in microelectronics) to the macroscopic (high performance structural components). Understanding structure property relationships has always been the "holy grail" in polymers. Fundamentally, the behavior of long chain molecules in the bulk or in solution represents a significant challenge. Polymers can exist in a wide variety of phase states: liquids, semi-crystalline solids, glasses and gels. Block copolymers, two polymer chains covalently linked at one end, form well-ordered morphologies on the tens of nanometer scale that are model systems for investigating the fundamental chemistry and physics of phase transitions. Polymer chains pervade tens of nanometers in space which has made x-ray scattering methods an invaluable tool for their study. Due to their large size, polymers inherently move slowly and the trapping of nonequilibrium states is common.

The high flux, brilliance and resolution of synchrotron x-ray sources has afforded a unique tool for the investigation of polymers in solution, in the bulk and at surfaces. High flux and brilliance permit more rapid experiments on the static structure of polymers and allow the investigation of specimens with limited volume. Synchrotron sources have, also, permitted the measurement of the real time response of polymers to an imposed field, e.g. heating, cooling and stretching, and the simultaneous use of two different methods, e.g. small angle x-ray scattering with wide angle diffraction or differential scanning calorimetry. Many nonequilibrium phenomena underpin the morphology and, consequently, the properties of polymers. Thus, both the real time and simultaneous measurement capabilities of these sources represent distinct advantages in the characterization of polymers. The high brilliance and resolution have made the characterization of polymer surfaces possible using grazing incidence scattering and reflectivity methods.

The use of synchrotron radiation for the study of polymers began in the early 1980's with several research groups. At CHESS, time resolved scattering studies were being pursued to investigate crack propagation in glassy polymers and, in fact, studies on single cracks were possible. At SSRL, the kinetics of phase separation in polymer mixtures were being investigated using time resolved small angle x-ray scattering following a rapid thermal quench into the spinodal envelope. Anomalous small angle scattering experiments were being employed to characterize the ion aggregation in polymers. In Europe, scientists at LUBE were just beginning the investigation of the solution properties of ion containing polymers. These initial efforts and others were discussed at the first workshop on synchrotron radiation applications in polymers in 1984. Since that time there has been a tremendous increase in the use of synchrotron radiation for the investigations of polymers. In addition, the sophistication of the experiments has also increased.

The simultaneous measurement of thermal or mechanical properties of a polymer along with the small angle x-ray scattering represented the first serious efforts to combined two distinctly different experiments. Experiments performed at SSRL in the mid- 1980's demonstrated the viability of such measurements and paved the way for other studies. In particular, these studies uncovered the origin of multiple endotherms observed in polyurethane elastomers during heating. At CHESS and at SSRL crazing studies and tensile deformation studies were coupled with small angle scattering. Both efforts were geared to coupling the macroscopic mechanical properties of a polymer to its microscopic structure and morphology. Subsequently, small angle x-ray scattering was measured simultaneously with wide angle diffraction by scientists at NSLS and at DESY in Hamburg which permitted the characterization of polymer structure from the tenth to hundreds of nanometer size scale. More recently, at SSRL, x-ray scattering studies were performed simultaneously with compression in a surface forces apparatus thereby coupling the mechanical and structural properties of fluids confined between two solid walls. Dramatic effects of reduced dimensionality, deformation and fluid surface interactions on liquid crystals have been observed. These studies have been extended to polymers and complex fluids.

Despite the significant progress over the past decade in using synchrotron sources to study polymers and the enormous potential that these sources offer for in situ structural characterization of polymers, the number of users in 1997 at each United States facility totals only in the tens. Consequently, the current first and second generation sources are being underutilized by polymer scientists. Several reasons underlie this. First, synchrotron sources are viewed as a characterization tool and are not the mainstay of research for the typical polymer scientist. Therefore, if facilities are not set-up in a truly user friendly mode, many polymer scientists will use other techniques or operate without the information rather then investing a large amount of time in technique development. This is particularly true for scientists in industrial laboratories. With the exception of companies with large research efforts, industrial scientists simply do not have the time, the funds or the management commitment to be dedicated to one technique. Multi-purpose beamlines often discourage general users from the polymer community. Small angle scattering or wide angle diffraction are the dominant techniques used. If the beamline must be reconfigured to doing such experiments, the driving force to use the facility markedly decreases. While there are facilities dedicated to small or wide angle scattering at different light sources, it is either difficult, or it is perceived to be difficult, to get beamtime on such facilities. It is for this reason that a private research team effort was formed at NSLS establishing the first beamline dedicated to scattering research in polymers. This beamline was commissioned in 1997.

One overriding aspect of the arguments given above is that for many polymer problems, unique and very important information can be obtained from the second generation sources. The polymer activities at these facilities are still largely in their infancy and will grow significantly over the next decade. In addition to scattering, second generation sources offer capabilities that have been used only marginally, i.e. by the experts in the field. Very few polymer scientists have used grazing incidence x-ray scattering, a technique that provides information on the surface structure of materials. Even though the information provided is important for understanding the interdiffusion, healing or adhesion of polymers, the use of grazing incidence scattering is marginal. The same holds true for near edge x-ray absorption fine structure. Again, here is a technique that provides unparalleled information on the chemical composition or bond angle orientation at the surface, both of which are essential for understanding the surface properties of polymers but this technique is used by only a very few polymer scientists.

Does this mean that third generation sources are of no use in polymer science? Emphatically no. The x-ray microscopy methods originally developed at the NSLS are currently also available and under development at the ALS. These methods are ideal for addressing numerous fundamental and applied problems in polymers. X-ray microscopy measures chemical differences in multicomponent polymer systems with submicron resolution and, capitalizing on the polarized nature of the synchrotron beam, can be used to measure dichroism which is related to chain orientation. For any polymer that has been processed by injection molding or extrusion, fibers that have been spun, or polymers that have been compression molded, x-ray microscopy comes to the fore as an ideal tool for characterization.

The most dramatically new prospect, but also rather speculative at the present time, is the development of x-ray photon correlation spectroscopy (XPCS) technique at the APS. It holds the possibility of providing unique, spatially-resolved dynamic information on the 5-50 nm scale out to long time. This window of momentum-time is not accessible by dynamic light scattering, inelastic neutron scattering or neutron spin echo spectroscopy. XPCS may be particularly important for systems since the length scales of interest are often in the 5-50 nm range.

Moreover, for high molecular weight polymer solutions, melts, blends, and self-assembling block copolymers, XPCS may provide previously-inaccessible dynamical correlations on length scales shorter than the size of individual macromoelcules. Such “internal dynamics” information is critical to understanding “entanglement” phenomena which are so pervasive in polymer science. The internal dynamics of clusters and aggregates in associating polymers and complex fluids may also be probed for the first time, and correlated with macroscopic structural, thermodynamic, and theological properties. Glassy polymers are ubiqutous. XPCS may provide a powerful and critical tool for probing the fundamental nature of the glass transition, in particular the question of intermediate range order. Several recent indirect experiments, and also computer simulations and novel theories, have suggested a type of inhomogeneous domain dynamics exists in fragile supercooled liquids with a characteristic length of 2-5 nm. Direct experimental probes of slow correlated motions on this length scale have not been available before.

XPCS requires the high brilliance and coherence of the APS, which raises several potential problems. In dense one-component polymer melts, the lack of signal intensity(contrast) may be a problem. Of most critical and generic concern is the issue of radiation damage. Simply put, will the polymer sample survive the intense x-ray radiation for the time needed to probe the long time dynamical phenomena of interest? At present, benchmark experiments on dense polymer phases are lacking, so the answer to this question is open.

5.4 Atomic, Optical, Molecular Physics & Chemistry (AMOC)

This section describes the scientific impact of synchrotron radiation on Atomic Physics, Molecular Physics, Optical Physics, and Chemistry (AMOC). Excluded from this section are subfields within these areas that are covered elsewhere in this report such as surfaces, materials, polymers, biological chemistry and structural biology, environmental chemistry, microscopy, and x-ray optics.

Synchrotrons have been less important to subfields of AMOC considered in this section than to other areas of science. Important major advances such as traps, coherent atom beams, Bose-Einstein condensation, behavior of matter in intense optical fields, and coherent control of chemical reactions have made little or no use of synchrotron radiation. It should be clearly understood that this is a criticism of neither AMOC nor the synchrotron facilities. There is no reason that a single technique should solve all the problems of science, nor is there a reason why all fields should make equal use of a given technique.

Synchrotron radiation has been used to study fundamental interactions of x-rays with atoms, particularly many body effects such as 2-electron excitation in krypton, elastic and inelastic scattering, interference between dipole and quadrupole allowed transitions, and the double ionization of helium. These involve high precision experiments where the intensity provided by synchrotrons greatly enhanced sensitivity of the experiment.

Infrared synchrotron radiation has been used in a variety of AMOC experiments. Included in these are vibration/rotation spectroscopy, work on solid and high pressure hydrogen, and infrared microspectroscopy. The infrared program at the NSLS seems to have been successful in developing an appreciable clientele, and this is not surprising considering the extensive use made by chemists of infrared radiation. Since laboratory sources of intense infrared radiation are inadequate, particularly at longer wavelengths, there is a need for infrared synchrotron radiation. Many of the most important infrared measurements on molecular dynamics have been made on high frequency (e.g. hydrogen stretching) modes, not because these are the vibrational modes of choice but because these were the only modes that could be excited by existing high intensity laboratory sources. Interactions of a molecule with its environment such as a solvent involve lower frequency vibrational modes, and studies of such interactions could be an important use of infrared synchrotron radiation.

One of the most interesting uses of synchrotron radiation in the area of AMOC is in the study of chemical dynamics. Two sophisticated end stations have been constructed at the ALS, one being a high-resolution multipurpose photoionization-photoelectron apparatus and one being a molecular beam/photodissocation apparatus. These have been or will be used for reactive molecular beam scattering, photochemistry, photoionization of rare gasses, photoelectron spectroscopy, and the imaging of reaction products. Laboratory apparatus of this kind has been of major importance in advances in our understanding of chemical dynamics. Most of the laboratory instruments use ionization, either by electron bombardment or multiphoton photoionization. High resolution single photon ionization would be preferable to these methods, but this has not been possible due to the lack of intensity from high-resolution laboratory sources. The use of synchrotron radiation makes one-photon ionization possible.

The two sophisticated end stations were designed to be multipurpose instruments for the use of the general scientific community. However, because of the complexity and variability of the experiments and the associated apparatus, there is some question as to how useful they will be for the general user. Thus far they have been used most successfully by the local groups responsible for their design, and it is likely that all experiments on these instruments will require heavy involvement of the local groups.

5.5 Molecular Environmental Science

The interdisciplinary field referred to as *molecular environmental science (MES)* has developed over the past decade in response to the need for molecular-scale information (molecular structure, composition, oxidation state, reaction mechanisms) on the chemical and biological processes that control the fate and transport of environmental contaminants. One of the most fundamental properties required for understanding the stability, toxicity, mobility, and bioavailability of an environmental contaminant is its speciation, or chemical form. For example, hexavalent uranium, U(VI), in contaminated soils is usually easily removed by washing the soil with a carbonate solution, but when uranium is present as a U(VI)-phosphate phase or as U(IV), it is insoluble and not removed by this process. Hexavalent chromium, Cr(VI), in soils and groundwater is highly soluble, mobile, and toxic, whereas Cr(III) is relatively insoluble, immobile, and has low toxicity to organisms. Thus, knowledge of the chemical form(s) of a contaminant can result in major cost savings in remediation efforts. Moreover, these and other heavy-metal contaminants (e.g., arsenic, mercury, lead) can pose dramatically different health hazards to humans and animals, depending upon the relative bioavailabilities of different contaminant species.

Although there are many probes that provide compositional and structural information on concentrated bulk materials and solutions or model systems, synchrotron x-ray methods, particularly x-ray absorption fine structure (XAFS) spectroscopy and micro-XAFS spectroscopy, have become indispensable for providing information on contaminant speciation and the processes that transform species as they react with soil particles, natural organic compounds, microbial organisms, and plants. This is true because the extremely high fluxes of modern synchrotron sources are required to detect the dilute levels (< 100 ppm) of metal-ion contaminants often present in environmental samples. XAFS spectroscopy has become a method of choice for speciation studies because it is sensitive to the chemical form of most elements in the periodic table, and XAFS measurements can be made on environmental samples without sample-altering preparation procedures such as drying, which may change the chemical form of a contaminant. Micro-XAFS measurements make use of the very high brightness of synchrotron radiation sources to provide unique information on chemical speciation of metal-ion contaminants in highly heterogeneous natural materials such as soils at relevant spatial resolution (mm to µm scales).

Figure 5.5.1 shows a micro-XAFS map of uranium species in a contaminated soil from the Fernald, Ohio, uranium processing plant before and after washing the soil with a carbonate solution designed to remove the uranium. This innovative study, which was carried out at the NSLS, showed that an insoluble U(VI)-phosphate phase and a U(IV) species remained after carbonate washing, which necessitated the use of different remediation methods. XAFS spectroscopy studies have been performed at SSRL on radioactive waste samples from the DOE-Hanford, Washington tank farm, which is the largest temporary storage site for high-level nuclear waste in the U.S.. These ground-breaking studies yielded some of the first detailed information on the chemical forms of radioactive strontium, uranium, neptunium, and plutonium in the tank wastes and showed that different species of the same element are present in individual tanks as well as in different tanks. This information is essential for developing cost-effective strategies for chemical separation of mixed wastes, which is required to reduce the volume of high-level nuclear waste prior to encapsulation in a waste form designed to isolate the waste from the biosphere for thousands of years.

Turning to more fundamental synchrotron x-ray studies of environmental processes, XAFS spectroscopy has provided unique insights into the reactions and transformations of common environmental contaminants such as chromium, cobalt, arsenic, selenium, lead, and uranium at mineral-water interfaces. In XAFS studies pioneered at SSRL, the molecular-scale details of these chemisorption reactions were unraveled in samples under the same conditions as in nature. Such reactions between aqueous metal ions and the surfaces of soil particles are often responsible for immobilizing or retarding the dispersal of important contaminants, and commonly represent the only protective “barrier” between a contaminated site and the rest of the biosphere. Soft x-ray spectromicroscopy at the ALS has recently been used to reveal changes in macromolecular conformations of humic substances (natural, high molecular weight organic compounds) in electrolyte solutions as a function of pH under ambient conditions. These substances, which are very common in natural waters and soils, play important roles in the chemisorption and transformation of metal-ion contaminants in the biosphere.

One of the most exciting aspects of MES research is the diversity of disciplines it has attracted, including agronomy, chemistry, environmental engineering, forestry, geochemistry, microbiology, plant ecology and botany, soil science, surface science, and synchrotron science. This breadth of expertise is required in addressing both applied and fundamental environmental issues because of the complexity and diversity of environmental processes. Synchrotron radiation sources have served as the focal point for this emerging research field due to the unique information provided by synchrotron-based methods. In fact, recent surveys of user demand at the four DOE synchrotron light sources have shown that MES is one of the two fastest growing fields at these sources, the other being structural molecular biology. MES user demand has doubled at the ALS, NSLS, and SSRL over the past 1.5 years, and MES research is a major focus of at least four APS sectors. We estimate that over two hundred scientists from various disciplines are currently involved in MES research at U.S. synchrotron light sources.

Among the most important recent accomplishments in MES made possible by synchrotron radiation methods are the following: (1) XAFS spectroscopy has provided the first direct speciation information on many environmental contaminants at dilute concentrations in heterogeneous natural materials. These studies provide a scientific basis for site risk assessment and improved remediation technologies; (2) XAFS studies have revealed that multiple species of the same element are often present under conditions where only one form would be expected to predominate, and that surface-bound contaminant species often comprise a major fraction of those present in environmental samples; (3) Micro-XAFS studies of heterogeneous environmental samples have provided the first detailed information on the spatial distribution (at 10-20 μm resolution) of different species of a given element; (4) Micro-XAFS studies of contaminant speciation in certain hyperaccumulating plants have revealed that transformations of highly toxic chromate and selenate ions occur in the cytoplasm and nuclei, respectively, of these plants. These types of studies are providing some of the first molecular-scale information on phytoremediation processes; (5) Micro-XAFS studies of lesions on diseased rice plants and wheat have shown that oxidation of Mn by fungi has occurred. Such plant diseases are responsible for billions of dollars in crop losses each year; (6) Photoemission studies of model metal oxide surfaces and adsorbate interactions on these surfaces have led to a deeper understanding of the reactions of water and aqueous metal ions with oxide surfaces, which are among the most important reactions in natural systems; and (7) Soft x-ray spectromicroscopy studies have revealed changes in Mn speciation on Mn-oxide surfaces caused by Mn-reducing bacteria. This finding has important implications for changes in the oxidation-reduction capacity of natural Mn-oxides, which are among the most important solid sorbents of environmental contaminants. Without modem synchrotron radiation sources, these types of studies would not be possible.

Future directions of MES research include: (1) XAFS studies of the speciation of contaminant ions at even lower concentrations than in the past, including more routine studies of radioactive and highly toxic samples; (2) surface-sensitive XAFS studies of contaminant ions reacting with defect sites on single-crystal metal oxide surfaces (such studies are essential for understanding the reactivity of surface defects, which control most chemisorption reactions at low sorbate concentrations); (3) x-ray standing wave studies of adsorbates on metal oxide surfaces and of the structure of the electrical double layer at solid-aqueous solution interfaces; (4) micro-XAFS studies of contaminant species distributions in heterogeneous samples at higher spatial resolution;

(5) micro-XAFS studies of the molecular-scale processes involved in phytoremediation and in microbially mediated contaminant transformations; (6) soft x-ray spectromicroscopy studies of reactive sites on environmental organic compounds, including humic and fulvic substances; and (7) photoemission studies of the changes in electronic structure of metal oxide surfaces after they react with water and aqueous contaminant ions.

Accomplishing these goals requires access to (1) higher flux insertion-device beamlines (XAFS studies of dilute samples are flux limited), (2) higher brightness sources (micro-XAFS mapping of contaminant species in heterogeneous inorganic samples, plants, and organisms is often brightness limited), (3) higher through-put and higher resolution x-ray detectors (to handle the higher fluxes and the high background scattering and x-ray fluorescence from typical environmental samples), (4) soft x-ray spectromicroscopy beamlines optimized for environmental samples (particularly wet samples), (5) special experimental enclosures on synchrotron beamlines optimized for environmental samples (to provide a safe environment in which to carry out studies of radioactive and toxic samples), and (6) technical support for MES synchrotron users (this was identified as one of the major needs of MES beamline facilities given the diversity of backgrounds of MES investigators). A new high-flux beamline and environmental enclosure at SSRL will provide a much-needed facility for safe XAFS and micro-XAFS studies of dilute radioactive and toxic samples, whereas new high-brightness beamlines at the APS will provide unparalleled facilities for high spatial resolution micro-XAFS studies. New infrared beamlines at the NSLS will provide the brightest sources of IR light available for IR spectromicroscopy studies of organic contaminants and metal-ion adsorbates in environmental samples. A 1997 workshop on soft x-ray synchrotron sources and molecular environmental science concluded that the construction of a new soft x-ray spectromicroscopy beamline at the ALS is needed to meet the increasing demand for this type of experimental facility by MES users.

Synchrotron radiation studies have provided much of what is known about the chemical forms of metal-ion contaminants in environmental samples, particularly radioactive elements at contaminated DOE and DOD sites. In addition, such studies have revealed a great deal about the chemical and biological processes that result in the transformation of contaminant species to less (or more) toxic forms. Such information is essential for improving existing or developing new remediation methods, including those that utilize plants and microbial organisms. Considerable progress in both fundamental and applied MES research is expected during the next decade as a result of new higher flux beamlines at second-generation synchrotron sources, higher brightness beamlines at third-generation sources, and special experimental enclosures and more advanced detectors at both types of sources.

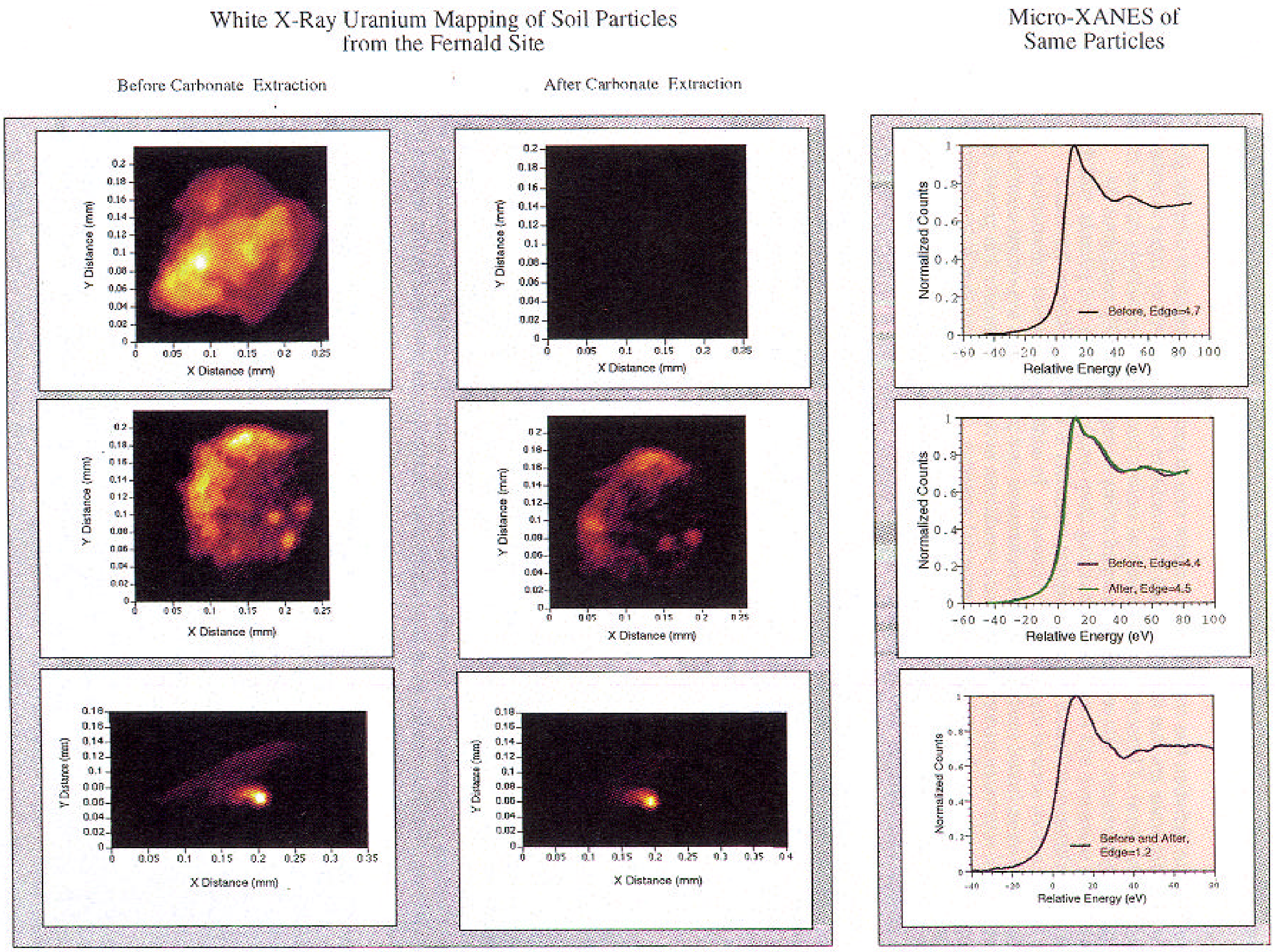


Figure 5.5.1 Uranium oxidation state maps of contaminated soil particles from the Fernald, Ohio uranium processing plant before and after washing with a carbonate solution. These maps were produced by micro-XANES spectroscopy on beamline X-26A at the NSLS. Micro-XANES spectra of 0.1 x 0.1 mm spots are shown and indicate that both U(VI) and U(IV) species are present in different parts of the sample. The upper panels show that U(VI) is removed by carbonate washing, where the lower two panels show that uranium is not completely removed when present as a U(VI)-phosphate phase (middle) or as a U(IV) species (lower).

5.6 Geosciences

Synchrotron radiation has come to play a major role in geosciences research over the past decade, and all indications are that its importance will continue to grow for many years to come. In part, this reflects the trend of laboratory and theoretical studies becoming increasingly central to the Earth and planetary sciences. The recently developed ability to experimentally reproduce the conditions of high pressures and temperatures existing deep inside the Earth and planets, and the application of synchrotron radiation to characterizing materials at these conditions, has had a significant impact across several disciplines, for example. In addition, the novel information provided by synchrotron-based methods on the mechanisms and products of important chemical reactions at mineral interfaces under Earth-surface conditions have led to considerable growth in research that impacts the geological and environmental sciences. Thus, although still comprising a relatively small fraction (< 20%) of synchrotron-based studies, the geosciences have grown to become an important and highly visible component of the research being pursued at synchrotron sources in Europe and Japan as well as in the U. S.

Four areas of research illustrate the application of synchrotron radiation to the geosciences: i) studies of mineral interfaces, especially in contact or after reaction with aqueous fluids; ii) in-situ determinations of the compositional variations and coordination chemistry of metal ions in fluid inclusions in minerals at temperatures and pressures of the Earths crust; iii) characterization of amorphous geological materials and their analogs; and iv) studies of mineral phases and phase transitions under conditions of very high pressures and temperatures. Some of the most important advances in these domains, and others in the geosciences, have only been possible due to the availability of synchrotron radiation.

The understanding of mineral interfaces and the chemical reactions that occur at these surfaces has been truly revolutionized by the use of synchrotron radiation. Of particular significance to geochemistry and environmental sciences is the ability to document the atomic-scale structure, ion speciation and transformations of species at mineral interfaces immersed in an aqueous fluid. This has now become a reality through the application of x-ray absorption spectroscopy, as no other technique offers the combination of element sensitivity and selectivity in the presence of an aqueous solution, and the spatial resolution required for such studies. Documenting the valence states of metals present in trace concentrations (< 1000 ppm) on mineral surfaces is of critical importance, for example, because valence can determine both the mobility and toxicity of the ions. Further details, as well as additional examples, are provided in the section on Molecular Environmental Science.

The use of synchrotron x-rays to probe the composition and coordination chemistry of metal ions in multi-phase fluid inclusions in minerals, in situ, at temperatures up to those needed to homogenize the fluid inclusions (I 600” C), is leading to new insights about the nature of hydrothermal fluids under the conditions at which they occur in the Earth’s crust. Such fluids are responsible for the transport and eventual deposition of many economically important types of metals (e.g., hydrothermal gold and silver deposits, porphyry copper deposits), as well as the transfer of heat from magma-hydrothermal systems to groundwater and overlying rocks. Recent x-ray absorption studies of actual fluid inclusions in natural quartz crystals from such deposits, and of simulated fluid inclusions at temperatures up to 600” C and pressures up to several hundred MPa, have made use of the ability to focus intense synchrotron x-ray beams to the small dimensions (< 1 mm) and to the select wavelengths required to probe the compositional variations within the fluid inclusions, and to determine the structural environments of aqueous metal cations like iron and zinc under hydrothermal conditions. Two important discoveries have resulted from these studies. One is the observation that the first-neighbor bond distances and coordination numbers of many aqueous metal cations decrease with increasing temperature, which results in significant changes in metal-ion speciation that are not predicted by conventional solubility measurements or first-principles electronic structure calculations. The other is the observation that ion pairing increases with increasing temperature, which again is not predicted by conventional indirect measurements of solution properties or theory. These types of in-situ measurements are simply not possible using non synchrotron-based methods, and will be markedly enhanced by the high brightness of third-generation hard x-ray sources, including APS, ESRF and SPring-8.

Synchrotron radiation provides one of the only means of documenting the atomic packing and coordinations of amorphous materials, with x-ray diffraction (including anomalous diffraction) and absorption spectroscopy being two of the most useful methods now available. One reason for this is the ability of synchrotron x-rays to penetrate the containers needed to hold a sample at high temperature and/or pressure; another is the ability to tune the wavelength of synchrotron x-rays to values required for certain types of x-ray scattering or absorption experiments. One of the distinct advantages of x-ray absorption spectroscopy and anomalous scattering methods relative to other structure-sensitive probes is their ability to provide pair correlation functions for a selected type of atom in a compositionally complex glass or melt, rather than all pair correlations as is often the case for x-ray or neutron scattering. This attribute has resulted in unique information on the structural role of weakly scattering, network modifying elements (e.g., Na, K, Ca) and "spectroscopically silent" elements (e.g., Ti(IV), Ga, Ge, Zr) in silicate, aluminosilicate, and borosilicate glasses and melts. The study of amorphous materials, both liquid and glassy, is important to geosciences because the geological evolution of planets depends on processes of large-scale fluid motion. Geochemical differentiation, the separation of planets into global regions of distinct composition, such as an atmosphere, rocky or icy mantle, and metallic core, is due to fluid migration, for example. Also, much of the Earth's internal heat is lost by volcanic eruptions, caused by magmas (high-temperature silicate melts) being buoyant and hence rising toward the surface; the same is thought to be true for other geologically active planets, such as 10 and Venus.

Because melts are usually far more compressible than the coexisting crystals, however, magmas at great depth are relatively dense and do not necessarily rise toward the surface. Indeed, changes in the structures of amorphous silicates at high pressures -- similar to the pressure-induced coordination changes found in crystals -- have been documented by synchrotron x-ray diffraction and provide new insights into the means by which silicate melts (magmas) become compressed at great depth. Given the differences in composition between melt and crystals for the multicomponent systems typically representing rocks, the melts can sink rather than rise; the long-term geological consequences of such "anti-volcanoes" deep within the Earth are currently being explored, and are thought to have played an important role in the early geological evolution of our planet.

Other studies have focused on the use of x-ray absorption spectroscopy (EXAFS and XANES) to characterize the coordination sites for specific ions within oxide melts and glasses. The speciation of these ions is of considerable importance to geochemists because the relative abundances of elements present in trace concentrations in naturally occurring magmas is used to reconstruct the processes by which rocks melt and release magmas at depth. Such studies have diverse applications, ranging from documenting the evolution of continental crust over billion-year timescales to the highly practical determination of how certain types of ore bodies have been formed (hence, how the resources might best be extracted). A related and important contribution of synchrotron-based studies, and one that is likely to increase in importance over the coming years, is the information that is being provided about the coordination environment of high-level radioactive waste elements (e.g., ^{90}Sr, ^{99}Tc, ^{238}U, ^{239}Pu)in amorphous or poorly crystalline waste forms (e.g., borosilicate glasses, cements, or radiation-damaged crystals such as zircons). Knowledge of changes in the local coordination environment of these elements in waste forms, as a function of time or after reaction between the waste form and groundwater, is essential for predicting the stability of the waste form in an underground storage repository, where it is likely that long-term exposure to energetic radioactive decay processes and groundwater will alter the waste form, potentially resulting in the release of these elements into the biosphere, X-ray absorption spectroscopy is particularly well suited to these types of studies.

The best means available for studying materials at the high pressures and temperatures of the Earths deep interior have traditionally required dynamic (shock-wave) techniques in which a sample is compressed for a short time period (< μs). With the advent of high-brilliance synchrotron x-ray sources, it has become possible to trade off sample dimensions in order to examine materials under sustained conditions that allow a close approach to thermodynamic equilibrium. Thus, laser-heated diamond cells can now be used to study ~μg quantities of sample materials at pressures (-100-500 GPa) and temperatures (to -6000 K) exceeding those at the center of the Earth. At the same time, multi-anvil ("large-volume") presses can be used to examine much larger samples (-mg) to pressure-temperature conditions of 20-30 GPa and about 3000 K; larger samples typically yield enhanced quality of data.

High-precision measurements of the unit-cell volumes of materials as a function of pressure and temperature have provided the first reliable determinations of thermal expansion coefficients at deep-Earth conditions of up to -30 GPa and 2000 K. These measurements have only been possible because of the availability of synchrotron sources for x-ray diffraction, applied to both diamond-cell and multi-anvil experiments, and the data are significant because it is the variation of density with temperature (thermal expansion) that provides the buoyancy forces which drive solid-state convection of the Earth's mantle over geological time periods. That is, the forces governing large-scale geological processes of the planet, including the movement of tectonic plates, and the associated earthquakes, volcanic eruptions and ore deposition, are being quantified through such work.

Recent experiments are revealing new ways of determining the shear stresses present in samples under pressure, thus offering reliable values for elastic moduli and yield strengths at very high pressures (10^{10}-10^{11} Pa range). The measurements depend on being able to quantify the angular-orientation dependence of x-ray diffraction patterns of polycrystalline samples loaded under nonhydrostatic stresses. The results are providing some of the first high-pressure (quasi-static) measurements of rheological properties, both for metals and for ceramics (e.g., oxide minerals). The importance for geosciences is that these properties, including yield strength and resistance to creep deformation, are what limit the rate at which the planet loses heat and therefore evolves geologically.

Needless to say, the determination of thermomechanical properties, such as equations of state, thermal expansivity and yielding strengths at high pressures and temperatures, is of considerable importance to materials science and applied physics as well as to the Earth and planetary sciences. In this regard, the $\sim 10^{11}$ Pa pressure range that can now be probed using synchrotron radiation is especially significant because the compressional work associated with such pressures is comparable to bonding energies (- eV). Thus, new chemical behavior is expected, and indeed observed at pressures of tens to hundreds of GPa, including insulator-metal transitions, transformations of crystal structures associated with changes in bonding character, and alteration of magnetic and electronic correlations reflected in novel spin states and superconducting properties. Pioneering determinations of 300 K equations of state to pressures exceeding 100 GPa on such planetary (and chemically important) constituents as hydrogen and H_2O are examples of this type of work that has only now become possible through the application of synchrotron x-ray diffraction. Moreover, comparisons of ultrahigh-pressure measurements with the results of first-principles quantum-mechanical calculations of material properties (e.g., stability and equations of state of different crystal structures) has provided significant tests of existing condensed-matter theory, applied both to geological and to nongeological materials.

Infrared Spectroscopy

One of the most spectacular applications of synchrotron-based infrared spectroscopy has been to characterizing hydrogen-bearing materials to pressures in the 100 GPa (10^6 atm.) range. In particular, changes in the vibrational modes, molecular structures and bonding in hydroxides, in H_2O and in hydrogen itself have been tracked as a function of pressure. As it is necessary to use small ($< 100\ \mu m$ diameter) samples in order to achieve ultrahigh pressures, the application of synchrotron radiation becomes essential for infrared absorption and reflectance spectroscopy: the brilliance of conventional sources is far too low, especially when working under diffraction-limited conditions.

Ice, for example, is characterized by an open structure associated with hydrogen bonding in H_2O near ambient conditions of pressure and temperature. At pressures above 60 GPa, however, the densely packed molecules become arrayed in a more symmetric configuration that can best be thought of as an “ionic” rather than a molecular solid. The existence of this symmetric form of H_2O was predicted more than 25 years ago, but it is only through the application of synchrotron radiation that this could finally be confirmed. The results are of broad interest because the nature of the interatomic forces is quantitatively recorded through the vibrational spectra, and can therefore be used to test and improve current theoretical models of the structure and properties of H_2O (e.g., Car-Parinello type first-principles molecular dynamics simulations). The rich details of the transition to the newly discovered high-pressure state, including soft-mode behavior and coupled vibrational modes (Fermi resonances) observed by synchrotron infrared spectroscopy, will further improve the understanding of H_2O. Also, as water ice is an important constituent of the outer planetary moons, its properties are of considerable importance to planetary sciences.

5.7 Structural Biology

In the past decade, the impact of structural biology in all areas of biological science has increased considerably. Commensurate with this growth in importance has been a major expansion in the use of synchrotron radiation. More than one quarter of the users of the four DOE-supported synchrotrons in the United States are currently life scientists (see Table 5.7.1).

Table 5.7.1: Life Science Users at Synchrotron Facilities

Facility	Total Users	Life Sciences
ALS	**300**	**4%**
APS	448”	30%
NSLS	2,261	26%
SSRL	860	31%
Total	**3869**	**26%**

* First year of operation.

Determination of the three-dimensional structure of a protein has become an integral part of information necessary to understand protein function. Even more than that, it has now become a critical factor in elucidating biological pathways and more complex biological processes. Macromolecular crystallography has also emerged as an important player in the drug design process. More groups are performing atomic resolution macromolecular crystallography and more structures than ever are being determined. For example, in 1996 the number of protein structures deposited in the Brookhaven Protein Data Bank was almost three times higher than in 1991.

In parallel with this broad expansion of macromolecular crystallography has been a dramatic increase in use of synchrotron facilities to solve protein structures. In the past several years, it has become routine to use synchrotron sources for x-ray structure determinations. The synchrotron, with its vastly more brilliant, broad wavelength source of x-rays, provides a number of crucial capabilities that are not otherwise available in the laboratory setting:

- The orders of magnitude increase in brilliance of the synchrotron sources permits experiments that usually require hours to days of data collections to be performed in minutes and even seconds. This corresponds to a major increase in throughput for structure determinations.

- The increased brilliance of the source permits data to be collected with very much smaller crystals than in house. This translates into more structures being solved since many proteins will not grow larger crystals. It also means many structures can be solved much sooner because it often takes several years of additional work, including the frequent requirement to re-engineer the protein, to produce larger crystals.

- Almost any crystal that is taken to the synchrotron will yield higher resolution data using this source. The typical improvement is in the 0.2-0.4 A range, but it can be more than that. This means better structures can be obtained with more of the important detail needed to understand the protein function or protein-ligand interactions for drug design.

- The synchrotron, with its highly intense extremely well focused beams, provides the best source for the very large unit cell structures that are currently under study. These are typically the leading edge work being performed on protein aggregates, such as viral particles, and multiprotein assemblies, such as the proteosome or ribosome. These studies cannot be performed on standard laboratory sources.

- The broad wavelength of the synchrotron source has made possible one of the most exciting developments in the solution of new protein structures in recent times. Multiple wavelength anomalous dispersion (MAD) methods for solving protein structures has revolutionized protein structure solution, accelerated the process dramatically, and has come the closest to making it a routine exercise. The need to collect full datasets at multiple wavelengths means this work can only be performed at a synchrotron.

- The highly intense source means that full datasets may be collected in seconds and in fractions of a second. This opens the exciting possibility of performing time resolved experiments where we can follow the complete three-dimensional structure of a protein during the course of its chemical or biological reaction. These are highly sophisticated experiments and they can also only be done at a synchrotron.

These capabilities combine to make access to a synchrotron beamline for macromolecular crystallography essential to almost any structure problem. In the light of vast amount of protein sequence information emerging from the Human Genome Project corresponding to at least 100,000 proteins, the only hope for producing three-dimensional structures for the most interesting of those proteins in a timely fashion is through the use of the synchrotron with its tremendous intensity of x-rays and MAD techniques for structure solution.

The unique properties of synchrotron radiation outlined above are also crucial for the application of crystallographic methods in the industrial environment. Structure-based drug design requires the determination of the structures of many different ligands bound to the macromolecule. These studies can be done with great facility and accuracy at a synchrotron source. Table 5.7.2 shows the current beamlines available for structural biology at the synchrotrons. Note the dramatic increase in the number beamlines available for macromolecular crystallography from 6 in 1990 to 25 in 1997. Another measure of the current importance of synchrotron sources to macromolecular crystallography is that only 16% of new protein structures published in 1990 involved use of the synchrotron. In 1995, this number grew to 40%, and it continues to increase.

Examples of the importance of macromolecular crystallography and synchrotron sources to biology abound. One interesting case occurred in the pursuit of HIV protease inhibitors. Many pharmaceutical companies determined the structure of HIV protease and used this information to aid in the design of novel and effective protease inhibitors. One of these was Norvir®, whose three-dimensional structure on the enzyme is shown in Figure 5.7.1. The critical problem with treating AIDS subjects is the rapid ability of the virus to mutate to become resistant to the drug. Studies of clinical isolates from patients treated with NorvirB indicated that mutation was possible and that the first residue of the protein to mutate was Val 82 with consequent loss of inhibitory effectiveness. The goal therefore was to design a follow-up compound to NorvirB which would have a different pattern of mutations on HIV protease. The critical question in order to design a new compound was which part of NorvirB is actually interacting with Va182 and thereby fostering this mutation. There was no other way to determine the answer to this question except by crystallography. The crystal structure, as seen in Figure 1, showed the answer immediately. Val 82 is interacting with a isopropyl group on NorvirB and this is the group that must be removed to avoid this mutation. The chemists were indeed successful in preparing molecules with this group removed and a follow-up compound, ABT-378, that has a very different mutation profile from NorvirB (see Figure 5.7.2), is currently in clinical trials.

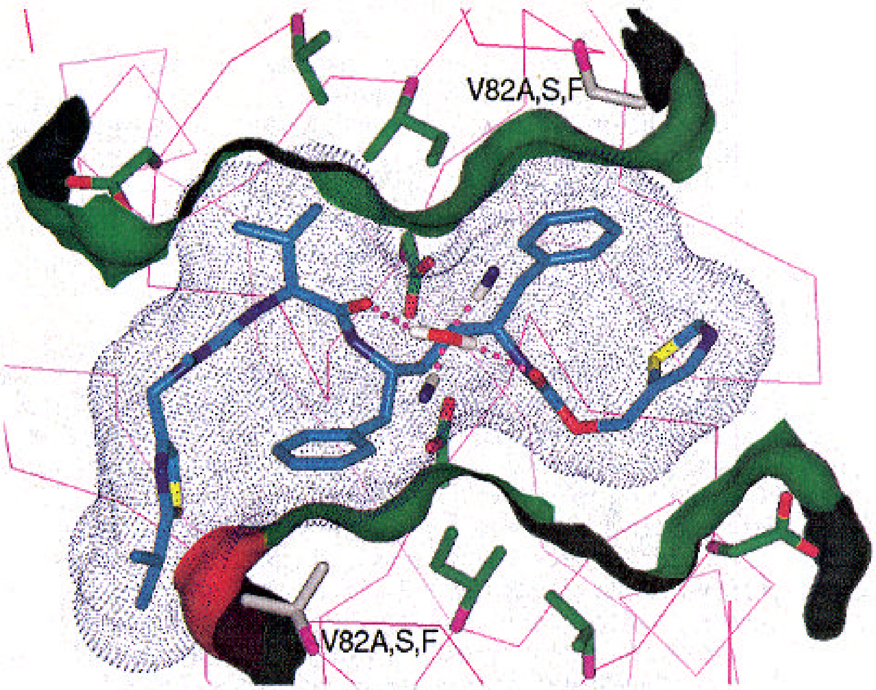
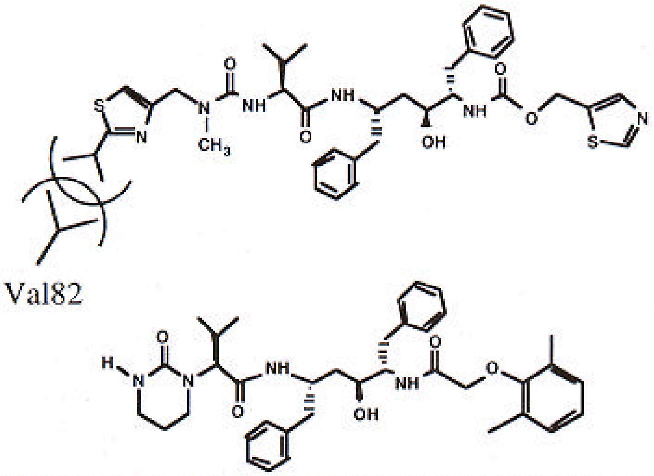


Fig. 5.7.1: Structure of the HIV protease inhibitor Norvir® (shown in blue) in the active site of HIV protease (shown in green). The side chain of Val 82 is shown in gray and is labeled. The protein mutates to either an alanine, a serine, or a phenylalanine at this site. The surface of the enzyme active and binding sites is shown by a green surface. That part of the surface which represents the interaction site between the Norvir® and the Val 82 is shown by a red surface.



Norvir

ABT-378

Fig. 5.7.2: Structure of Norvir® and of the follow-up compound that is currently in clinical trials, ABT-378. Note that this new compound does not have any group that approaches Val 82.

A beautiful example of the impact of structural biology and synchrotron radiation on the understanding of biological systems comes from immunology. The major histocompatibility complex (MHC) encodes a set of proteins vital to the immune system. In humans, these proteins are called HLA (human leukocyte antigen), and they are found on the surface of most cells in the body. Differences in HLA molecules between individuals leads to rejection of transplanted tissue or organs, and susceptibility to certain autoimmune diseases correlates with a person's HLA type. HLA molecules play an important role in immune recognition of virally infected cells. In an infected cell, viral proteins are cut into small fragments called peptides, which bind to HLA proteins on the surface of the cell. If the complex formed between the viral peptide and the HLA molecule is recognized by a receptor on the lymphocyte, the infected cell is destroyed. In order to understand the role of HLA in immune surveillance, autoimmune disease, and graft rejection, the structure of a specific HLA, HLA-A2, was determined by x-ray crystallography. However, the crystals of this protein were only -20 microns in size, and were far too small to use conventional x-ray sources for recording diffraction data. Consequently, synchrotron radiation was absolutely essential for data collection and the ultimately successful structural analysis.

Fig. 5.7.3 Structure of the HLA-A2 major histocompatibility complex protein involved in immune recognition. The binding groove for virally or self-derived peptide antigens is positioned at the top of the molecule between the two a-helices.

Once solved, the HLA-A2 structure revolutionized our understanding of the molecular basis of immune recognition. The most distinctive feature of the HLA-A2 protein structure was a large groove on the top surface of the molecule (above). A variety of evidence suggested that this groove was the binding site for peptides derived from the proteins of pathogenic organisms. Surprisingly, the groove was observed to be occupied in the structure, even though the HLA protein had not been purified from an infected cell. This observation suggested that the peptide binding pocket of the HLA contained a mixture of peptides that had been created during degradation of host cell proteins. Finding these host cell-derived or "self' peptides in the HLA molecule implied that HLA molecules always present peptides to the immune system, even when the peptides are not derived from a pathogen, and that the immune system must have a way to distinguish innocuous "self' peptides from potentially dangerous "foreign" peptides. This in turn suggested what goes wrong during an autoimmune disease: the body mistakenly recognize a "self' peptide for a "foreign" peptide, and destroy healthy cells and tissues. Subsequent biochemical work, together with further structural analyses (requiring synchrotron radiation) has established the rules for which types of peptides are likely to be presented by HLA proteins for immune surveillance.

Non-Crystallographic Methods in Structural Biology

In addition to the impact on crystallographic studies, synchrotron radiation has also had a significant impact on the structural characterization of non-crystalline biological samples. While crystallography is generally the method of choice for high resolution structural characterization of biological samples, there are a variety of cases in which crystallography has not, and in some cases, cannot be used. Among these cases are the many examples of proteins that have not yet produced diffraction quality crystals, despite tremendous effort, and transient reaction intermediates that are difficult to prepare and analyze even when crystals do exist. There are key applications, moreover, such as analysis of the solution structure, precise determination of metal-ligand distances, or direct visualization of individual objects of interest, where crystallographic methods are not applicable, and other methodologies must be employed.

Three of the most important approaches to the analysis of non-crystalline samples, X-ray absorption spectroscopy (XAS), small angle X-ray scattering (SAXS) and X-ray microscopy are based on the interaction of X-rays with matter, and thus share with crystallography a dependence on synchrotron x-ray sources. Specific examples of these techniques and the importance of synchrotron radiation, follow. While these illustrations are drawn from biological systems, it must be noted that these techniques can be quite generally applied to the characterization and analysis of materials, whether of biological origin or not.

X-ray Absorption Spectroscopy

XAS refers to the structured absorption on the high energy side of an X-ray absorption "edge". Analysis of these effects provides element-specific information on the oxidation state of the absorbing species, the local geometry, bond lengths to ± 0.02A, coordination numbers to ± 1, and the chemical identify of the neighboring atoms. Critical applications of XAS in structural biology have been to establish the metal coordination environment in the absence of crystallographic information, as for the copper sites in cytochrome c oxidase responsible for aerobic respiration and in the enzyme peptidylglycine alpha-hydroxylating monooxygenase that is involved in peptide hormone metabolism; characterization of metal-ligand distances in metalloproteins with an accuracy typically an order of magnitude better than can be achieved crystallographically, as in the iron-sulfur containing proteins rubredoxin and nitrogenase; and establishment of the oxidation states of metal ions, as discriminating between Cu(II) and Cu(III) in the galactose oxidase active site. An area of great impact has been in the time-resolved characterization of reactive intermediates that occur transiently during enzyme turnover. Some of the most impressive successes have been obtained for processes critical to biological energy metabolism, including intermediates associated with the mechanisms of cytochrome c oxidase, methane monooxygenase and manganese center of photosystem II that catalyze key reactions in the metabolism (consumption or production) of oxygen.

XAS measurements are absolutely dependent on having an intense, tunable wavelength x-ray source, with high energy resolution, to very accurately characterize the environment of a wide range of elements. Consequently, synchrotron radiation is indispensable for these studies. The development of cutting edge technology, such as the use of polarized XAS to provide angle-resolved bond-length information, could only be achieved with synchrotron radiation

Small-Angle X-ray Scattering

SAXS is the principal solution scattering technique that can provide information on macromolecular size and shape with high temporal resolution. Solution scattering used in conjunction with high resolution structural data can provide invaluable insights into the way individual components interact in the molecular assemblies and complexes, such as the binding of calmodulin to target proteins. SAXS studies are quite versatile and can be applied to the analysis of systems in the size range of 10-1000Å. Recent developments in the use of time-resolved SAXS measurements have been critical for the study of protein folding, where the collapse of the denatured protein during the refolding process to the native structure has been monitored in real-time to provide structural information not accessible by other methods.

In addition to solution studies, the beamlines used for SAXS can be utilized for the analysis of fibers. Fiber diffraction is the primary technique used to structurally characterize the amyloid fibrils formed by aggregating proteins and peptides associated with Alzheimer's and other amyloid diseases. These studies have provided an important and unexpected observation that, despite the diverse nature of proteins forming amyloid fibrils, they all contain polypeptide chains organized in a beta sheet arrangement. SAXS techniques can also be used to collect diffraction data from crystals with very large unit cells, where the highly focused and narrow beam is essential for resolving the diffraction peaks. Complete collection of the very low resolution data from virus crystals allows the determination of a high resolution structure direct from the diffraction data, by utilizing the symmetry of the virus particle and approximate knowledge of the overall shape of the virus.

The high intensity of the synchrotron source is essential for these SAXS studies, by allowing the collection of higher angle scattering data, the use of highly focused x-ray beams, and by improving the signal to noise ratio sufficiently to conduct time resolved studies.

X-ray Microscopy

Recent advances in x-ray optics have resulted in the development of synchrotron X-ray microscopes that can permit the direct visualization of objects with resolutions approaching 30 nm. Through the use of tomographic methods, it is possible to obtain three-dimensional reconstructions of biological systems. The tunable wavelength of synchrotron sources also has the capability of conducting these studies in an element specific fashion, i.e. as in X-ray microprobe experiments. While these developments are detailed elsewhere in this report, x-ray microscopes have had several promising applications to biological systems, including imaging of whole cells, analysis of fungal pathogen - host interactions and monitoring of bone structure during the development of osteoporosis. The high intensity of synchrotron x-ray sources are essential for determination of high resolution structures with good statistics.

Synchrotron Radiation in Structural Biology - Critical Issues

The past decade has seen a great increase in the number of beamlines available for structural biology. What are the critical issues for a proper evaluation of the needs of the structural biology community in the field of synchrotron radiation?

- The major impediment to use of the synchrotron has been timely access to beam time. In the past, the waiting time has typically been 6 months. This is too long for most interesting biological projects. For the drug industry, desirable access time should be measured in days since immediate responsiveness is crucial. The increased number of beamlines at the various facilities (see Table 5.7.2) should permit a better access time in the near future.

- The requirement of performing experiments on biological specimens that are labile and with crystals that are very delicate dictates that experiments will most successfully be performed at a facility which is easily reached and close to the home site of the experimenter. The large number of graduate students and postdoctoral fellows that train at these facilities also makes regional facilities of considerable importance to the user community.

- For several reasons, it is expected that structural biology use of the synchrotron will continue to increase dramatically for the next decade:
  -> Use of the user beamlines for structural biology has become more facile over the past several years as user friendly interfaces have been introduced and more skilled support staff have been provided to run these user beamlines. Accordingly, it is becoming more common for non-crystallographically trained biologists to come to user beamlines with their favorite protein to determine the crystal structure. This pool of biologists is, of course, much larger than the crystallographic community and represents a very large latent pool of users of the structural biology beamlines that are just beginning to appear.
  -> The literal flood of new protein sequences emerging from the Human Genome Project will provide a large number of protein targets whose structure will need to be determined to properly understand their function. Synchrotron radiation is the only crystallographic technology that gives hope of providing atomic resolution structures quickly. The very highly intense x-rays sources, the power of MAD phasing, and the promise of exceedingly rapid data collection times using Laue strategies means that macromolecular structures may soon be determined in less than a day rather than the months to years it has taken in the past.
  -> Rapid and frequent access to beamlines also means that there will be dramatic increase in the use of these facilities by the industrial community and especially the pharmaceutical industry.

  All told, the evidence indicates a continued large expansion in the structural biology use of the synchrotron sources for the foreseeable future.

- There is a continued need for research into improved methodology for synchrotron use. The most important is probably detector development. For many applications, the rate limiting step is detector sensitivity and read out time. In some cases, the beam has to be attenuated because of limitations of the detectors. This is a critical area for continued research to permit maximum advantage to be taken of the third generation sources. This is discussed further in Section 6.3.

The past decade has been an exciting one for structural biology at the synchrotron. Structural biology use of the synchrotron has matured from an esoteric exercise to a relatively routine one. It has become a scientific stage where the excitement emerges from the novel biology that is elucidated rather than from the arcane physics of the synchrotron. The next decade promises to be even more rewarding and stimulating. The many synchrotron advances of the past decade will reach fruition in fascinating new biological discoveries and the rational design of novel pharmaceutical agents using synchrotron driven structure-based drug design.

Table 5.7.2: Structural Biology Beamlines as of 1990*

Synchr.	Macromol. Crystallog. (XTAL)	Fixed Wavelen. Crystal (XTAL)	Non-Cryst Diffract (SNM)	X-ray imaging (IMG)	Spectros. (XAS)	Other	Run Schedule (Days/year)	% Struct. Biology
CHESS	None	A1,F1	A1,A3,C2, F1	None	A3,C2	Laue B2	130	60
NSLS	None	X19A	X9,X12B	X1A	X9, X11A, X12C, X19A	U9B	200	60
SSRL	BL1-5AD	BL7-1	BL1-4, BL2-1, BL4-2, BL7-2	None	BL1-5, BL2-3, BL4-1, BL4-2, BL6-2, BL7-3	None	--	25

Structural Biology Beamlines as of 1996†

Synchr.	Macromol. Crystallog. (XTAL)	Fixed Wavelen. Crystal (XTAL)	Non-Cryst Diffract (SNM)	X-ray imaging (IMG)	Spectros. (XAS)	Other	Run Schedule (Days/year)	% Struct. Biology
CHESS	F2	A1,F1	A1,F1,F2	None	None	None	165	30
ALS	5.0.2,5.0.1	None	None	6.1.3	4.0	None	210-230	12
APS	17ID,17BM, 19ID,19BM, 14ID,14BM	5BM	18ID	None	18ID	None	200-250	25
NSLS	X4A,X8C, X12B,X12C, X25,X26C	X4C	X9B,X12B, X27	X1A	X9, X11, X18B, X19A, X10C	LAUE X26C, IR Micro U2B, CD, Fluor. U9B	210	15
SSRL	BL1-5,BL9-1, BL9-2	BL7-1	BL4-2, BL10-2, BL1-4	BL3-4, BL10-2	BL2-3, BL4-3, BL6-2, BL7-3, BL9-3, BL5-2, BL8-2	LAUE BL9-2	220	35

* Taken from 1991 Biosync report.

† Taken from 1997 Biosync draft report.

5.8 Microscopy

Microscopy adds spatial resolution to a broad variety of synchrotron radiation techniques, including absorption spectroscopy, fluorescence analysis, photoemission and scattering. At the same time the elemental, chemical and structural sensitivity of X-ray techniques provide unique capabilities and contrast mechanisms to new forms of microscopy. By definition one is dealing with complex, heterogeneous samples, and this leads to a style of research that requires substantial amounts of beam time. Microscopy benefits particularly from the brightness of the source, especially when spatial resolution is obtained with scanning microprobes.

Soft X-ray microscopy

The energy range between 90 eV and 1 KeV covers the K absorption edges of carbon, nitrogen and oxygen, and the L edges of the elements from silicon to copper, among others. These elements form the bulk of biological and polymer materials, and play a major role in geology, the environment, and in modern technology. With the development of high-resolution optics (zone plates, mirrors, and electron columns) and bright sources, the spatial resolution of microscopes operating in this energy range is now routinely in the 50 nm range at several instruments around the world, with further improvements to the 20 nm level on the way. This corresponds to the highest far-field resolution with photons of any wavelength by far.

Scanning microscopes focus synchrotron radiation to form a microprobe, the size of which determines the spatial resolution. Generally the specimen is raster scanned to collect the image, or, with the specimen held fixed, an absorption spectrum or photoemission spectrum may be collected from the small illuminated area. Scanning transmission microscopes are bulk sensitive, while scanning photoemission microscopes provide information on surface and near-surface structures. Zone plate based scanning microscopes have been developed at the NSLS since 1983, and additional instruments of this type have started operation at the ALS. These operate most efficiently between 250 eV and 800 eV. An additional photoemission microscope based on Schwarzschild mirror focusing has moved from Wisconsin to the ALS. It operates in a restricted energy range below 250 eV. X-ray photoemission spectroscopy with 1 micrometer resolution is being pursued by Intel at the ALS with the capability of homing in on specific defects on large silicon wafers.

Other instruments illuminate the entire object area to be imaged and use the optics to form an enlarged image. Transmission microscopes of this type use zone plates to form the image on a CCD camera. The prime example is XM1, operating at the ALS. Photoelectron emission microscopes (PEEM) use an electron optical column to form the enlarged image. A microscope of this type is also operating at the ALS.

The combination of spatial resolution with XANES spectroscopy has opened new areas of microchemical as well as elemental analysis with important new applications in biology (Sec. 5.7), environmental science (Sec. 5.5), polymer research (Sec 5.3), surface science (Sec 5.2), geochemistry, and various areas of technology (Sec 5.9). It is of particular importance in some of these applications that specimens up to several microns thick may be analyzed wet, and with minimal preparation. In the study of magnetic materials and crystalline polymers the polarization characteristics of the radiation provide additional important information. To overcome limitations due to radiation damage in sensitive samples, an instrument operating at liquid nitrogen temperature has been developed at the NSLS, and another one is under development at the ALS. Such microscopes open the way for three dimensional imaging by nanotomography. Techniques to label important structures within the sample have been demonstrated and are under additional active development.

Soft X-ray holography has also been developed into a high resolution imaging modality, and shows particular promise for three dimensional imaging of relatively thick specimens.

The soft X-ray microscopy community has grown rapidly, especially in the last year or two. While as recently as three years ago there was a single dedicated beamline devoted to this technique at DOE facilities (at the NSLS), today there are eight additional beamlines at various stages of operation, construction or design at the ALS, and one is being commissioned at the APS. With new applications areas opening up and new communities of users getting involved, even more facilities will be needed in the future.

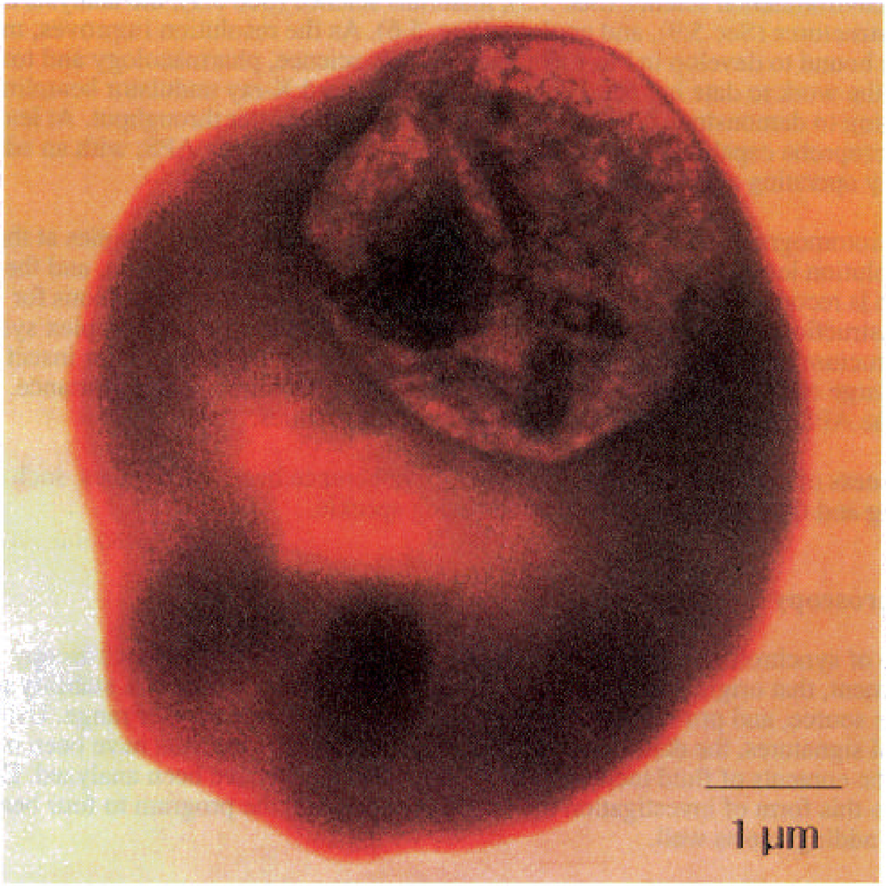


Figure 5.8.1 High resolution image of a malaria parasite in a human red blood cell. The image was taken as part of the ongoing study of malaria, with the soft x-ray microscope XM-1 at the ALS. In this study researchers (i) detected newly elaborated structures in the cytosol of the cells, (ii) measured the mass redistribution in infected cells, (iii) studied the change of parasite morphology due to potential chemotherapeutic agents and in red blood cells with skeletal protein mutation. The findings demonstrate conclusively for the first time that constituents of the red blood cell membrane play a role in parasite development and extend our understanding of the relationship between the host blood cell membrane and the parasite.

Hard X-ray Microscopy

The development of hard X-ray focusing devices (zone plates, Kirkpatrick-Baez mirrors, Bragg-Fresnel optics and capillaries) has led to ever-finer microprobes of hard X-rays. Routine work today involves a resolution of 2 - 3 micrometers, with a few instruments (notably at the SRI CAT at the APS) already capable of 0.5 micrometer or even finer resolution. Microdiffraction is being performed at the ALS with 1 micrometer resolution. Further improvements in resolution to the 0.1 micrometer level can be expected. These microprobes are used in highly sensitive trace element mapping using fluorescence detection, chemical state mapping using XANES contrast, and the study of the microstructural environment using diffraction techniques. There are numerous applications in environmental science (Sec 5.5), materials science (Sec 5.1), the analysis of artificial microstructures (Sec 5.9), and geology (Sec. 5.6). As the resolution improves, more applications are bound to develop in bio-medicine, forensic science, pharmacology and toxicology. While much of the work to date has been done at the NSLS, hard X-ray undulator beamlines at the APS are beginning to demonstrate considerably higher speed and better throughput. At least five CAT s have microprobe capabilities at various states of completion at the APS, with an additional dedicated facility operating at the ALS.

Hard X-ray microtomography provides three-dimensional information about samples at the few micrometer resolution level. The whole sample is illuminated with a parallel beam, and the attenuation-map is recorded on a CCD camera at a complete set of angular orientations for computer reconstruction. This technique is particularly useful for the study of complex systems such as bone structure in osteoporosis (SSRL), the structure of the head of a major insect pest (NSLS), and a large class of porous and composite materials of technological importance. At least five CAT's at the APS are developing microtomographic capabilities.

The high brightness of the sources can be exploited for coherence based techniques, such as phase contrast imaging and time resolved investigations using speckle.

Infrared Microscopy

The use of synchrotron radiation for infrared microscopy and micro-spectroscopy is a recent development, that originated at the NSLS. It makes use of the brightness, stability and tunability of the source, and provides spatial resolution in the 2 - 3 micrometer range. Using infrared spectral signatures, the distribution of different chemical constituents have been mapped in live cells, and the contents of fluid inclusions in geological samples have been analyzed. Due to the broad interest in this form of investigation the NSLS is expanding the program to four beamlines, and the ALS is adding one as well.

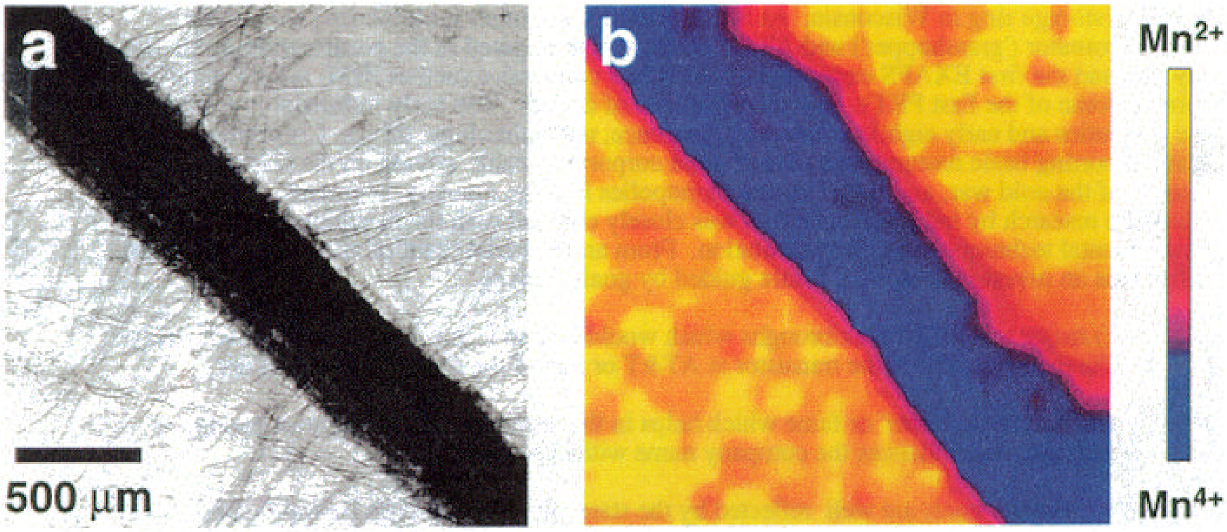


Figure 5.8.2 Take-all disease, one of the world's major wheat diseases, has been studied at NSLS beamline X26. The disease is caused by the soil borne fungus *Gaeumannomyces graminis*. It has been hypothesized that fungal oxidation of soil Mn is an essential step in the infection process. (a) Photograph of an infected wheat root (upper left to lower right) growing in agar amended with 50 mg / 1 Mn^{2+}. Root hairs radiate perpendicularly from the main root. (b) An Mn oxidation state map of the same area obtained using micro-XANES spectroscopy showing that the interior of the root contains physiologically inactive Mn^{4+} due to fungal infection, while the surrounding agar still contains the essential nutrient in the active Mn^{2+} form.

5.9 Technological Impact

This section outlines the historical development in the use of synchrotron radiation for technology (which to a large degree is synonymous with its industrial use), in particular, the significant changes which have occurred since the Eisenberger-Knotek and Seitz-Eastman reports. We discuss specific cases where a technological impact can be directly demonstrated. Finally we discuss the anticipated future development.

Industrial use of synchrotron radiation: from the 70's to the 90's

Industry has had a presence in synchrotron radiation research from the very beginning. In the seventies IBM and AT&T scientists participated in the early photoemission experiments at the Tantalus storage ring in Wisconsin. At SSRL XEROX scientists built the first soft x-ray monochromator ('grasshopper') and AT&T scientists participated in the construction of the first x-ray line and the first EXAFS experiments. At NSLS companies such as IBM, AT&T and EXXON formed some of the first PRT's, investing millions of dollars. The early industrial investments in the seventies and early eighties were mostly science, not technology, driven. Corporate America was supporting basic research in an era of great corporate wealth, relying on the technological hunger of the cold war, and broad virtual monopolies in large industry segments. The pursuit of scientific research by industrial scientists was closely coupled with the development of experimental techniques and instrumentation. From an industrial point of view the synchrotron effort was an investment into the future guided by goals such as

(i) major scientific breakthroughs which would lead to technological shifts or advantages like the discovery of the transistor at AT&T or that of the nylon fiber at DuPont.

(ii) scientific 'luster' or fame which helps in the attraction of the brightest young scientists and enhances the company name with customers.

These early goals are well reflected by the stated goals of the IBM Research Division at that time 'To be famous for science and technology and to provide value to IBM'. Until the time of the Eisenberger-Knotek and Seitz-Eastman reports the question on 'technological impact' was largely synonymous with 'scientific impact'. One of the few exceptions was the x-ray lithography program of IBM at the NSLS which was clearly initiated with a technological mission, as discussed below.

The last decade has witnessed enormous change in the political and economic landscapes. Companies with significant synchrotron research investments have reduced their commitments as financial pressures have mounted and 'science for fame' has become an unaffordable luxury. Economic considerations led to restructuring and changes in mission in some of the major US industrial research laboratories with early involvement in synchrotron radiation research, in particular, AT&T, IBM, EXXON and XEROX. The shift was marked by the desire of a quicker return on investment. This led to a shift in research goals from long-term to short-term, from basic to applied, from science to technology. For example, the goal of IBM's research division became simply to 'provide value to IBM'. In addition, some high-tech companies shifted emphasis from hardware to software and services because of their higher profit margins, leading to a relative de-emphasis of materials science based research and development.

On the other hand, many new companies recognized the potential value of synchrotron radiation for technology and invested in synchrotron facilities. This second generation of companies invested with the goal of technological, not scientific, impact. The NSLS, in particular, covers a wide range of companies including Air Products & Chemicals, Allied Signal, BP, Bechtel, Chevron, Dow, Hoechst, Mobil, Northrop Grumman, Dupont, and UOP in addition to the early users EXXON, Lucent, and IBM. At the APS significant investments have been made by 32 companies ranging from health care and biotechnology companies, mostly grouped together in the Industrial Macromolecular Crystallographic Association (IMCA) CAT, to oil companies, high-tech companies and chemical companies. At the ALS investments have been made by Intel and the biotechnology companies Amgen and Roche. Hewlett-Packard, Genencor, Agouron, Bristol-Myers and Genentech have established research programs at SSRL.

The end of the cold war also played a significant role in increasing the emphasis on technological impact. Here the emphasis shift was from strong national defense to strong national industry. This led to restructuring of research at DOD funded labs, the creation of the technology reinvestigation program (TRP) by ARPA, and the creation of federally supported technology programs such as the advanced technology programs (ATP) and corporate research and development associations (CRADAs). The clearly stated mission of these programs is research for US technological advantage.

It is interesting to point out that while the total number of industrial users has grown from 334 in 1990 to 560 in 1997, the relative percentage of industrial use of the synchrotron facilities has declined from 19% in 1990 to 12% in 1997.

Areas of Technological Impact

Synchrotron radiation has played an important or at least significant role in the following technology areas:

Development of exploratory lithography methods.

Exploratory x-ray lithography experiments performed by IBM at NSLS convinced IBM to build the Helios storage ring which was commissioned in 1991 at its East Fishkill semiconductor manufacturing facility. The ring parameters were optimized for soft x-rays suitable for proximity x-ray lithography. In this technique a mask is brought in close proximity to the wafer and projected with 1: 1 magnification by forming a shadow of the mask onto the wafer. The switch-over from optical projection to x-ray proximity lithography has been postponed by extension of optical lithography through innovative optics and by going to shorter wavelengths. The delay allowed the development of an alternative method at somewhat longer wavelength (about 13nm), pioneered, among others, by AT&T at NSLS. Extreme ultra-violet, EUV, projection lithography uses reflective optics to form a demagnified image of a mask onto a wafer. A 250 million dollar joint program including Intel, Advanced Micro Devices, Motorola, Lawrence Livermore National Laboratory, Sandia National Laboratory, and Lawrence Berkeley National Laboratory was announced to further develop EUV lithography. At present, the source is envisioned to consist of a high power laser plasma rather than a synchrotron radiation source. The LIGA (short for ‘Lithographie-Galvanik-Abformung’) process was developed in Germany for the production of micro components. In this technology x-rays are used to cut a mold, consisting of micron-sized features of large depth, into a suitable material which is then used for repeated casting. A dedicated ring for LIGA has been constructed in Karlsruhe Germany. In the US, the LIGA process is presently used for micromachining at CAMD and NSLS in collaboration with industry.

Analysis, development and optimization of semiconductor processing.

The work in this general area has been quite broad, and only a few representative examples are given here. Researchers at IBM used the UV ring at NSLS for studies of dry etching of silicon wafers, an important technological process. After reactive exposure of the wafer to fluoride containing gases the different fluorine containing reaction products could be identified by their chemical shifts in XPS spectra, and the kinetics of the etching reaction could be established in considerable detail. X-ray diffraction studies at SSRL by scientists at Lucent were instrumental in obtaining a better understanding of the epitaxial growth of compound semiconductors under realistic growth conditions using metal-organic precursors at high pressures. Traditional surface science methods had only succeeded in studying this process at much lower pressures. X-ray diffraction experiments at NSLS by IBM scientists, were used in time-resolved rapid thermal annealing studies of $TiSi_2$ films as used for metallic interconnects on silicon microelectronic devices contributed significantly in establishing processing conditions that result in the lowest possible resistivity of the silicide.

Corrosion analysis in aerospace industry.

Most structural metals are chemically very active and without a passivating or protective layer would soon oxidize or corrode. Corrosion problems are becoming acute in the aerospace industry where frames of structures are lasting longer than their outer skins. EXAFS and XANES studies carried out at SSRL on various aluminum alloys by Boeing researchers have enhanced the understanding of the basic nature of the corrosion processes and their control in the aerospace industry. Because of weight and fatigue life advantages, future aerospace structures will make increased use of components which have been adhesively bonded together. Conventional processes to treat titanium and aluminum surfaces for bonding applications include immersion-based anodizing and conversion coatings. Because these processes use strong acids or bases and toxic materials (such as chromates) an environmentally safe sol-gel process has been empirically developed that produces structural adhesive bonds with equivalent or superior strength. The details of the interactions at the sol gel - surface interface remained unknown. Again, EXAFS and XANES measurements by Boeing scientists have uniquely shown that the sol-gels chemically bond to the Al or Ti surfaces to which they are applied.

Catalysis

At companies like EXXON, in the area of catalyst development, x-ray absorption spectroscopy, XAS (EXAFS and XANES), is used as routinely today as IR, NMR or (in house) x-ray diffraction. These synchrotron radiation techniques therefore have been incorporated into the mainstream of characterization activities. XAS has been extensively used by EXXON scientists, working at SSRL, for the characterization of supported bimetallic catalysts. These catalysts, consisting of platinum and a second metal (Ir, Re, Sn), are widely used in commercial petroleum reforming processes. The addition of the second metal to platinum results in improvements in a wide range of performance characteristics of the catalyst, e.g. enhanced activity and lifetime. XAS has provided valuable insights into the structure of these important commercial systems. One theme emerging from these studies is that the second metal enhances the metal dispersion relative to pure platinum catalysts. In addition, it imparts resistance to agglomeration of the metallic clusters through the formation of interfacial structures between the metal clusters and the support. In other studies XAS has been used to successfully identify the competing chemical structures formed during halogenation of the support, and thus identified those structures associated with the desired acid catalysis reaction. This work was also helpful in optimizing the halogen content of the commercial catalyst. At DuPont hydrogenation catalysts have been studied by powder diffraction under true operating conditions, using thick-walled pressure vessels. In a separate experiment dispersive EXAFS was used to follow the oxidation state changes in a vanadium based catalyst. The experiments clearly demonstrated that V^{+5} was the key component in initiating the reaction.

Synchrotron radiation experiments at NSLS and APS are also playing an important role in the research into new and improved catalysts at the Dow Chemical Company. The vast majority of this work is performed using proprietary beamtime in which Dow pays full cost recovery. Because of the proprietary nature of the work, only general examples can be given here. In the past two years, XANES and EXAFS data have been used to support better key patent positions for

Dow catalysts. NEXAFS studies carried out under a Dow-NIST CRADA agreement on the NSLS UV ring have been used to probe the bonding of reactive molecules on supported materials. Some of the important advances made using synchrotron techniques have been funded in part by a grant through the Advanced Technology Program. The work has provided timely structure and characterization information and is having a significant impact on the catalyst development cycle. Dow expects an increased need for access to synchrotron radiation facilities in the future.

Polymers

Synchrotron radiation has been used by several companies for the characterization of polymers, materials with widespread industrial use. Many of the polymers made by DuPont are crystalline in nature and control of the crystal structure and morphology has significant impact on the performance of the final products. DuPont scientists have used the NSLS to carried out small angle x-ray scattering and wide angle x-ray diffraction to study the crystallization and melting behavior of polymers such as nylon, polyethylene and polyesters. In a related program the structure evolution during polymer processing such as fiber spinning and drawing has been investigated. At EXXON, XAS has successfully identified the chemical environment of organically bound halogen impurities in commercial polymer products. The work provided guidance to process engineers in altering the process to mitigate the effects of these impurities. At IBM, rubbed polyimide films are used for the alignment of nematic liquid crystals (LC) in flat panel displays. Because of the disordered nature of the polymers used in practice, the microscopic origin of the LC alignment by the rubbed polymer surface, has been a mystery since its discovery in 1911. Polarization dependent NEXAFS studies carried out at SSRL by IBM researchers revealed that the LC alignment direction is set by the microscopic alignment of bonds, e.g. phenyl rings, at the polymer surface. This understanding has led to the development of new non-polymeric alignment materials and to the development of non-contact alternatives to the mechanical rubbing method, which are key to the implementation of novel LC display technologies.

Polyurethane flexible foams are highly versatile materials used in great quantities (well over 5 billion pounds) in transportation components (e.g. seating, padding), furnishings (e.g bedding, carpets), and packaging. The stiffness and other physical properties of polyurethane foams are greatly influenced by precipitates whose characterization has been difficult in the past. Dow scientists, in collaboration with various scientists from Universities and the ALS, have studied the chemical nature of precipitates in polyurethane foams, at the submicron level, by means of scanning transmission x-ray microscopy at NSLS and the ALS. The images were also used to visualize different filler particles through spectroscopic contrast and to study the influence of additives on phase segregation processes. This information, which could not be obtained previously, is helping define structure-property relationships useful in improving these materials. The unique capability of x-ray microscopy to image materials at ambient pressure while dry or swollen in water is being used by Dow scientists to examine the distribution of differently cross-linked phases in an otherwise identical polymer matrix. This work is being accomplished through a combination of general user access time (for technique development and project demonstration) and proprietary beamtime. The proprietary experiments are helping refine the manufacturing process and are playing a role enabling new product development.

Biotechnology

The impact is described by the following quote from the 1997 BioSync Report: “Structure-based drug design, which seemed a trendy buzz phrase a few years ago has become a reality. The design of new medically important drugs, such as HIV-protease inhibitors and the influenza neurominidase inhibitors, is a direct consequence of research in structural biology”. Biotechnology is one of the most promising areas for future application of synchrotron radiation. This subject is covered in detail in section 5.7.

Metrology

Sematech has placed the synchrotron radiation techniques total external reflection x-ray fluorescence (TXRF) and micro-XPS on its roadmap of critical metrology technologies. This has resulted in benchmark TXRF experiments at SSRL, in particular in a collaborative CRADA with Hewlett-Packard. At this time the technique continues to be evaluated. In a joint CRADA with Intel and Applied Materials a micro-XPS facility has been constructed at the ALS. The facility is operating at 2 micrometer spatial resolution and analytical work is being performed by Intel.

Materials science in general

As discussed in section 5.1 a large body of work both by academic and industrial users has been directed at improving our understanding of materials in general, often without specific applications in mind. While the impact of this work on technology is hard to measure and quantify, there is little doubt that advances in materials science in general have a profound impact on the competitiveness of US industry. Synchrotron radiation research has played a key role in the development and studies of such diverse materials as high temperature superconductors, polymers, man-made fibers, semiconductor materials, magnetic materials, chemical precursors, and new alloys.

Fire fighting

While the use of synchrotron radiation by industrial users to solve problems ‘at home’ (i.e. in manufacturing plants) is by nature hard to document and quantify, there is enough anecdotal evidence to suggest that this role of synchrotron radiation has been of sufficient importance to the industries involved to assure their future commitment (if sometimes at reduced levels) to synchrotron radiation research. It is important to realize that in this context synchrotron-based techniques are part of a much broader array of sophisticated analytical methods that are at the user’s disposal. Microscopy techniques play a particularly important role. The development of synchrotron based microscopies such as Photo Electron Emission Microscopy, X-ray and soft X-ray microprobes and microdiffraction capabilities is therefore particularly significant.

Transfer of storage ring technology

Synchrotron radiation research in the US has resulted in numerous new technologies related to synchrotron radiation research that have been exported to and/or copied at synchrotron radiation sources in both the US and abroad. The first wigglers were developed and tested at Lawrence Berkeley National Laboratory and SSRL. US-developed electron beam alignment, focusing and steering technologies are the basis of the most advanced sources worldwide. Vacuum technologies developed for APS are used in Europe and Japan. Efforts are underway at the APS to develop an advanced vacuum technology venture company for production of electronic microchip fabrication chamber.

The Future

Compared to the enormous contributions of synchrotron radiation research to fundamental science the impact on technology is significant, but much more modest. To a significant degree this is a reflection of the mostly academic community in which synchrotron radiation research first developed, as discussed above.

Synchrotron radiation is one of the most versatile tools for the study of the electronic and structural properties of matter. At the same time, synchrotron radiation techniques continue to develop and improve, becoming increasingly attractive for applications in industrial research.

Improved brightness allows studies of smaller crystals, smaller features on microelectronic devices. X-ray tomography enables the scientist to obtain 3-dimensional views of new man-made materials and disease-carrying organisms alike. Micro-beams are used to create ever-more-detailed images of the material world, with information on chemical composition, chemicalm state, strain distribution, grain structure, defect structure, and numerous other properties. Using the unique properties of polarized light, magnetic materials can be analyzed and imaged with unprecedented accuracy and detail. The use of x-ray diffraction for drug design, reflected by the formation of IMCA (industrial macromolecular crystallography association, consisting of 12 companies) at the APS appears to be of particular future importance. Next generation problems involve the development of models for smaller molecular weight agonist/antagonists or the answer to questions whether small molecules can inhibit protein-protein binding events. Biotechnology applications such as the design of enzymes to degrade pollutants or to be usable as thermostable industrial catalysts or the design of insecticides with increased efficacy have huge environmental and economic impact.

While synchrotron radiation appears to offer enormous opportunities to US industry, it is the view of many in the industrial community that the synchrotron radiation management does not always engage industry in a manner that is conducive for effective research and utilization of these national resources. While many US industries have learned the dangers of too narrow a view of the virtues of basic science, the synchrotron radiation community has remained strongly entrenched in its academic roots. The achievement of technological impact remains one of the great challenges for synchrotron radiation research in the next century. Strong, deliberate efforts must be made to ease the utilization of the national synchrotron radiation facilities for industrial research, proprietary and non-proprietary.

6.0 MACHINE & INSTRUMENTATION ISSUES

6.1 Machine Issues

All of the four facilities are operating for users at or beyond specifications. The older machines, SSRL and NSLS, have developed through continuous improvement programs, to well beyond the original specifications. They also operate with very high reliability and beam availability for users. It is expected that the newer machines, the APS and ALS, will follow a similar continuous improvement process.

The Advanced Photon Source (APS)

The new facility already operates at design specifications of 100 mA of positrons, beam lifetimes of 10–40 hours, and a horizontal emittance of less than 10 nm-rad. The vertical emittance achieved is 0.24 nm-rad, corresponding to 3% coupling, and is expected to improve further.

The near term goals for the machine are concentrated on reliability and availability. These goals can be stated as, "deliver $>$ 5000 hr./year to users with 95% availability and $>$ 24 hours mean time to beam loss." There are programs underway to improve system performance towards these goals.

Another important machine issue is orbit stability where the goal is to maintain orbit stability in the insertion devices and other source points to better than 5% of the beam size. This has been achieved through continuing development of RF and X-ray beam position monitoring and real time orbit feedback systems. These developments will continue and, as the coupling or vertical beam size is decreased, the requirements on orbit control are tightened.

A major issue is the development of the top up mode of operation. The near term goal is to achieve a beam current stability of 10^{-3} and a longer term goal of 10^{-4}. There are several challenges which will be studied in this development program. Radiation protection on the beam lines and of the insertion devices will demand high injection efficiency and reliability.

In the longer term, the machine is capable of operating with higher currents. The vacuum chamber was designed to handle 300 mA. However, this will require more RF power to sustain the beam and multibunch instabilities will probably require damping of modes in the RF cavities and/or the development of transverse and longitudinal feedback systems. To maintain good, long beam lifetimes at higher currents, some vacuum and aperture improvements will be required; and lower beta functions in the insertion devices are under study.

The National Synchrotron Light Source (NSLS)

The NSLS has both an 800 MeV VUV ring and a 2.5 GeV X-ray ring. The performance of both rings far exceeds the original goals through continuous improvements over the last 10 plus to 15 years.

The VUV ring has been developed as the worlds most intense infrared source. With 1 A of current at 800 MeV and its small bending radius, it is several orders of magnitude more intense in the IR region than any existing or potential competitors. The addition of a fourth harmonic RF system has increased the beam lifetime and the use of orbit feedback systems has made for a very stable source. Future developments on this ring are directed more in the development of more IR beamlines.

The 2.5 GeV X-ray ring has again made significant gains in performance over the years. The operating beam current has steadily increased to 350 mA with near term plans to further increase this to 450 mA along with new RF cavities and more RF power systems. The emittances have been reduced from 110 to 90 nm-rad in the horizontal and from 2 to 0.1 nm-rad in the vertical. This has been achieved with fine tuning of the magnet lattice. With further tuning and corrections of the lattice, it is expected that the horizontal emittance will be halved, 45 nm-rad, by 1999.

The NSLS has been a leader in the development of orbit feedback and stabilization. This work has led to short and long-term orbit stability in the range of a few microns. This type of stability is important in allowing the development of state of the art insertion devices. Recently, an undulator with a gap of only 3 mm was successfully tested with only a small reduction in beam lifetime as was expected. Another recent development is a time varying elliptically polarized wiggler. With this wiggler switching at 100 Hz, the residual orbit distortion has been corrected to a few micron.

Last, but not least, is the continuing efforts to optimize operations, i.e., reliability, stability and injection efficiency.

Stanford Synchrotron Radiation Laboratory (SSRL)

The SPEAR storage ring was designed as an electron-positron collider and, therefore, had a relatively large design emittance. However, it had a large number of straight sections suitable for insertion devices. Some of the first wigglers were installed even when synchrotron radiation usage was parasitic to high energy physics. After SPEAR became dedicated to synchrotron radiation use, the emittance was reduced from 540 to 160 nm-rad. With its own dedicated injector and continuing development, operation became extremely reliable, 95% delivery, with improved beam stability and very long lifetimes. This machine has one scheduled fill per day and 40 hr. beam lifetimes. Orbit control using analog and digital feedback systems is under continuous development, and higher resolution beam position monitors are being installed in the ring. New insertion device beam lines are being added at an approximate rate of one per year.

The plans for improvement of the SPEAR ring over the next decade are primarily focused on a major upgrade of the ring. A proposal for this upgrade, called SPEAR3, is to be submitted for funding in FY99. This upgrade replaces all the magnets and vacuum chambers of the ring but on the same footprint. That is the ID beamlines are unchanged. This new lattice design would bring the emittance down by an order of magnitude to 18 nm-rad, 3rd generation source territory. The new vacuum chamber is designed for 200-500 mA, at 3 GeV, limited initially to 200 mA by the beamlines. Some parts of the older beamlines will be upgraded as part of this upgrade.

The proposed schedule for this upgrade is a three-year project requiring only six months of downtime of the ring when the magnets and vacuum chambers are replaced. This would be in 2001. During subsequent years, beamlines and other ring systems would be slowly upgraded to handle higher currents with the goal of operating at 500 mA with long beam lifetimes.

Advanced Light Source (ALS)

The ALS is performing at or above its design parameters, i.e., 400 mA in multibunch mode with a horizontal emittance of 3.6 nm-rad at 1.5 GeV. The vertical emittance is less than 0.1 nm-rad and any further reduction would be a trade-off with beam lifetime which is limited by Touschek scattering to a few hours. Using closed orbit feedback systems, the beam is stable to less than 10% of the beam size. Although the design energy is 1.5 GeV, the ring has operated from 1 .O to 1.9

GeV to optimize conditions for users. It has also operated in a few bunch mode with 20 mA/bunch or a mixed mode with more than 250 bunches of nominal bunch current and one bunch of higher current with empty buckets on either side.

Near term machine development includes investigation of beam stability at high frequencies, > 100 Hz, top off operation, operation up to 2.1 GeV and lattice correction and modifications which will reduce the horizontal emittance from 3.6 to 2 nm-rad and the vertical to < 0.02 nm-rad.

In the next two to three years, a third harmonic RF cavity system will be added to control the bunch length and increase the Touschek lifetime. There is also a plan to increase the booster injector energy to 1.9/2.1 GeV to allow top off and increase fill-to-fill reproductivity. Other upgrades under investigation are specialized optics for different bend or insertion device sources and superconducting high field dipoles to replace some bend magnets.

A study has begun of the feasibility of fourth generation storage rings with 100 times the brightness of the ALS for kilovolt X-rays. Here the issue is to identify the ultimate limiting parameters of the storage ring approach.

6.2 **Beamlines**

The sources have various models for allocation of beam line resources, e.g. for deciding who specifies, builds, owns, operates, maintains and uses the beam lines. Beam line allocation models cover the spectrum from facility beam lines, which are fully built, owned and operated by the facility, to Participating Research Teams (PRTs) and Collaborative Access Teams (CATs), in which consortia of outside users build, own and operate the beam lines. Another factor in beam line allocation is if the beam line is constructed to serve a specific group of scientists (science specific), as is typically the case at the NSLS, or if it is constructed to service a specific experimental technique (technique specific), as is the case at the ESRF. Beam line allocation models are among the most important factors texturing the use of storage ring facilities.

SSRL presently has 26 experimental stations on 22 beam ports with 4 more stations under construction. Ten stations are soft x-ray VUV stations. There are 4 PRT stations, where the PRT share of the beam time is either 1/3 or 2/3; thus, most stations are facility stations. SSRL participates significantly in the definition, design, construction, maintenance, support and improvement of all beam lines. It performs the scheduling on all beam lines (after receiving information from each PRT about who is to be scheduled in the PRT lines). SSRL constructs new experimental stations at an average pace of l-2 per year. It currently has 8 remaining straight sections that could be used for insertion devices and 14 remaining bend magnet sites. SSRL has proposed an ambitious upgrade to the ring, called SPEAR3, to 3 Gev, 200 mA, low-emittance operation, which would require that the beam lines be upgraded. SSRL's beamline allocation model is flexible and accommodates to both science specific and technique specific operation. SSRL proposes no overall change to their beamline allocation procedures.

The NSLS has 82 operational stations, with an additional 10 under construction or being commissioned, 6 in planning, and 6 stations available for future use. Thirty-five stations are on the VUV ring. Of the 82 PRT stations, NSLS is the sole participant on 5 stations and is a member of 18 others. In addition, there are 6 stations devoted to NSLS R&D programs and 6 diagnostic stations. Thus, most stations are PRT stations without facility membership. The standard PRT arrangement is that 75% of the time is available for PRT use and 25% is available to general outside independent investigators. Proposals by the independent investigators are funneled through the facility.

The PRT model at the NSLS evolved because there was insufficient funding when the NSLS was built to construct both the ring and the beam lines. Construction and operations of the ring was the primary NSLS obligation and funding, construction and operation of the beam lines fell mostly to PRTs. This strategy was successful in populating the ring, but as time evolved, it has become subject to several criticisms: (1) It is difficult to remove ineffective or disinterested PRTs. There is no simple, clean mechanism to provide for PRT turnover when there is a change in focus of the original PRT participants. Beam lines have become moribund when support diminished due, for example, to a change of interest of industrial participants or when some PRT members became interested in operating primarily at the APS. (2) Independent Investigators often feel that the PRT system gives them inadequate access to the source. (3) One of the most significant changes in the usage of synchrotron radiation has been the growth of user communities, such as protein crystallography and environmental and molecular science. Much of this growth has come from users who do not wish to become synchrotron experts but rather simply wish to use the facility to do experiments. In consequence, much of the growth in use of the NSLS is coming from user communities who do not have the inclination or expertise to manage and operate beam lines and, therefore, are not PRT members.

The NSLS strategy in response to the criticisms of the PRT model has been to identify beam lines which are being under utilized and to convert them to use by the growing user communities. Since much of this growth is in areas where the users do not wish to operate the beam lines, more responsibility for beam line operation falls to the NSLS, which, in turn, will require additional resources. The trend for the NSLS to gain more responsibility for beam line upgrades and operations is likely to increase when planned ring improvements (higher currents and brightness) put additional budgetary pressure on marginally-active PRTs.

The APS consists of 35 sectors, each containing an insertion device port and bend magnet port. As is the case at the 2nd generation machines, the radiation from each port can be sub-divided further so the number of eventual stations will certainly be considerably larger than the number of ports. The CAT system in place at the APS has many similarities to PRTs in that CATs must fund, design, build and operate the beam lines. However, one quantitative feature which distinguishes CATs and PRTs is that it is very expensive to develop an APS sector (c.a. $8-12M). Hence, CATs tend to have more members than PRTs, so each participant can expect less beam time. Presently, CATs are commissioning 20 sectors. The APS is primarily responsible for the SRI-CAT beam lines (sectors 1-3), which are mostly used for instrumentation development. Requests for the remaining sectors range from well-developed requests to initial feelers and letters of intent. Since most of the sectors now being commissioned are science specific, the APS has suggested that most of the remaining sectors should be devoted to technique specific applications.

CATs are allowed a 1 year grace period for 100% usage of beam lines after commissioning; thereafter, 25% of the time must be awarded to non-CAT independent investigators. An aspect of planned operation which has raised much concern among independent investigators is that review of independent investigator proposals and scheduling of beam time will be done by the CATs via a facility approved procedure. Another concern is if the CAT system will eventually be subject to the criticisms which have befallen PRTs.

The ALS has 8 bend magnet and 6 insertion device stations in operation and 5 bend magnet and 7 insertion device lines under construction. There are an additional 3 straight sections available for future insertion devices and many of the 48 bend magnet ports are available for future use. In general, stations at the ALS do not fit a rigid separation between PRT and facility beam lines because their construction and operation is supported by a mixture of PRT and ALS resources, with the division varying over a wide range from beam line to beam line. Accordingly, the amount of beam time available to PRT members and independent investigators varies. Some of the beam lines are essentially PRT beam lines with little time for independent investigators, some are essentially facility beam lines with a large fraction of time for independent investigators, and some are hybrids with the distribution of beam time covering the range between the extremes. The general feeling at the ALS is that the increased requirements at 3rd generation sources exceed the resources of most PRTs, and therefore, the facility must play a larger role. This appears to be a marked contrast in philosophy between the APS and the ALS.

A final, significant note about beamline utilization is that users apparently place great value upon nearby access to synchrotron radiation facilities. In the early years when only SSRL was available, users came from all parts of the country. Increasingly, however, all facilities have become regional facilities, with most of the users from the local region. Even the APS has nearly half of its CAT members from the state of Illinois. Although several interpretations of this trend are possible, the simplest is to accept that regional facilities, be they 2nd or 3rd generation, appear to be going a long way towards serving the needs of the local user communities. When combined with the increase in demand at all the sources, one is forced into the conclusion that there is great latent demand for regional storage ring facilities in all parts of the country.

6.3 Detectors

Synchrotron radiation experiments involve four essential components: The storage ring to generate the x-rays, x-ray optics to select and guide the x-ray beam, the specimen being examined, and the detector to record the resultant signal. The type, rate and quality of data collection is constrained by each of these components; therefore, effective data collection demands that each component be well matched to the others. The intensity and brightness of the available beams have jumped by many orders of magnitude over recent years and continue to outpace developments in detector technology, such that for many experiments effective utilization of the available flux is constrained by the detectors.

Protein crystallography provides a representative example. Usage of synchrotron radiation by the protein crystallographic community has been growing exponentially to the point where roughly half of all new published protein structures involve storage ring data. The primary factors enabling this growth are the availability of bright beam lines, the development of rapid crystal freezing techniques to mitigate radiation damage, and, most significantly, the development of image plate and CCD detectors to handle the high data rate flowing from the specimens. Even so, for many crystals at second generation sources, more time is spent reading out the detectors than exposing the crystal; this situation is expected to worsen as third generation stations come on-line.

Surveys across the broad spectrum of synchrotron user communities have consistently indicated detectors as the most significant limitations on experiments at synchrotron sources. Yet resources devoted to detector development are a very small fraction of those devoted to the x-ray source and other beam line equipment. This is to be contrasted to the situation in high energy physics where detectors may consume 10-20% of the budget of new accelerator facilities. The interplay of three reasons have led to the current lack of emphasis on x-ray detector development: (1) The national laboratories were endowed with a wealth of accelerator physics talent; there were far fewer instrumentation groups with a background readily adapted to x-ray detector development. In consequence, there was a natural emphasis at the national laboratories on the storage rings, which largely determined DOE funding priorities. The result has been, in contrast to the development of the storage rings, that very few of the developments of modern x-ray detectors were generated with Basic Energy Sciences support. (2) The PRT and CAT models encouraged a division of instrumentation effort at the primary shielding wall of the storage ring, with the result that detector responsibility fell primarily to user teams. However, detector development is complex and requires long term commitments which few user teams could support. (3) With limited detector development coming from either the national laboratories or user teams, detector provision fell to commercial vendors who attempted to adapt existing radiographic or analytic detector product lines for storage ring use. Unfortunately, many such products were ill-suited for the needs of storage ring users. Radiographic detectors typically lacked the required quantitative response or rapid readout time and analytical detectors designed for home laboratory x-ray generators were overwhelmed by the count-rates available at storage ring sources. Commercial detectors designed specifically for storage ring use have begun to emerge only in very recent years. However, the limited market for such products, and the magnitude of effort required to develop new advanced detectors may be expected to severely limit future development.

Better detectors, and better detector integration into the beam lines, will be needed to realize the potential of many synchrotron radiation applications. Specifically, detectors are needed with larger and more flexible active areas, better quantitative recording ranges, higher spatial resolution, higher overall count-rate and data through puts, better energy resolution, the capability of working at higher x-ray energies, and faster and more versatile readout capabilities. Significant work needs to be done on radiation damage of detectors, as well as on improvements in electronics for detector data handling. Detector software and user interfaces are still primitive and poorly serve the needs of specific communities. Computer platform independent and standardized data formats and storage protocols are needed to replace the existing menagerie. Network-compatible detector tools are sorely needed.

A number of promising detector technologies have been suggested, including amorphous silicon devices, superconducting detector arrays, new wide band-gap detective materials, microlithographically fabricated x-ray stopping screens, and rad-hard silicon processes. These technologies can be integrated into custom fabricated pixel array detectors (PADs), consisting of x-ray detective layers bonded to electronic processing arrays fabricated on single silicon wafers. PADs are enabled by the wide-spread availability of commercial silicon foundry services for custom integrated circuits and the capability of bump-bonding exotic x-ray detective materials to the silicon chips. PADs are a flexible detector approach towards meeting the diverse needs at storage rings.

However, it must be emphasized that the rate at which these promising approaches become available to users will be entirely limited by the priority given to detector research and development. Given current priorities, detector limitations at storage ring sources can be expected to worsen as the third generation sources continue to improve. The simple solution, namely of giving more resources to the national laboratories to solve the problem, has had limited success in the past and is unlikely to succeed in the near future. The primary reason is that there is a very limited human infrastructure of detector talent at the national laboratories and there is no ready, external pool of such talent which can be easily imported. Rather, detector talent in key technologies is spread over a small number of groups in universities and industry, as well as in the national labs. In the absence of critical mass, detector groups at the national laboratories have been relatively ineffective at introducing new developments and unable to defend against losses to more powerful groups when lab budgets became tight.

A more coherent approach toward detector development is needed to ensure that the investment in storage ring sources is effectively utilized. The first step is for DOE to give priority to detector development and to set aside long-term resources for this purpose. The next step is to put in place a continuing procedure to identify the best detector talent in key technologies, wherever it may be found, to provide support for collaborative efforts at developing detectors, and to ensure that detectors actually get into user's hands. This necessarily will involve a wise spectrum of support decisions, ranging from long-term development of speculative technology to the short range needs of technologies nearly ready for application at beam lines.

6.4 Fourth Generation Sources

Synchrotron sources have a remarkably successful history of providing electromagnetic radiation from infrared to x-ray wavelengths for scientific and industrial research. Bright electron beams have been generated from continually improving storage rings with the increasing brightness of the first, second, and third generation sources. While further advances are possible, they are limited by the fundamental characteristics and expense of ever larger storage rings. A new approach using the free electron laser (FEL) mechanism appears to be much less expensive and may increase x-ray brightness and intensity by many orders of magnitude.

FEL has been developed in parallel to synchrotron sources over the last twenty years, but at substantially longer optical and infrared wavelengths. From the beginning, it was clear that the gain medium of the FEL is transparent to x-rays and could become an impressive x-ray laser. Recent experimental advances in laser driven photocathodes and electron pulse compression indicate that a linear accelerator can generate a more intense, higher quality electron pulse than can be achieved in a storage ring. When such a pulse is accelerated to many GeV energy and injected into a long undulator, the spontaneous radiation emitted from the early sections of the undulator begins to feedback on the electron beam so that stimulated emission becomes important. As the electrons in the beam respond to feedback, they bunch at the x-ray wavelength and radiate coherently. The combination of the high peak current and the long undulator length causes high gain amplification of the co-propagating x-ray pulse. As a result, the emitted x-ray power increases by many orders of magnitude and develops a high degree of longitudinal and transverse coherence.

The SLAC proposes to carry out research on the Linac Coherent Light Source (LCLS) using the FEL gain mechanism and self-amplified spontaneous emission (SASE). The improvement and distinction of the fourth generation over third generation sources is expected to be so significant that new frontiers in science will be opened. The LCLS design uses the last 1 km of the SLAC electron accelerator and two magnetic pulse compressors to create a short electron pulse of 280 fs length with 3400 A peak current, 1.5 π mm-mrad normalized rms emittance, and 15 GeV energy. The intense electron pulse is injected into a 100 m long undulator. At the beginning of the undulator the electron pulse spontaneously emits a spectrum of x-rays characteristic of a conventional synchrotron undulator. As the x-rays and electrons travel further along the undulator, stimulated emission begins to dominate and narrow the x-ray pulse spectrum. Both the spontaneous and stimulated x-ray spectra are anticipated to be useful to the user community. The improved brightness of the fundamental's 1 Angstrom wavelength is expected to be ten orders of magnitude greater than conventional synchrotron sources, as shown in Figure 6.4.1. The x-ray FEL wavelength will be tunable from about 1 to 15 Angstroms with a 0.2 % bandwidth and has 10 GW of peak power in the radiation pulse containing 10^{12} coherent photons. Because there is expected to be full transverse coherence, the pulse can be focused to a small spot creating intense electromagnetic fields at the sample.

There have been four international workshops from 1992 to 1996 on the applications of the LCLS. The main attributes are high brightness, short pulses from stimulated emission, and the intense spontaneous emission spectrum from the 100 m long undulator. The short 280 fs pulses can be used for pump/probe experiments either with a synchronized external laser or by splitting and delaying part of the LCLS x-ray pulse. Applications include high resolution power diffraction from a single pulse, fast non-reversible chemical reactions, holograms of explosions, anharmonic lattice motion, stimulated x-ray Raman scattering, 3D holograms of biological materials, and examination of hot, dense plasmas. The LCLS represents such a large improvement in brightness that the most exciting experimental possibilities may take time to develop. The instantaneous power loading and strong fields acting on optical elements and samples may require new techniques. The number of users supported by a single LCLS undulator may be limited, but more undulators could be added in the future driven by a series of pulses from a single accelerator.

An enabling technology is the laser-driven photocathode producing a high quality, low-emittance electron pulse with high peak current at 100 Hz repetition rate. Current guns are close to demonstrating the necessary emittance and research is ongoing at LANL, SLAC, BNL, U. Rochester, and UCLA. The peak current from the gun is further increased to the necessary levels with pulse length compression by a factor of 50. This technology has been developed by the high energy physics (HEP) community for future particle beam colliders. The 100 m long undulator requires only state-of-the-art technology and is only 4 times longer than a 25 m undulator built several years ago. The SASE mechanism has already been studied at centimeter wavelengths, and is now being explored at infrared wavelengths at UCLA, BNL, and LANL. High-gain FELs are studied at LLNL, LANL, BNL, and Orsay. The LCLS R&D has been going on for several years at a low level at several research laboratories. A detailed design of the complete LCLS will be completed in late 1997 including collaboration with ESRF, LBNL, LLNL, LANL, UCLA, SLAC, and U. Rochester. SLAC wants $2.52M in 1998 and $3.25M in 1999 to continue the LCLS research. Beginning as soon as year 2000, SSRL and SLAC proposes to begin building LCLS over four years at a cost of about $70M to $100M.

The NSLS at Brookhaven National Laboratory has a long history of contributing to FEL science and technology. In 1986, BNL started the Accelerator Test Facility (ATF) supported by HEP at $1.5M per year. The ATF has excellent electron beam diagnostics for analyzing experiments and has graduated 9 PhD students and now has 7 PhD students working towards their degrees. The ATF has achieved record electron beam brightness from its RF photocathode gun, which has been used to generate 1 micron SASE. Central to the NSLS plans is the development of sub-harmonically seeded FELs, in which harmonic generation converts a laser seed to much shorter wavelength radiation.

Proof-of-principle SASE and high gain harmonic generation (HGHG) experiments are planned to be carried out at the ATF in the infrared, using an undulator borrowed from Cornell and upgraded at Argonne. An important advantage of HGHG over SASE is that HGHG will produce a beam with much higher longitudinal coherence. BNL has also just started the Source Development Laboratory (SDL). Both the SASE and HGHG work will be extended into the ultraviolet at the SDL. The SDL was established to pursue the science outlined in the NSLS Deep Ultraviolet Free Electron Laser (DUV FEL) conceptual design report. The cost of the SDL facility has been minimized by using an existing 210 MeV linac and 10 m long undulator. For a number of years, BNL has proposed developing a fourth generation DUV FEL using emission from higher frequency harmonics as shown in Figure 6.4.1. In the near future, a $2M experiment at SDL will study the SASE process from 1 micron down to 2000 Angstroms wavelength. The 10 m undulator is proposed as the basis for a user facility in the UV at 750 Angstroms at a cost of $10M over 2 to 3 years. Applications for the UV FEL include atomic and molecular stabilization in superintense fields, UV radiation damage of DNA, pump-probe kinetics, VUV photodissociation of C02, photoelectron spectroscopy of laser excited surface states, UV resonance Raman spectroscopy of proteins, trace protein identification, and time-resolved phosphorescence with researchers from FOM Holland, U. of Maryland, Princeton, Cornell, NRL, and Albert Einstein College of Medicine.

The APS at Argonne National Laboratory proposes to perform fourth-generation FEL R&D using its Low-Energy Undulator Test Line (LEUTL) system. An existing 700 MeV linac, which uses a high-brightness electron gun, will feed the LEUTL. High-performance beam diagnostics would also be available along the length of the linac and in the beam transport leading to the new 50 m long LEUTL enclosure. These diagnostics will allow further improvements in the quality of the electron beam exiting the linac and thus minimize any possible dilution of the high-brightness beam during acceleration to 700 MeV. Over time, the present high-brightness electron source will be improved as new capabilities become available.

The current plan proposes to transport the electron beam accelerated by the linac through a long undulator line, consisting of an 30 m long undulator and focusing/diagnostic equipment. The APS has accumulated unique experience and expertise in the area of design, construction, and operation of undulators and associated radiation diagnostics. Twenty state-of-the-art undulators are currently in use at the APS. The experience and well-developed technical infrastructure at the APS will be used to build and bring into operation a long undulator system on the LEUTL. The APS high-performance electron beam delivery system and the long undulator system are ideally suited to perform planned SASE FEL investigations and experiments at (or below) 100 nm wavelength as shown in Figure 6.4.1. Provision has been made to extract the radiation for leading-edge experiments. Research funding at $2M per year for four years is requested to test the SASE concept.

APS also proposes to study the use of a superconducting linac at 20 to 30 GeV energy as a fourth-generation FEL driver. A superconducting linac can deliver a much higher pulse rate with an order of magnitude higher average current. This capability is required to support the ultimate multiple-beamline user facility. A joint international research effort would incorporate the TESLA accelerator design at DESY, which has recently achieved an accelerating gradient of 23 MV/m from their 9-cell cavity in the course of R&D work. A multiple-beamline fourth-generation user facility will also require a beam-splitter system, which splits a long chain of linac beam microbunches into several branches. Each branch is transported to a designated undulator system, where photons are generated. Conventional magnets do not appear appropriate for this purpose because of the tolerances required for an FEL. APS proposes to pursue a solution to this problem using the deflecting mode of a radio frequency cavity system. The cost of performing the R&D on a superconducting fourth-generation FEL driver linac would be $4M per year for five years.

The ALS at the Lawrence Berkeley National Laboratory is studying several options for next-generation light sources. One option under study is a new storage ring with stabilized permanent bending magnets resulting in a factor of 10 to 100 improvement in brightness. The new ring would be about twice as large as ALS and uses conventional undulators. The permanent magnets and the small-aperture vacuum system technology that would be used in this machine are could make it relatively less expensive than other large next- generation rings, such as the Swiss Light Source, the Shanghai Light Source, and the Soleil project (France). Studies are also underway to develop a practical source of short (fsec) pulses of light in the range of roughly 100 eV to 10 keV. These approaches include: laser manipulation of electron beams and a new machine optimized for producing short bunches, possibly at rather modest emittance. The applications here involves x-ray beams overlapping with relatively large laser beams on the sample, so there is no need for super-low emittance, but rather a need for the highest possible peak current. Studies are also underway to use a mm-wave FEL to produce fsec bunches in a special storage ring, as well as the possible use of a recirculating beam linac to produce short pulses. There is no FEL development work at the ALS, but the LBNL Center for Beam Physics does excellent theoretical FEL research on fourth generation concepts.

Laser manipulation of electron beams is being actively pursued at LBNL, and the Center for Beam Physics is one of the world’s leader centers in this area. Compton scattering of a terawatt infrared laser producing fsec x-ray pulses from the ALS injection linac has already met with success, and a project using a fsec laser to modulate electrons in the ALS storage ring so as to make a fsec synchrotron pulse is underway. Experiments aimed at making an x-ray “switch” by modulating crystal reflectivity are also in progress, with preliminary results to appear in Science in the near future. These are all low cost ideas for improving x-ray synchrotron sources, and their feasibility should be pursued.

Synchrotron sources and FELs developed at Stanford University in the 70's. The development of radar led to coherent microwaves tubes like the Motz undulator in 1951 and the Phillips Ubitron in 1960 both preceding the FEL, while the parasitic x-rays from the bending magnetics used in HEP preceded modem synchrotron facilities. In the last twenty years, synchrotron sources have become increasingly bright in their second and third generations. In parallel, the FELs have developed high-gain theory and experiments at long radiation wavelengths, as well as brighter photocathodes than were thought possible a decade ago, and electron pulse compression techniques for use in HEP. Five years ago, the LCLS concept became feasible to propose. For fifty years, the development of radiation sources from beams of free electrons has been led by source physicists, not users. Yet, the success of synchrotron facilities, microwave tubes, and FELs have proven the value of this approach to generating radiation. The fourth generation LCLS FEL will be the next step to shorter wavelengths and significantly brighter beams of photons.

The National Academy of Science's National Research Council Committee on "Free Electron Lasers and Other Advanced Coherent Light Sources" in 1994 recommended a national effort supporting the R&D necessary for an x-ray FEL. Each facility points out that fourth generation R&D is synergistic with the operation and future developments of the existing sources. As we shall discuss in Section 10, this panel recommends continuing support of fourth generation R&D on x-ray FELs be at a modest level. The R&D plan should emphasize small experiments establishing the capability of reaching the electron beam quality necessary for an x-ray FEL. The laser-driven photocathode gun, electron pulse compression in the accelerator, electron pulse transport in the undulator, and SASE experiments at longer wavelengths are all important technologies. Building a prototype FEL at longer wavelengths is not as important as understanding the basic physics for the 1 Angstrom FEL. The decision for a start date on an x-ray FEL would depend on the success of these small experiments. The research should be a national effort involving universities and national laboratories. The actual distribution of research funds and schedule should be determined by another panel made up of potential users, accelerator and FEL physicists.

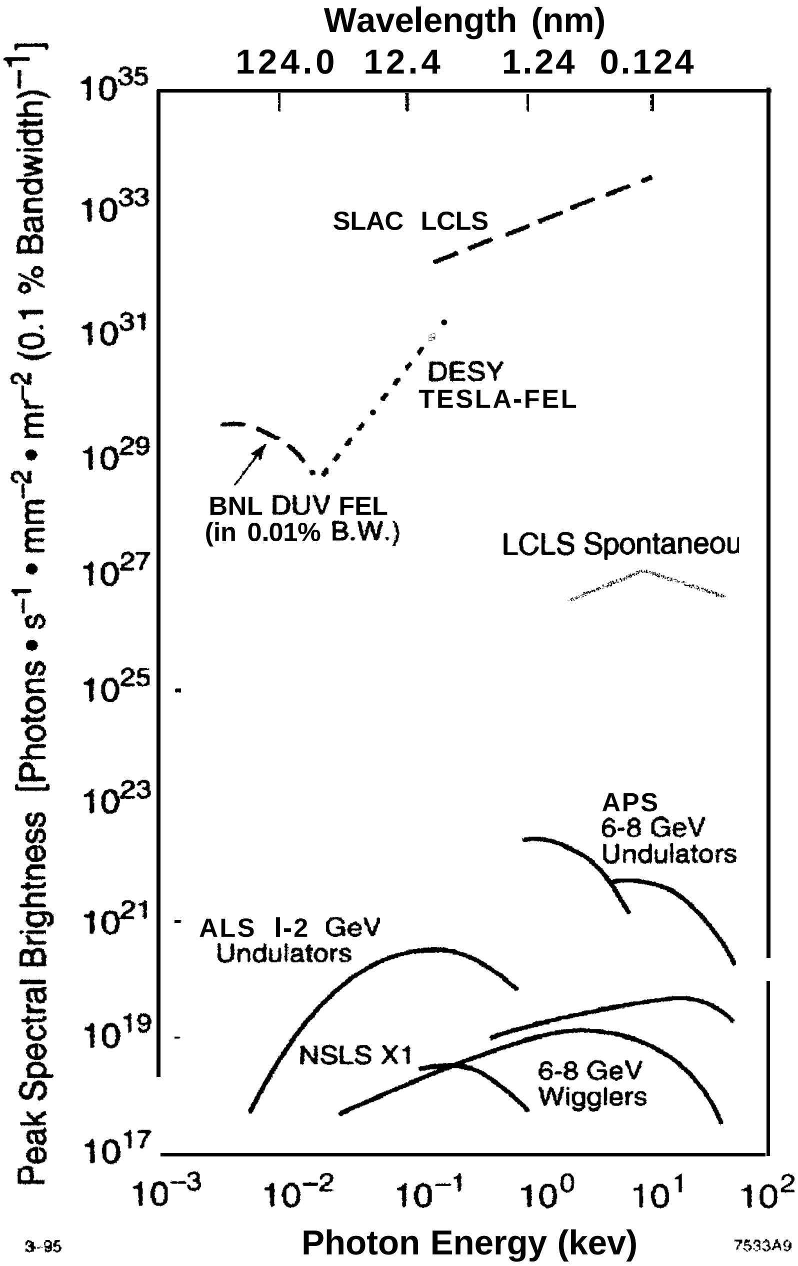


figure 6.4.1 A source such as the proposed SLAC/SSRL LCLS would offer extraordinarily high, unique peak brightness - up to 10^{10} over 3rd generation sources with extremely short sub-picosecond pulse length and full transverse coherence based upon the SASE effect. The spontaneous emission from such a source would be 3-4 orders of magnitude above 3rd generation sources but with the much shorter time structure.

7.0 USERS, PUBLICATIONS AND EDUCATION

Users at the National Synchrotron User Facilities

In response to the charge to this committee, we looked at the user community for the synchrotron light sources in some depth. This review largely focused on user demographics. In addition, we elicited the opinions of the user community through presentations by a representative of the user group at each facility, meetings with users at each of the light sources, and an e-mail survey involving about 25 users from each facility. The information compiled from these sources is discussed in this portion of the report.

User Demographics: Since 1990, the number of users at the BES synchrotron facilities has more than doubled. The actual distribution of users for FY97 is shown in Figure 7.1. In FY97, there were over 4,500 users at the four light sources, with over 50% at the NSLS. For comparison, there were 1,642 users in FY90 (more than 90% were at the NSLS and the balance at SSRL). Considering only the SSRL and the NSLS, the number of SSRL users has increased by a factor of 8 and NSLS users have doubled since 1990. [A user is generally defined as someone who is actually badged and performs experiments. For the compilation of data used in this report, however, a "user" at the APS is defined as a member of a collaborative access team (CAT). This exception was made in order to give a better picture of where the APS will be as the beamlines are commissioned. The actual number of APS users during FY97 was less than 500, compared to about 1,000 CAT members. Finally, note that a weakness in these data is that users of multiple facilities are counted multiple times... a person who uses all of the BES facilities will be counted as four users.]

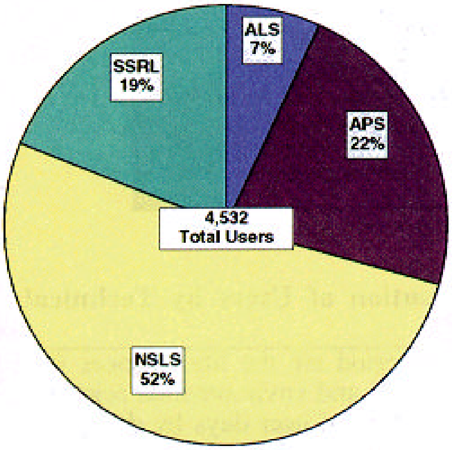


Figure 7.1: Distribution of FY97 Users by Facility

Another view of the user demographics is "user days," defined as one day of beamtime at an experimental station. The distribution of user days by facility is shown in Figure 7.2. Of the over 25,000 user days in FY97, nearly 70% were at the NSLS and 18% were at SSRL. It is expected that the number of user days will increase significantly as additional beamlines and experimental stations are commissioned at the APS.

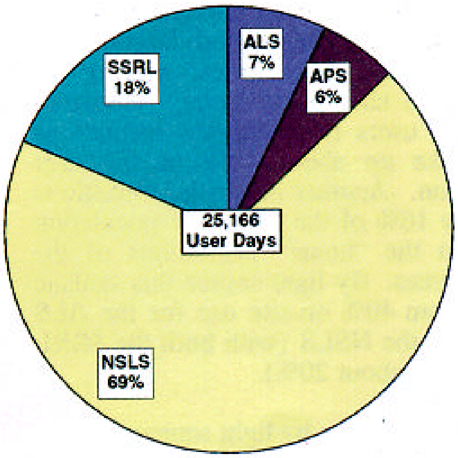


Figure 7.2: Distribution of FY97 User Days by Facility

The light source user population can be defined in terms of technical disciplines. BES has maintained statistics on the number of users from materials sciences (including condensed matter physics), chemical sciences, life sciences, geosciences/ environmental sciences, applied science/engineering, and optical/nuclear/general physics. As shown in Figure 7.3, the largest number of users are from the materials sciences community, although the percentage of materials science users in the total community has decreased since 1990. The communities that have seen the largest growth over this period are the life sciences (an increase from 6% in FY90 to 29% in FY97) and geosciences and environmental sciences (from 4% to 8%). A review of the estimates of the distribution of user days by discipline showed no significant differences compared to the user distribution. [This analysis did not include NSLS data.]

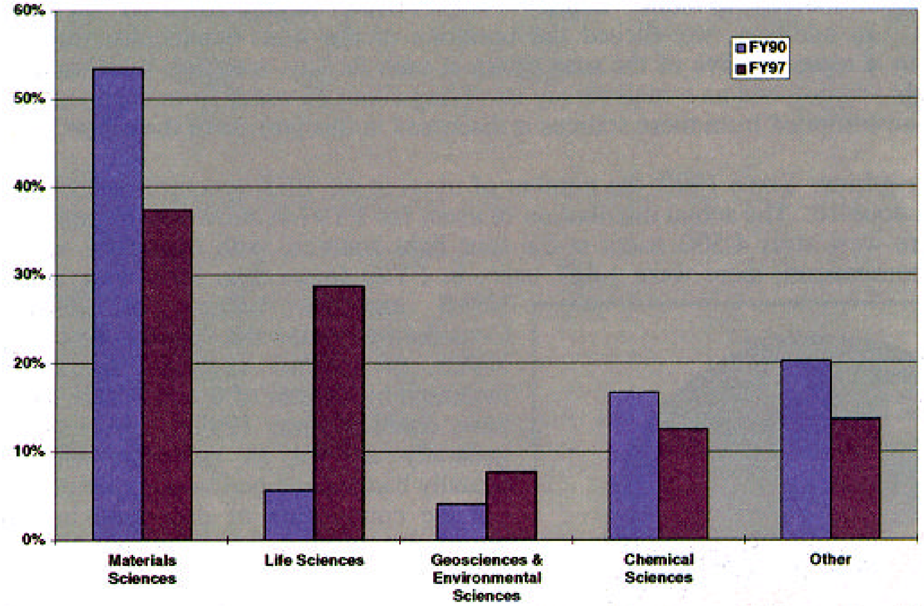


Figure 7.3: Comparison of the Percentage Distribution of Users by Technical Discipline for FY90 and FY97.

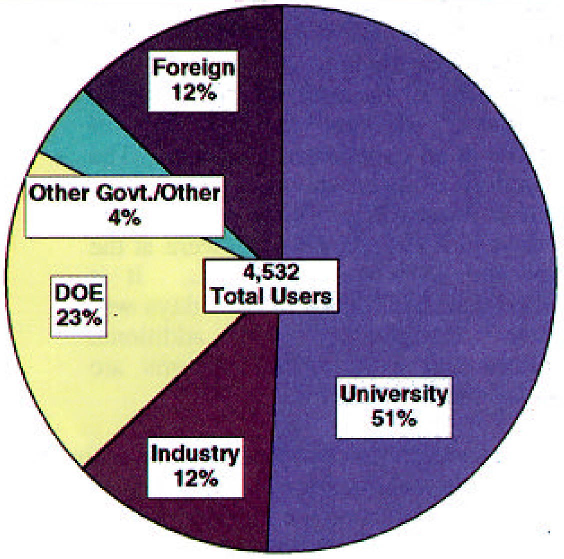


Figure 7.4: Distribution of FY97 Users by Home Institution

Another metric monitored by BES is the distribution of users according to their home institution. For FY97, as shown in Figure 7.4, half of the users of the synchrotrons were from universities in the United States. The second largest user group is DOE laboratories, making up 23% of the user populations. Industrial users and users from non-US institutions each make up about 12% of the user population. Another interesting statistic is that only 16% of the total user population are from the "home" institutions of the light sources. By light source this statistic varied from 40% on-site use for the ALS to 9% for the NSLS (with both the SSRL and APS at about 20%).

Based on estimates by light source staff, the distribution of both users and user days for FY97 by technique are shown in Figure 7.5. For the users, over 80% are using hard x-rays in their experiments, compared to 15% for VUV and 1% for IR. On the basis of user days, the VUV and

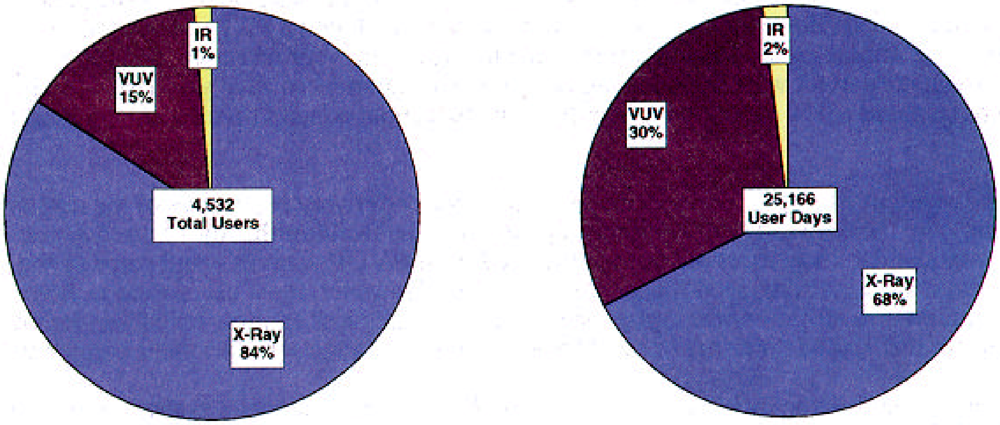


Figure 7.5: Distribution of the Users (left) and User Days (right) by Technique Used.

IR percentages are nearly double the user percentages, an indication of the requirement for longer experiments for these techniques.

Publications Data: Beyond the numbers of users, one measure of the success of synchrotron research is publications. For FY96, there were 950 publications from ALS (15%), NSLS (60%), and the SSRL (25%). Since the APS began operation in FY97, there were no publications tracked for FY96. From an historic perspective, during 1990-96 there were 5,284 publications from NSLS (74%) and the SSRL (26%). Of these, over 8% were in Physical Review Letters, Science, and Nature. These data are summarized in Table I below. [Note: Since the ALS began operations in FY94, their publications were not included in this evaluation. During FY94-96, ALS had 344 publications, of which 14 were in the journals cited above.]

Table 7.1: Publications data for 1990-96 for the NSLS and SSRL. The APS and ALS were not included in this summary since these facilities were not operational during the total period.

Facility	Total Publications	Physical Review Letters	Science	Nature
NSLS	3,884	234	55	51
SSRL	1,400	49	27	17

Of the FY96 publications, approximately 65% were related to x-ray experiments and 28% VUV experiments. The remaining publications were largely "general" technique oriented publications, with less than 1% related to IR experiments. [Note that these data are based on best estimates provided by the facilities. No exact tracking is performed by the facilities.] It is interesting to note that the percentage of publications by technique can be approximately correlated with the distribution of the user days.

User Issues and Concerns: In addition to presentations to the committee by representatives of the users from each facility, the committee met with the user communities at each facility and conducted a brief e-mail survey of 25 users from each facility. The questions asked in the e-mail survey were: (1) What is the optimal balance between PRTs or CATS and facility-owned and operated beamlines. (2) How can the general user (not associated with a PRT or CAT) be best served? (3) What impact would closing different facilities have on your research: and (4) Of the facilities that you have used, what favorable and unfavorable experiences have you had? There was excellent response to the survey with over 60 responses about equally divided among the four facilities.

Based on all of the input received, the users were generally very supportive of the quality of the facilities and the desirability of continued operation of the facilities that they currently use. Obviously, some of the x-ray users did not see the need for the VUV sources – and some of the VUV users did not see a strong need for the x-ray sources. However, most users were in favor of continued operations at all four of the current synchrotrons. The most extreme response was one from an industry that said that closure of the APS would result in a lawsuit from their company.

One early observation by both the facilities and the user communities was the importance of **regional facilities.** Regional users made up over 50% of the users for all of the facilities. For the SSRL and ALS, 60 to 70% of the users were from the west coast. In fact, home state users were nearly 50% - or more - of the user population for the ALS, APS, and SSRL. The in-state use of the NSLS was 25%. Very diverse parts of the user population favored the need for a geographical distribution of facilities. Educational issues that favored having a light source that was within "driving" distance were the cost of long distance travel and the need for on-site faculty supervision. Cost and convenience were also issues from industrial users. Portions of the life sciences user community were concerned about transporting short-lived and fragile specimens. The emerging community in nuclear waste research expressed an unexpected concern – difficulties with transporting actinide wastes, especially those containing plutonium, across multiple states.

With regard to the new, third generation sources, while some users planned to move their research from the NSLS to the APS or ALS, the more general observation was that the NSLS would continue to play an essential role in their research. It was felt that the APS would be restricted to research that required the higher brightness (due to the limited availability of beamtime and the many members of the CATs). Likewise, relative to the ALS, geographical concerns were an issue with respect to moving research. Finally, there were concerns that developmental work (to establish new techniques or new areas of research) would have difficulty in getting enough beamtime at the APS. Graduate students were concerned about the scheduling of adequate beamtime to complete their studies.

At all facilities, there was user involvement in decisions about the operations of the facility. All facilities have some type of user group that meets regularly with the management of the facility. These systems appear to be working at most of the facilities. There was some user dissatisfaction at the ALS about the degree to which their concerns were addressed in the operation of the facility. At the NSLS, however, a management concern was the difficulty in getting user input in a timely way about operational decisions.

While the purpose of this committee was not to determine whether the **CAT/PRT system** was working, questions about the approach to R&D at the synchrotrons were unavoidable. First of all, each synchrotron operates in a slightly different mode. At SSRL, most of the beamlines are operated by the facility. This is generally viewed as satisfactory by the users and has the advantage of more uniformity in both software and technical support. At NSLS, most of the beamlines are operated by PRTs, with at least 25% of the time at the PRTs available for general users. User concerns at the NSLS were the changes occurring in the PRT membership (with the commissioning of the APS beamlines), the aging of the equipment at some of the beamlines, and the inconsistency of user support for some PRTs. The ALS has a mix of facility and PRT beamlines, but the mix is weighted toward facility beamlines (the time available to general users is proportionate to the support of the beamline... the more facility support for the beamline, the more general user time is available). One concern expressed by users relative to the ALS was a perceived lack of scientific community involvement in decisions about the focus of the ALS beamlines. At the APS, the majority of the beamlines will be CATs. As at the NSLS, at least 25% of the APS beamtime will be available for general users.

The CAT/PRT system is generally regarded by the users as a system that provides innovative beamlines with strong science programs. Generic concerns about the PRTKAT approach are the long-term maintenance, technical support for the beamlines, and inconsistent software and equipment among the beamlines. The latter issue is being addressed at the APS to some degree through application of a consistent operating system for most of the beamlines. The need for a strong scientific review was also expressed by users. At the NSLS, a system of review for the PRTs is in place to assure the scientific quality and health of the beamline organization. Currently, as beamlines become available at the NSLS there has not been a shortage of new groups to take them over. For the ALS and APS, the issue is the availability of funding to complete the beamlines and associated facilities. The APS has an external review board that assesses all proposed CATs. Although funding for PRT/CATs is a major concern of many users, these issues are addressed elsewhere in this report.

The concerns of general users and of users who are members of the PRT or CAT (for the bearnline that they want to use) are different. Access for PRT/CAT members to their own beamlines is based on the amount of funding that they are contributing to the PRTKAT. For PRT members there are restrictions for general access to similar beamlines. This creates the possibility that general users (people who have no affiliation with PRTs) could actually get more instrument time (by using multiple beamlines) than a PRT member who is paying for beamline operations. One issue for this group is the continuing difficulty in getting programmatic support for beamline operations as part of work funded by NSF or other agencies. (Funding for initial construction of the beamline is more straightforward than obtaining funding renewals for multiple year operations.) One concern expressed by the PRT/CATs was that general users who are frequent users of a specific beamline should be “encouraged” to join the PRTKAT and should thereby contribute their fair share of the operations cost of the beamline(

For the NSLS, SSRL, and ALS, general user access to a beamline requires a proposal that is reviewed by a central scientific committee to determine (based on the quality of the work proposed) who gets beamtime. Exact review procedures vary from facility to facility. At the APS, however, it is proposed that the general user proposal will be reviewed by the CATs themselves. The details of this procedure are evolving. There are concerns from the general users about the proposed process in terms of possible favoritism towards friends and collaborators and in terms of time requirements from the CATs themselves (the same proposal could be turned in to multiple beamlines).

The first desire of the all users *is* to have lots of beamtime that is available with a “quick” response and to do experiments on the “best” beamlines with adequate operational assistance. Industrial users were concerned about reducing the delay between proposing an experiment and getting beamtime for both proprietary and non-proprietary research. Some of the general users have concerns about the reliability of the beamline equipment and quality of the user support that they receive. It is expected that the CAT/PRT will provide equipment in good working order and the staff necessary to insure that the user is able to do his/her experiments. Clearly this concern reflects individual experiences at specific beamlines. Likely many beamlines provide excellent user experiences, and others do not. While systems are in place to identify problems, preventing these may be impossible due to changing conditions at the PRTs. The ALS has used facility funds to place postdoctoral staff at some of the beamlines to help these concerns. A related series of comments from users suggested that the facility should have funding set aside to help first-time users of a light source. The belief was that this would help all of the staff, would encourage users from new fields, and would enhance the quality of the science.

In terms of the balance between PRT/CAT and facility operated beamlines, the responses of the user community varied from all facility operation beamlines (particularly at the 2nd generation sources) to "mostly" CATs/PRTs (particularly at the 3rd generation sources). Some industrial users want all facility operated beamlines. However, it appeared that most users liked the current CAT/PRT system with allocation of around 75% of the beamtime for the PRT/CAT members and the balance to the general users.

Housing, parking and availability of meals, etc., were other areas commented on by many users. In general, users want inexpensive, good quality housing that is close to the facility. NSLS is the leader in providing good services this area. The lack of available parking near the facility was a concern for many ALS users. Across all facilities there were comments about the need for meals and technical services (especially repairs) to be available during late night – early morning hours and over weekends. It should be noted that the users were very sensitive to the responsiveness of the facilities to their concerns – many of the negative comments about experiences at the light sources focused not on the problem itself, but instead on a perceived "we don't care" attitude of the facility staff about the problem/concern.

Education

As with any area at the cutting edge of science, synchrotron-based research contributes broadly to education by providing the essential material -- facts and insights -- that will be taught in the future. Already, the results of synchrotron research is causing textbooks to be re-written. The area of molecular biology, for example, is being revolutionized by the quantity and quality of structural data now becoming available, from which entirely new paradigms are emerging. A similar impact can be noted in materials chemistry and many other disciplines.

Synchrotron radiation sources also contribute directly to the education of a large number of undergraduate students, graduate students and postdoctoral fellows in a wide range of fields, from chemistry, physics and materials science to biology, geology and environmental sciences. All sources have strong ties with academia, including close links with individual universities (e.g., Stanford University, University of California, University of Chicago) as well as with consortia led by or involving universities (e.g., the CATs at APS). More than 100 universities participate, and the fraction of synchrotron users from academia ranges between approximately 33 and 70 percent at the various sources; the more established sources (NSLS and SSRL), which are perhaps more representative of the long-term steady state, report that 65-70% of their users are from academia. Although difficult to estimate precisely, the number of students utilizing synchrotron sources for their research undoubtedly exceeds 1000/year within the U. S., since NSLS alone reported -700 students/year for the period from 199 1- 1996.

Another measure of educational impact is the number of theses that are completed annually based on work partially or fully performed at synchrotron sources. SSRL reports 20-30 Ph. D. theses per year since 1993, with a total of 349 Ph. D. plus 11 M. S. degrees awarded based on work done at SSRL over the period 1974-1997. ALS reports 3-5 doctoral theses per year since 1995. NSLS estimates of order 70 theses per year based on research carried out at that facility. As APS is just starting to gear up, steady state numbers are not yet available, and it is reasonable to expect that students will constitute a significant fraction of the more than 4000 researchers who may ultimately work at the APS.

One of the special characteristics of synchrotron-based research is that it tends to be highly interdisciplinary. Thus, students typically work with several collaborators, often on more than one project, thereby being introduced to a much greater variety of scientific problems and techniques than is normally the case in smaller-scale individual research. Because many different scientific disciplines benefit from a given source, students are introduced to a wide range of science both at user groups' meetings and simply while working at the synchrotron.

In addition to providing resource facilities for experimental work, a specialized program exists at SSRL to provide graduate training in accelerator physics. This program was originally initiated by SSRL and the Stanford Applied Physics department, and now includes SLAC high energy physics faculty. Three of the six former graduate students are now working as accelerator physicists at APS and NSLS. One student's thesis actually worked out the basis for the SPEAR3 upgrade that is currently proposed by SSRL. Two additional Stanford graduate students are performing longitudinal feedback and nonlinear map fitting studies using SPEAR; SSRL also hosts accelerator physics graduate students from other universities for various accelerator studies.

8.0 BUDGETS

BUDGET SUMMARIES: SCENARIOS AND OPPORTUNITIES

In this section we first summarize the budget information for fiscal years 1997 and 1998 made available to the Panel by the DOE synchrotron facilities and by DOE/BES. We also present parallel information on personnel and beamlines at each facility. Secondly we present a brief review of the costs of various proposals by the Facilities to enhance source, instrumentation and user support capabilities over the next 5 to 10 years. We also briefly summarize the responses of each facility to a hypothetical funding increase of 20% above inflation over five years and to a flat budget. More details on the accelerators, beamlines and instrumentation briefly mentioned in the summaries below are included in other sections of this report

Budgets for FY 97 and 98

The total DOE/BES budget for operating and capital equipment for the four DOE Synchrotron Facilities (including accelerator improvement projects) is 163.4M$ in 1997. This number does not include DOE/BES funding for instrumentation, operation and science programs for beamlines at the synchrotron sources, which amount to 30+M$ a year. The FY 1997 and projected 1998 budgets for the four DOE facilities are shown in table 8.1, broken down into separate costs for accelerator operation and maintenance, beamline operations and support, research and development efforts, and capital expenditures. The number of beamlines which are projected to be operational by the end of FY '98 and the number of personnel funded by each facility budget in FY '97 are also included for comparative purposes. There are slight inconsistencies between the numbers provided by BES and the facilities, but they have little impact on the overall picture.

The numbers in table show some significant, not unexpected, differences between the budget profiles for the third generation sources (APS and ALS), which are still at an earlier stage of development and commissioning and the second generation sources, SSRL and NSLS, which are also engaged in accelerator and instrument improvements or replacements at a slower pace.

At its early stage of operation, the newest, largest, and most complex source, the APS, spends a larger fraction of its budget on R&D, in part because of the challenges in operating at a much higher brightness, with more insertion devices and instruments which require new developments in optics, heat removal, detection, etc. A larger R&D component can be expected for a number of years at this facility. In addition it should be noted that the operations expenditures for direct scientific and technical assistance for users is much larger for the ALS and the SSRL than it is for the NSLS, which has participating research teams (PRT's) providing technical and instrument science support for over 70% of its beamlines. In addition, the APS, with its CAT system will provide a great deal of generic user support (including R&D) for CAT users, but will generally not directly support experiments as is done on most beamlines at ALS and SSRL. It should be noted that the scientific teams engaged in PRT or CAT arrangements also expend funds (aside from scientific research costs) maintaining and operating beamlines. For example BNL estimates approximately 1 8M$/year (-300K per beamline) in such costs for their PRT's at the NSLS.

Table 8.1: DOE Synchrotron Facility Budgets ($M) - FY97 and FY98

Facility	Beamlines	Total Budget*		Acc. Ops & Maint.		Beam Ops/Support		R&D		Capital**		Staff
	FY98	FY97	FY98	FY97	FY98	FY97	FY98	FY97	FY98	FY97	FY98	FY97
SSRL	26	20.5	21	7.1	7.3	8.0	8.0	2.9	2.5	2.4	3.2	136
NSLS	80	28.6	30.8	18.7	19.3	3.4	4.3	2.3	2.5	4.1	4.1	166
ALS	26	33	35	17.9	18.7	7.3	7.6	2.5	2.5	5.6	6.4	179
APS	40	81.3	84.7	55	57.3	21.0	21.8	***	***	5.4	5.7	402

FY98 budgets are the Presidential budget recommended levels.

*Folds administrative support costs into Operational and R&D costs (generally 5-6% of budget)

** Includes Equip. Funds and ARIM

*** Major R&D included in the costs in the first two columns.

Cost of Proposals for Facility Improvements

As part of the Panel's visits to each of the DOE Synchrotron sources we were briefed in written and oral presentations on various proposals to enhance the accelerator and instrumentation capabilities at their facilities, all of which would increase U.S. and DOE capabilities and opportunities in this field. What follows is a summary of the proposed projects by each laboratory with estimated costs. Further details are available from the written materials presented to the Panel, which are available to BESAC. Each of these proposals would also require an increase in operational costs, which are estimated where possible.

1. Stanford Synchrotron Radiation Laboratory

Full implementation of upgrade opportunities at SSRL would include the upgrade of the accelerator to "third generation" character with increased brightness and flux and development of 22 straight and bending magnet sections. The estimated costs for these improvements (FY '97$) are:

SPEAR 3	~50M$
Develop 22 lines including instruments	~90M$
Upgrade of beamlines for SPEAR 3	~10M$
Total	~150M$

It should be noted that smaller continuing improvements would occur at SSRL, including development l-2 beamline per year under anticipated funding profiles. Increased operating funds required if the above improvements are funded are uncertain, but in excess of 5M$/year. Therefore the summary costs of proposed or projected opportunities at the four existing DOE facilities are:

ALS- ~100M$ - largely from DOE/BES
APS - ~200M$ - many funds anticipated from outside sources
NSLS - ~70M$ - largely from DOE/BES
SSRL - ~ 1 50M$ - largely from DOE/BES

Total ~500M$ over 5-8 years if all opportunities were to be pursued. Increased operating funds required if these projects are carried is again uncertain, but is likely greater than 20M$ per year.

2. National Synchrotron Light Source

BNL projects the need for a broad beamline upgrade and proposes a Phase III NSLS upgrade for the accelerator, to improve brightness and reliability, insertion devices, and some beamline improvements. The projected costs are as follows:

Phase III (costs validated by DOE) =	~34M$
General Beamline Improvements	~35M$
Total	~70M$

It should be noted that BNL also anticipates some additional need for operating funds for the new capacity from the upgrades and to compensate for the need to assume responsibility for some PRT stations being reprogrammed. Again these costs are estimated at 300K$ per beamline. A complete figure is not available, but again of the order of $5M per year would be required.

3. Advanced Light Source

The ALS management has devised a roadmap for full development of the ALS facility between FY 1998 and FY 2005 with installation of a full complement of insertion devices, full instrumentation of insertion device beamlines, and a number of front ends for bend magnet lines. They also propose to upgrade the performance of the ALS accelerator. The most expensive part of the proposed roadmap is a 60M$ project to improve the infrastructure for research, including completion of the unfinished second floor of the ALS building to provide office and laboratory space for users and a new building to house ALS staff, along with related improvements - power, cooling, etc. The ALS management feels that these latter improvements are critical to allow the Facility to properly serve its user community. The summary of costs to complete the roadmap over 8 years follows (as spent dollars).

Instrumentation	$ 24M
Accelerator Upgrade	$ 22M
Infrastructure Improvements	$ 60M
Total	**$ 106M**

Over these eight years ALS would also provide some additional expenditures from capital and ARIM funds to cover part of the beamline development.

4. Advanced Photon Source

The Advanced Photon Source projection for desired additional funding is complicated by the strong ANL view that the existing operating budgets in table 1 are already 15% too low to allow the APS to meet its accelerator performance, insertion device development and other tasks to optimize operation of the APS for the user community. However, previous experience with development of the first 20 sectors allows APS management to project a cost of about 210M$ over the next 5-7 years to fully develop the remaining 14 sectors of the APS. The expenditure estimates are as follows (FY '97).

New Beamlines	APS (DOE)	~ 45M$
	Users .	~ 150M$
Additional APS Lab-Office Modules	(DOE) =	~ 5M$
Total		~200M$
Additional Operating Funds to serve new CAT's:		5.4M$

Facility Responses to 20% Real Increase Over Five Years

We will now briefly summarize the response of the Synchrotron Facilities to a hypothetical increase in funds over 5 years of 20% above inflation. This would amount to an overall increase of ~40M$/year for the four laboratories.

<u>SSRL</u> - Under such a 20% increase, SSRL would be able to provide major new capabilities based on state-of-the-art insertion device lines. They would also strengthen their staff with 7 FTE's for more effective R&D and user support in molecular environment science and materials research. SSRL could not, however, proceed with SPEAR 3 unless alternative funding was found.

NSLS - A 20% increase would fund two thirds of new science and beamline opportunities and allow some retargeting of PRT beamlines. The proposed Phase III upgrade and beamline modernization would not be achieved.

ALS - Such a 20% increase would cover their scientific roadmap over the next five years (see above) but would not allow construction of new lab, office and other facilities to effectively serve users. In addition, there would not be an adequate increase in support staff under such funding.

APS - Such an increase would restore APS after five years to their originally anticipated budget in FY '98. Accelerator, undulator and user support goals would be met. However 10-12 sectors would remain undeveloped due to a shortfall of ~40M$ in construction and 5M$ a year in operating funds.

Facility Responses to a Flat Budget

Each of the facilities were also asked to project the consequences of a flat budget (no inflation increase) over an extended period of years. The following summarizes the responses to such a constrained budget.

SSRL - The SSRL management would immediately curtail instrumentation development. They would attempt to increase and diversify the operational support base from BES sources beyond the current 20% and re-target capabilities to serve more "full cost recovery" users. If not successful, operations and facilities would erode significantly in both reliability and capability.

NSLS - It is estimated that station hours would have to be cut 50% over 3 years, along with the loss of up to 30 FTE's over 5 years. The reliability of accelerator and beamline operation would also be seriously impacted.

ALS - Under such a curtailed budget beamline development would stop. There would also be a loss of 8 FTE's per year and a curtailment of operating hours which would greatly impact existing users and compromise possibilities to serve new users and needs.

APS - Full performance goals would be postponed indefinitely, greatly diminishing competitiveness with new 3rd generation sources in Europe and Japan. In addition, the facility would operate less reliably for less hours. Furthermore, there would be a major cutback on services of the XFD division and full development of the remaining 14 sectors would be impossible.

Fourth Generation Source

Each of the DOE synchrotron sources has some plans and activity underway to develop or participate in the development of next generation sources. Very briefly, the status of each effort is as follows.

SSRL - Stanford is spending 1M$ in FY '97 on R&D for a linac coherent light source (x-ray FEL). They propose to request DOE funding for R&D to allow start of construction in 2000 on a dedicated ~1.5A FEL, using part of the SLAC beam.

NSLS - Brookhaven would like to continue to perform R&D, using capabilities at the Accelerator Test Facility. They are also working toward development of SASE and HGHG FELs for UV wavelengths at the Source Development Laboratory. Cost estimates are ~2.5M$ to demonstrate SASE and an additional 10M$ to produce useful photons in a user mode.

ALS - Some exploratory research is underway with LDRD funds, but there are no plans for an expanded effort unless the DOE funding situation changes.

APS - R&D is currently being carried out with LDRD funds on the APS undulator test line. This project is part of an interlaboratory effort aimed, if funds are available, at developing and testing a uv FEL.

9.0 CONSEQUENCES OF FACILITY SHUTDOWN

Note that the following subsections in the 9.0 Consequences of Facility Shutdown section were adapted from the responses by the individual facilities to question number 12 in Appendix B.

9.1 Stanford Synchrotron Radiation Laboratory

In considering shutting down SSRL, one must remember that it is the primary source of hard x-ray synchrotron radiation for the western United States, serving about 1400 scientists. In addition, SSRL is the only provider of long lifetime VUV/soft x-ray radiation for the West, complementing the radiation provided by ALS. Closing of SSRL means that most of its users would have to severely compromise their scientific programs because the remaining facilities would not be able to support these users in the foreseeable future given the relatively small amounts of beam time the users could expect to obtain as general users at other synchrotron facilities. These users would lose, in addition, about 200 million dollars worth of scientific instrumentation which has been improved constantly over a 20 year period. Some beamline capabilities have no replacement (e.g., the soft x-ray l-4 keV line). Lost, as well, would be the very special scientific support teams and specialized instrumentation for: a) structural molecular biology; b) molecular environmental science and analysis, and c) thin film, interface and surface analysis. One must also remember the context in which SSRL functions. It serves three great western national laboratories, and provides unique capabilities for scientists at these laboratories for XAS studies relevant to cleanup of radioactive contaminants within the DOE weapons complex, which is one of the major current missions of the DOE. Being a part of Stanford University and within driving distances of many western universities, SSRL has paid enormous attention to the education of graduate students. Students trained here have taken leadership roles at national labs, industry and academia. The training of graduate students in synchrotron radiation science would be severely compromised. The unique experiences and perspectives gained by graduate students working in a multidisciplinary laboratory with strong ties to industry and national laboratories would be lost. Lost as well, are the successful medical synchrotron-based programs which have been those coupled closely to appropriate local university or hospital groups. Finally, SSFU is in the center of one of the United States' great high technology areas which supports semiconductor, magnetic storage, biotechnology and petrochemical research on a grand scale. All of these communities would lose ready access to hard x-ray synchrotron radiation. Closure of SSRL would eliminate a strong tradition of excellence and ongoing effort in technological development of synchrotron radiation sources. SSRL was the first storage-ring based source for x-ray science in the Nation, developed the first wiggler insertion devices for x-ray science on storage rings, and developed the first undulators which have become the basis for third generation synchrotron radiation sources throughout the world. The Nation's ability to develop in a cost effective and timely manner a fourth generation source of sub-picosecond, pulsed, coherent x-rays would be lost. In summary, a well-functioning facility, which has become extremely valuable to about 1400 scientists, which continues to produce excellent science and thrives in educating students, which excels in engaging new communities, developing new capabilities and pioneering new directions, would be eliminated in spite of its success. This outcome would represent a great loss of science, and a great loss in educational opportunities for science students and postdoctoral fellows in western US universities. It would represent a great loss in industrial applications of synchrotron radiation science, particularly in the semiconductor and biotechnology areas where proximity to the activities is a strong facilitating factor. And, it would represent a great loss in the vitality and breadth of synchrotron radiation research in the US.

9.2 National Synchrotron Light Source

The two storage rings at the National Synchrotron Light Source were the first light sources in the world built with the innovative Chasman-Green magnet lattice which was later adopted by all three of the larger third generation light sources. Throughout the 1990s the NSLS user community has dominated the field of synchrotron radiation based science providing over three-quarters of the DOE station hours in each of the last two years. The NSLS has over 6500 users, -800 newcomers each year, and the facility accommodates about 2200 users each year. The users have produced more than 4000 publications since 1990 including more than three-quarters of all the DOE synchrotron radiation based research papers in quality journals such as Physical Review Letters, Nature and Science. Our large user community could not be accommodated at the other synchrotron radiation facilities, hence many research programs at universities, industrial corporations and other national laboratories would be severely damaged if the NSLS were shut down.

Industrial use is strong; about one third of the beamlines were constructed by industrially based Participating Research Teams (PRTs), and each year 250 shifts of proprietary beamtime are purchased on a full cost recovery basis. The large investments made by industry in beamlines at the NSLS were based on assurances that the facility would run steadily and reliably well into the next century. Shutting down the NSLS would be to break a commitment made to these companies who have made large investments at the NSLS. 86% of our national users reside east of a line drawn from the eastern border of the Dakotas to the eastern border of Texas. Since 1990 more than 450 theses have been awarded to graduate students who worked at NSLS.

Because the NSLS is two storage rings, NSLS is the only facility in the world which can provide optimized photon beams from the infrared to hard x-rays. The unique opportunity to use both extremes of the electromagnetic spectrum is crucial , for example, in research at very high pressures in materials sciences, solid state physics, geosciences and in biology. Spectroscopy across the entire periodic table requires both VUV and X-Ray radiation; that is why several PRTs (including for example Albert Einstein College of Medicine, AT&T, Carnegie Institution Washington, Exxon, IBM, LANL, NIST, NRL, Smithsonian Astrophysics Observatory, SUNY Stony Brook) have built beamlines on both storage rings. The infrared programs on the VUV ring are world beating and will remain so for the foreseeable future because the storage ring has a unique combination of high current (almost 1 A), small bend radius (1.9m) and extraordinary stability (ca. 1 micron r.m.s over 1000s). The X-ray ring is the only facility in the USA which provides radiation at fm wavelengths (300 MeV) for research in particle physics.

This world renowned, high quality, productive and cost effective resource would be lost to the country if the NSLS were closed. The opportunity to work at both high and low photon energies in the same facility cannot be optimized at any site with a single storage ring. The NSLS is sited at the heartland of the national synchrotron user community.

9.3 **Advanced Light Source**

The ALS was the first of several third-generation VUV/soft x-ray sources (10-1500eV) in the world to become operational. It is still nationally and internationally regarded as the premier source (flagship) in this spectral range. Closure of the ALS would eliminate the international leadership role of the United States in exploring and defining the scientific and technological utilization of high brightness soft x-rays. The emphasis would shift to facilities in Italy (ELETTRA), Sweden (MAX II), Taiwan (SRRC), Korea (Pohang Light Source), or the upcoming BESSY II facility in Germany. While some of the present VUV/soft x-ray programs at the ALS, which depend more on flux than brightness, could be accommodated by other US facilities like ALADDIN, CAMD, SSRL, NSLS or APS, the major consequence of an ALS closure would be the loss of unique scientific and technological opportunities afforded by its high spectal brightness. Also some programs which are "flux-limited" (the ALS offers a two orders of magnitude advantage in the flux*resolving power product) would be eliminated. The following major programs would be lost: (1) Microscopy and spectra-microscopy programs. These programs are aimed at understanding complex heterogeneous systems on a length scale ranging from 2 - 2000nm with elemental, chemical, and magnetic specificity. Important contributions are anticipated in biology, environmental and molecular science, polymer science, and in microelectronics and magnetic storage technologies. The technological utilization of the ALS by near-by Silicon Valley companies, in particular, presents great opportunities that would be lost. (2) Ultra high resolution photoemission spectroscopy programs. The high brightness of the ALS enables photoemission spectroscopy with unprecedented spectral resolution (at sufficient photon flux) in the region above about 40eV where grazing incidence optics need to be used. Of unique importance is the spectral region around 100eV where the 4d - 4f transitions in the rare earths can be probed, promising unique insight into the Kondo and heavy fermion problems, two of the great problems in solid state physics. Other important physical insight is expected from high resolution spin polarized photoemission studies of surfaces, ultra thin films, and multilayers. (3) Programs utilizing lateral coherence. The soft x-rays emitted by the ALS offer a degree of coherence unattainable at other US facilities. The ALS coherence is used effectively by the Center for X-Ray Optics in the evaluation of optical elements crucial for the implementation of EUV projection lithography. At a time when the future direction of lithography is under active evaluation this program plays an important role in the decision making process of the US microelectronics industry. (4) The thrust in soft x-ray spectromicroscopy in conjunction with synchrotron based molecular environmental science suggested in the 1997 update of the Airlie workshop would be lost.

9.4 **Advanced Photon Source**

Irreversible consequences of shutting down APS: Construction of the APS was completed in 1996 at a total project cost to the DOE of $812 million. Since 1996, the APS accelerator systems have been successfully operating and meeting or exceeding all technical design objectives. The APS users are actively installing, commissioning, and initiating the first operations of their research beamlines. Premature shutdown of this facility would represent an immediate loss of DOE’s promising investment before the U.S. scientific community could derive any significant benefits from it.

The APS is this nation’s premier synchrotron radiation source, designed to produce the brightest x-ray beams available with energies from about 1 keV to 300 keV. Loss of this state-of-the-art capability would place all U.S. x-ray experimenters at a technological disadvantage to their foreign colleagues in Europe and Japan where comparable sources of x-rays have begun operations.

Fourteen teams of research users involving more than 169 academic, governmental, and industrial institutions have invested $156 million to construct their experimental beamlines. These funds have come from other federal agencies, U.S. industrial corporations, state governments, private institutions and foundations, and foreign sources. Scientists and industrial engineers numbering in the thousands have formalized plans to use the APS and have developed research programs for the next decade. Shutdown of the APS would be disruptive of these plans and would represent an extraordinary public relations problem. And the technological and health advances anticipated form this research and their corresponding economics benefits would be delayed or entirely lost.

10. CONCLUSIONS AND RECOMMENDATIONS

Conclusions and Recommendations

The most straightforward and most important conclusion of this study is that over the past 20 years in the United States synchrotron radiation research has evolved from an esoteric endeavor practiced by a small number of scientists primarily from the fields of solid state physics and surface science to a mainstream activity which provides essential information in the materials and chemical sciences, the life sciences, molecular environmental science, the geosciences, nascent technology and defense-related research among other fields. The user community at U.S. synchrotron facilities continues to grow exponentially, having reached more than 4000 on-site users annually in FY97. The research carried out at the four D.O.E. synchrotron sources is both very broad and often exceptionally deep. The breadth of the research is well indicated by NSLS data which show that research results obtained at NSLS since 1990 have been published in more than 250 journals. Furthermore, the high quality of synchrotron-based research is illustrated by the large number of publications in premier journals such as Science. Nature and Physical Review Letters. This is especially true in the life sciences where in recent years more than 60% of the biological crystal structures published in that field's lead journals were obtained using synchrotron techniques. The growing significance of synchrotron radiation research is well-illustrated by the following quotes from 2 Nobel laureates, Arthur Komberg of Stanford and Phillip Anderson of Princeton.

Arthur Komberg states:

> "Molecular anatomy will be the foundation of medicine in the 21st century, as was human anatomy five centuries earlier. Some life processes are already understood in molecular terms, but the truly great insights have yet to be made into biologic form, function and cognition and their aberrations in disease. Understanding how enzyme, antibodies, and even more complex macromolecules work will depend on knowing their 3D structures, and subcellular architecture. The design of drugs to facilitate or interrupt these interactions will demand a sophisticated knowledge of molecular anatomy. For assays of drug efficacy and safety in animals, comparable knowledge of their 3D structure is essential.
>
> Just as powerful as the importance of structural biology for human health is its need for advances in all the biologic sciences. From viruses to bacteria to mammals, understanding evolution and function demands knowledge of chemistry at a structural level. The profound understanding of the universality and diversity of form and function throughout Nature will be one of the great revelations of the next century. In as much as synchrotron radiation is the primary means by which large scale biologic structural information will be obtained in the future, continued support is of utmost importance."

Phillip Anderson, in his discussion concerning the mechanism of high temperature superconductivity observes the potential of synchrotron based photoemission experiments:

> "If I had my choice of smoking guns, I would ask for two things. First, better photoemission data, both sample and resolution wise. Angle-resolved photoemission spectroscopy is, for this (high T,) problem, the experiment that will play the role that tunneling played for BCS...."

Synchrotron radiation facilities play a central role in education, especially at the graduate level. Since 1990, approximately 100 PhD's per year have been granted based on research performed at SSRL and the NSLS. With the initiation of research at ALS (1993) and APS (1996) this number is expected to grow considerably.

We believe that the growth in the number of participants in the synchrotron field and, most especially, its increasing diversification will continue for at least the next decade and accordingly facilities must be provided to accommodate these users. It is notable that much of this growth has been fostered by the second generation facilities. One of the side-effects of this growth is that there has been a marked increase in the number of novice, non-specialist users who require significant technical support in order to carry out their experiments This development will be reflected in our funding recommendations.

Each of the four D.O.E. synchrotron research centers is a national facility which serves both the nation as a whole and a significant number of international users. Nevertheless, the facilities have a surprising "regional" character. For example, about one half of the APS CAT members reside in the state of Illinois while more than 40 per cent of NSLS users are from the New York - New Jersey - New England area. Thus, NSLS is in good measure an East Coast facility, the APS serves predominately the Mid-West and similarly SSRL and the ALS serve primarily West Coast synchrotron radiation users. This regionality has several origins, including travel and living costs, the necessity for many experiments of transporting cumbersome equipment, ease of access for very brief trips by university faculty, and, especially in the life sciences, the fragility of samples. Of course, scientists will travel to a distant site if that facility possesses a unique and essential capability and if the experiment is transportable over long distances. Accordingly, all DOE sources continue to serve a large number of non-regional users.

It is self-evident that research which requires very high brightness will be carried out overwhelmingly at the third generation sources. This includes, for example, experiments which exploit the partial coherence and high brightness of undulator radiation such as fluctuation spectroscopy. Various high resolution microprobe and microspectroscopy experiments also require undulator radiation. Nevertheless, most current synchrotron research requires high flux as opposed to high brightness and therefore can be carried out equally well at second and third generation sources. Finally, the third generation sources could not possibly accommodate the more than 3000 users currently carrying out research at the second generation sources, especially since the overall community is expected to continue to grow in size.

As discussed in sections 6.2 and 7.0 of this report, there are various models for allocation of beamline resources, that is, for deciding who specifies, builds, owns, operates, maintains and uses the beamlines. Beamline allocation models cover the spectrum from facility beamlines which are fully built, owned and operated by the facility (FOOB's) to PRT's and CAT's in which consortia of outside users build, own and operate the beamlines. Each facility has a mixture of FOOB's and PRT/CAT's although, for example SSRL is overwhelmingly FOOB's while the APS is exclusively CAT's albeit with some of these entirely facility owned. This diversity seems to serve the community well provided that the PRT/CAT beamlines are properly maintained and operated and that appropriate support is provided to outside users. This turns out to be an emerging problem at the NSLS and one of our funding recommendations is aimed at ameliorating this situation. Otherwise, we do not recommend any significant changes in the current FOOB-PRT/CAT system.

As noted above, the panel believes that all four D.O.E. synchrotrons are essential to the national scientific and technological enterprise. The panel was very impressed by the outstanding performance of the second generation facilities, by the number of users they serve well, by their ability to renew and improve themselves, by their ability to continue cutting-edge research even though the storage rings themselves are not the most advanced, by their commitment to education, and by their abilities to engage new users and address new problems. Given the outstanding track record and clear vision demonstrated by these facilities, the panel expects these facilities to continue to thrive scientifically in a cost-effective manner. These centers are national resources and they should be adequately funded, upgraded and modernized in a timely fashion to serve better the national needs.

These second-generation facilities will complement the third generation synchrotron sources by providing first-rate x-ray capabilities for a very large number of users whose experiments are not brightness limited. Furthermore, these x-ray capabilities are reinforced by the large number of existing beamlines, end stations, detectors, as well as time-tested user support mechanisms and user support teams. This combination of x-ray capability and the support infrastructure will continue to allow the users to do cutting-edge science.

The APS is newly commissioned and therefore it is difficult to evaluate at this time the full impact of the research which will be carried out there. It is clear, nevertheless, that it will be the premier hard x-ray facility in the U.S. and indeed the world for the foreseeable future. The panel was impressed by the APS's ability to build the facility and achieve the design capability "on-time and on-budget." The CAT system has attracted of order 1000 participants from 85 U.S. universities, 32 industries and 25 research laboratories. The CATs will operate 40 of the 68 available beamlines. Continual development and implementation of the remaining 28 beamlines will occur over the next five to ten years given adequate funding. It is essential that these beamlines be properly funded by D.O.E. and other sources. We believe that a number of the open sectors should remain undeveloped until at least the first generation of experiments are completed so that one can assess any new and unexpected scientific and technological opportunities.

The ALS is a third generation synchrotron radiation user facility of very high brightness optimized for the UV and soft x-ray regions. It will be the U.S.'s premier UV and soft x-ray source for the foreseeable future. Again the ring was built "on-time and on-budget." In contrast to the APS which has only two international competing facilities (ESRF in France and Spring-8 in Japan), the ALS will have at least 7 international competitors. Currently 16 out of a total of 80 possible beamlines have been instrumented. To-date the ALS user community is relatively small, 7% of the U.S. total, and more than one third of the users come from Lawrence Berkeley National Laboratory itself. There seems to be limited participation in ALS research by U.C. Berkeley faculty. It appears that since the time of the Seitz-Eastman report, important scientific issues which require UV radiation have decreased in number compared to those which require hard x-rays; the UV community has correspondingly decreased in relative size now representing only about 15% of the total community. The ALS must therefore be very aggressive in seeking out new scientific opportunities and it must cooperate more effectively with its existing user community in this endeavor. On the other hand, the ALS has an impressive industrial research program centered on the needs of the semiconductor-microelectronics, magnetic storage and bio-technology companies in Silicon Valley and the San Francisco Bay Area.

It is a truism in scientific research that significant increases in scientific capability, be it a factor of ten in temperature, pressure, or instrumental resolution etc. inevitably yield new and unexpected science. This has certainly been true of x-ray sources as demonstrated by the results reviewed in section 5 of this report. It appears likely that "fourth generation" x-ray sources will be based on the free electron laser concept. If successful this technology could yield improvements in brightness by many orders of magnitude. It is our strong view that exploratory research on fourth generation x-ray sources must be carried out and we give this item very high priority.

Before coming to our detailed funding recommendations we have two observations about the overall budget situation. First, normalized U.S. expenditures are on average comparable to those of other G7 countries and lower than those of some countries such as Switzerland and Taiwan. It is evident, therefore, that if U.S. investment in this field does not at least increase with inflation, then we will rapidly lose our leadership position in this most important field. Second, as we have emphasized throughout this report, one of the most impressive features of current synchrotron radiation research is its remarkable diversity. One might therefore expect that the sources of research support would be equally diverse. This is in general true for the PRT/CAT beamlines and other ancillary facilities. However, the full operations costs of the four synchrotrons are supported exclusively by D.O.E./BES. We, therefore, considered whether or not for example if 30% of the research carried out at the synchrotrons is in the life sciences, should not NIH provide 30% of the operating costs. This would certainly mitigate the D.O.E. funding problems. After extensive discussions, we concluded that this is not practicable. D.O.E. has considerable expertise and experience in the management of large national facilities that is not found in other agencies. The stewardship role played by D.O.E. of its synchrotron facilities has been outstandingly effective and ensures that only one agency has responsibility for the efficient operation of these facilities. D.O.E./BES should take political advantage of the broad and successful impact of its facilities, especially in health-related fields, to increase its own base budget. We do, however, recommend diversification of the funding sources for special initiatives such as the proposed SSRL and NSLS upgrades.

We now discuss our explicit recommended funding priorities. We preface this by emphasizing that the committee concludes unanimously that shutdown of any one of the four D.O.E./BES synchrotron light sources over the next decade would do significant harm to the nation's science research programs and would weaken our international competitive position in this field.

Recommended Funding Priorities

The committee has divided its recommendations for on-going funding of the facilities into three sections. The three sections are in priority order, but all items within each section have the same priority. We have separately evaluated the requests for upgrades by SSRL and NSLS. Since the requisite funding for these upgrades need extend only over three years, we treat this recommendation on a different basis.

Priority 1

The panel recognizes the extreme importance of operating effectively the three hard x-ray sources for their very large user communities as well as the importance of a modest investment in research and development of a fourth generation x-ray source. The recommended funding levels for FY98 are as follows:

A.	SSRL	$21.0M
B.	NSLS	$33.8M ($3M increase)
C.	APS	$84.7M
D.	4th Generation X-ray Source R&D	$ 3.0M

The SSRL and APS figures are the FY98 DOE requests. The NSLS figure is increased by $3.0M above the FY98 DOE request figure. The panel recognizes the dire need for increased general user support at the NSLS PRT beam lines. The $3.0 M is to be used by NSLS to fund user support personnel for the PRT beamlines to facilitate their use by general users. Items A., B. and C. must increase at least at the rate of inflation for these facilities to remain viable. For item D, we recommend that the actual distribution of the 4th generation x-ray source research funds be determined by another panel made up of potential users, accelerator and FEL physicists. The present panel suggests a focused approach to this development given the limited funding available. This funding should extend over five years.

Priority 2

The second set of priorities concerns the development of CAT beamlines at the APS and he modernization of PRT and facility beamlines at the NSLS.

A.	APS front ends	$ 4.0M
B.	APS facility beamlines	$ 4.0M
C.	NSLS PRT and facility beamlines	$ 3.0M

The APS should be provided with $4M per annum to develop the insertion devices and front ends for the remaining sectors. In addition, the APS should be provided with $4M per year o develop facility CAT beamlines; this should make possible the development of one facility sector every two or three years. Funding for outside user APS CAT beamlines should be raised through he normal peer review process. $3M per annum should be provided to modernize and upgrade facility and PRT beamlines at the NSLS. These $3M should be distributed both through the facility and directly to the PRT community itself via a competitive peer review process in consultation with the facility.

Priority 3

The ALS as a third generation source provides the highest brightness in the UV/soft x-ray range. The panel recommends funding at the DOE's requested FY98 level.

A.	ALS	$35.0M

2nd Generation Facility Upgrades

Both SSRL and NSLS have proposed upgrades which, in the view of the panel, would be very cost effective. The panel recommends:

A.	NSLS	$12M per annum for 3 years
B.	SSRL	$15M per annum for 3 years

It is recommended, however, that the funding for these upgrades should be carried out under a special initiative which is separate from the routine budgeting process. For example, BES might seek partnerships with other divisions within DOE and with other agencies such as NIH for these upgrades. Alternatively, the funding for the upgrades could appear as a 3 year add-on or "spike" analogous to the peak in the overall BES synchrotron budget in 1994 due to the construction of the APS.

In the above prioritization scheme, the priority of this recommendation is 2.5, that is, intermediate between priority 2 and priority 3, for funding beyond 1998.

Funding of priorities 1, 2, and 3 requires a total of $188.5M per annum in FY98 dollars. This represents an increase of 11% over the requested FY98 budget; we note that the budget in FY94 was $224.2M. We believe that funding at the level of $188.5M per year for the four DOE synchrotron facilities is fully justified and indeed is required for the U.S. to retain its leadership role in this most important field. At the same time, upgrade and modernization of the second generation facilities are essential. In the event of inadequate funding levels, the facilities should be funded in the priority order given above.

Finally, we have not attempted to prioritize requests beyond those listed above. In the event of an unexpectedly generous Federal largesse for DOE synchrotron research, there are additional opportunities put forward by each of the facilities which would strengthen even further synchrotron research in the United States.

Appendix A

Charge Letter from Dr. John Stringer to Dr. Robert Birgeneau

EPRI
Electric **Power**
Research Institute
Powering Progress through Innovative Solutions

April 25th, 1997

Professor Robert Birgeneau
Dean of Science
Department of Physics
Massachusetts Institute of Technology
Cambridge, MA 02139

Dear Bob:

The Basic Energy Sciences Advisory Committee has been asked by Dr. Martha Krebs to help in the reassessment of the need for and the opportunities presented by each of the four synchrotron light sources operated by the Office of Basic Energy Sciences. She has asked us to report to her by the end of September. To that end she has asked us to assemble an expert balanced panel, and I am delighted that you have accepted the demanding task of convening and chairing it.

As part of the panel's work, it would be desirable to visit each of the four synchrotron light sources and meet with members of the management, staff, and user communities.

We would specifically like the panel to address the following issues and questions:

1. What has been the scientific impact of synchrotron radiation-based research during the past decade, and what is it expected to be during the next decade?

2. What is the scientific and technological demand for synchrotron radiation? From what fields and sectors? Who are the newcomers? How has the demand changed since the 1984 Seitz-Eastman report, and how might it change in the future? Please provide quantitative information whenever possible, e.g., how has structural biology, geosciences, environmental sciences, or x-ray microscopy changed during the past decade at the various light sources?

3. What is the user demand at each of the Department of Energy (DOE) synchrotron light sources? What is the distribution of users? Are there special needs served (e.g., scientific, industrial, geographical) at the different light sources, and, if so, are these needs growing or declining?

4. What is the expected future capability of each synchrotron light source over time? How do the capabilities complement one another?

5. What does each light source see as its own vision of the future? How do the visions complement each other? How well do the visions accommodate potential changes found in- item 2?

6. In a constant budget scenario, what is the appropriate level of research and development (R&D) funding for efforts related to continuously improving current facility operations such as accelerator R&D, the design of insertion devices, the design of advanced instrumentation, etc.? How should these funds be apportioned between the facilities themselves and the user community, including the broader accelerator R&D community? What is the priority between support for such R&D and direct support for users?

7. In a constant budget scenario, what level of investment should DOE/Basic Energy Sciences (BES) make in R&D for fourth-generation synchrotron sources and how should this effort be distributed among the facilities and other research sectors?

8. In a constant budget scenario, is the level of DOE/BES support of synchrotron radiation- related research for users and user-controlled beamlines appropriate and, if not, how should it be changed?

9. If additional funds were available to DOE/BES, should they be invested in items 6, 7, and 8 and, if so, what should the priority be among them?

10. What would be the consequences of the shutdown of one or more of the four DOE/BES synchrotron light sources?

The Committee believe that this is a most important task, and we believe that the report will play a key part in the evolution of synchrotron radiation in this country for some years. Once again, I am very grateful to you for your help, and I look forward to the panel's report.

Sincerely,

John Stringer,
Chairperson, Basic Energy Sciences Advisory Committee

FAX: (415) 855-2287
e-mail: jstringe@epri.com

Appendix B

Information Requested from the Facilities

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
School of Science, 6-123
77 Massachusetts Avenue
Cambridge, Massachusetts 02139-4307

Robert J. Birgeneau
Dean of Science
Cecil and Ida Green Professor
of Physics

phone: 617-253-8900
fax: 617-253-8901
e-mail: robertjb@mit.edu

MEMORANDUM

TO: BESAC Synchrotron Panel

FROM: Bob Birgeneau
MIT, 6-123

Z.-X. Shen
Stanford, McCullough 232

DATE: June 4, 1997

RE: **Scientific, Technical, Educational and Budgeting Information to be provided by each Facility to the BESAC Synchrotron Panel**

Enclosed is a list of questions that should be answered by each facility. This information should be provided to the panel members at least one week in advance of each site visit.

1. Scientific Impact: Document the scientific impact of research carried out at your facility during the past decade. Give the total number of publications for each year plus the number of articles published in Physical Review Letters, Nature and Science. Provide a complete publication list for FY96. Give the five most significant contributions based on research carried out at your facility as well as your view of the five most important contributions of synchrotron radiation overall.

2. Future Science: Discuss the manner in which the science done at your facility is likely to evolve over the next decade; for example, what is the probable distribution of users one decade from now between biology, materials science, chemistry, etc.? How will these changing needs impact the relative demand for radiation across the

electromagnetic spectrum from IR to hard x-rays? Are specific theoretical developments needed to facilitate the optimum use and scientific productivity of your facility?

3. Technical Impact: Document the impact on technology of research and development carried out at your facility during the past decade. If possible, give the total number of technical publications and patents. Discuss the likely evolution of industrial / technological research at your facility over the next decade.

4. Education: Document the educational impact of your facility over the past decade including the number of Ph.D. theses based on research carried out at your facility. Give information on direct support which your facility provides to graduate students and, if appropriate, undergraduates.

5. Users: Document user demand at your facility for the past decade; here a “user” is defined as a person who actually showed up at least once to do an experiment each year. Provide data on the distribution of users over different fields of science and technology and over the different regions of the electromagnetic spectrum (IR, UV, X-ray). Also provide data on user distributions between academia, industry and government laboratories. Finally, provide data on the geographical distribution of your facility users both national and international.

6. Budgets: Give budgets for FY97 and FY98 including breakdown of costs and staff associated with:
   a) operation and maintenance of accelerator/ring and insertion devices
   b) operation and user support of instrumentation, including scientists and technical engineering staff.
   c) any research efforts funded by the facility budget.
   d) equipment budget.
   e) administrative/clerical costs.
   f) funding from other agencies

7. User and Facility Beamlines: Document in detail PRT/CAT beamlines together with facility beamlines at your facility at present and, where appropriate, as anticipated over the next decade. If additional funds are available, how will you strengthen/rearrange the

PRT/CAT organizations? What level of funding is required to produce state-of-the-art beamlines at all of your facility's ports?

8. Machine Issues: Document machine developments over the past decade including beam quality improvements and insertion devices. What are the machine improvement plans at your facility for the next decade?

9. Fourth Generation Sources: Describe efforts at your facility contributing to Research and Development of 4th generation synchrotron sources; what level of investment in advanced source development is appropriate at your facility currently and in the future?

10. Flat Budget: How would you would organize your facility and activities if faced with a flat budget (no inflation) for the next 5 years.

11. Increased Budget: Describe new initiatives which you would undertake if your overall budget was increased by 20% above inflation over the next five years.

12. Facility Shutdown: What are the likely irreversible consequences of shutting down your facility?

Appendix C

Program of May 9-10 General Information Meeting

PROGRAM

BESAC PANEL ON SYNCHROTRON RADIATION SOURCES AND SCIENCE

Inaugural Meeting
May 9-10, 1997

Massachusetts Institute of Technology
Room 34-40 1

9May

8:30 a.m.	Continental Breakfast	
9:oo - 10: 15 Process	Robert J. Birgeneau	Welcome and Outline of and Procedures
	John Stringer	Committee Charge
	Patricia Dehmer	Perspectives from the Office of Basic Energy Services
10:15 - 10:30	Coffee Break	
10:30 - 11:00	Executive Session	

Facility Presentations

11:00 - 11:30	NSLS	Michael Hart
11:30 - 12:00	SSRL	Arthur Bienenstock
12:00 - 1:00 p.m.	Lunch (sandwiches provided)	
1:00 - 1:30	ALS	Brian Kincaid
1:30 - 2:oo	APS	David Moncton

Reviews of International Facilities		**Speakers**
2:00 - 2:30	U.V.	Ingolf Lindau
2:30 - **3:00**	X-rays	Jochen Schneider
3:00 - 3:20	Coffee Break	

National Facility Issues

3:20 - 3:30	HERAC/ BIOSYNC Activities	Keith Hodgson
3:30 - 4:30	User Issues	David Shuh, Lou Terminello Mark Sutton, Peter Stephens
4:30 - 5: 15	Machine Issues	Facility Directors' Roundtable
5: 15 - 6:00	Beamline Issues	Facility Directors' Roundtable
6:30 p.m.	Dinner - Royal East Restaurant	

May 10

8:00 a.m.	Continental Breakfast	

Science and Technology Reviews

8:30 a.m. - 4:15 p.m.		**Speakers**
8:30	Solid State Physics/Magnetism	Sunil Sinha
9:00	Soft Condensed Matter / Biophysics	Cyrus Safinya
9:30	Materials Science	Slade Cat-gill
lo:oo	Coffee	
10:30	Photoemission / Electron Spectroscopy	Jim Allen
ll:oo	AMO	Bernd Crasemann
11:30	Geosciences	Mark Rivers
12:oo	Lunch/Executive Session	
l:oo	Chemical Sciences / Surface Sciences	Anders Nilsson
1:30	Structural Biology	Steve Harrison
2:oo	X-ray Microscopy / Molecular & Environmental Sciences	Brian Tonner
2:30	Circuits / Electronic Materials	Jim Harper

3:00	Coffee	
3:15	Biotechnology	Tony Kossiakoff
3:45	Other Industrial Applications	Richard Harlow

Executive Session - 4:15 - 5:15 p.m.

Adjournment - 5: 15 p.m.

Appendix D

International Facilities

Appendix D International Facilities data were provided by H. Winick and A. Robinson and incorporated into this report as received.

SYNCHROTRON RADIATION FACILITIES OUTSIDE THE U.S.

Outside the U.S. there are about 35 storage rings in operation for research with synchrotron radiation in 13 countries. This includes two third-generation rings comparable to the APS at Argonne (the multi-national 6 GeV ESRF constructed in France at a cost of ≈$800M and the 8 GeV Spring-8 constructed in Japan at a cost of ≈$1B) and four 1 S-2 GeV third-generation rings comparable to the ALS at Berkeley (in Italy, Korea, Sweden and Taiwan ranging in cost from ≈$35M to ≈$185M).

Eleven rings are under construction including third-generation 1.5-2.5 GeV rings in Germany, Japan, and Switzerland at costs ranging from ≈$50M to ≈$110M. About 15 more rings are in various stages of design but are not yet funded. Three of these are 2-3 GeV third-generation rings for which funding approval is expected in the near future in Canada, China, and France with projected construction costs ranging from ≈$85M to ≈$233M.

To compare the level of activity and investment in synchrotron radiation research abroad with that in the U.S., we attempted to collect data from foreign facilities. A questionnaire was sent to these facilities soliciting detailed information about costs and other data for construction, operations, administration, beamlines, in-house research, outside users, graduate students, publications, etc. Unfortunately the response was poor. Those who did respond generally filled in only parts of the questionnaire and interpreted the questions differently. For example, although data were supplied on the initial construction costs of many rings, it is difficult to use these numbers for comparisons since the various countries compute their construction costs differently. Items such as staff salaries, land costs, overhead, administrative costs, and industrial contributions are handled differently in different countries. For this reason, the construction costs quoted above are given as approximate numbers, although they are the costs reported by the facilities themselves. Because of these differences and the incompleteness of our data, it became clear that meaningful comparisons on the many topics on which we solicited data would be difficult.

In an attempt to develop some measure of the relative support for synchrotron radiation research, we focused on a single item - operations costs for each country for its national facilities. For countries participating in the ESRF, we included the funds provided for their share of ESRF operation in their total synchrotron expenditures per annum. We tried to minimize the differences in accounting procedures in the different countries by including salaries and overhead as consistently as possible, going back to original sources as needed to clarify these points. The results are presented in Table D. 1 below. In addition to the costs themselves, we also present costs normalized to the population and gross national product of each country considered. In addition, we include the number of user facilities supported by each country, counting the ESRF as one facility for each member country.

A complete list of synchrotron radiation sources in operation, construction, and design is included as Table D.2 at the end of this report.

OBSERVATIONS

We offer several observations based largely on the statistics presented in Table 1. We consider the most meaningful comparisons to be those among the G7 countries, and have emphasized those below.

TABLE D.1. STATISTICS ON SYNCHROTRON LIGHT SOURCE OPERATION COSTS—USA AND INTERNATIONAL

Country	GNP, billion $[1]	Population, millions [2]	Number of Synchrotron Light Rings3	Total SR Operations, million $ [4]	Operations Cost/GNP, x 10^6	Operations cost per Capita, $
G7 Nations						
USA[5]	6,740	250	9	183	27	0.73
Japan6	4,690	125	9	126	27	1.01
Germany7	1,910	8	6"	55.5	29	0.68
France8	1,317	58	3 ”	41.0	31	0.71
Italy[9]	1,134	57	2"	32.6	29	0.57
UK[10]	1,040	58	2 *	41.8	40	0.72
Canada1 [1]	574	29	1	8.7	15	0.30
Total G7	17,405	658		488.6	28	0.74

*Includes ESRF as one source.

TABLE D.1. STATISTICS ON SYNCHROTRON LIGHT SOURCE OPERATION COSTS-USA AND INTERNATIONAL

Country	GNP,. billion $ [1]	Population, millions [2]	Number of Synchrotron Light Rings[3]	Total SR Operations, million $ [4]	Operations Cost/GNP, ¥ 10^6	Operations Cost per Capita, $
Non-G7 Europe						
Spain[12]	533	39	2 ”	10.5	20	0.27
Netherlands [13]	316	15	1 *	1.88	5.9	0.12
Switzerland[14]	254	7	2 *	17.8	70	2.54
Sweden[15]	216	8	3 *	4.44	20	0.56
Belgium[16]	213	10	1 *	1.88	8.8	0.19
Denmark[17]	137	5	2 ”	1.82	13	0.36
Norway [18]	115	4	1 *	0.35	3.0	0.09
Finland[19]	96	5	1 *	0.4	4.2	0.08
Non-G7 Asia						
Korea[20]	337	44	1	18.1	54	0.41
Taiwan[21]	245	21	1	20.4	83	0.97
Non-G7 Americas						
Brazil [22]	472	155	1	5	11	0.03
Total non-G7	2,934	313		82.6	28	0.26
Grand Total	20,339	971		571.2	28	0.59

*Includes ESRF as one source.

TABLE D.1. FOOTNOTES

[1] Source: 1997 Encyclopedia Britannica. Figures are for 1993, except 1994 for USA, Japan, France, and Taiwan.

[2] Source: 1997 Encyclopedia Britannica. Figures are for 1995.

[3] Number of synchrotron light source rings in operation, under construction, and expected to be approved. For European countries contributing to the European Synchrotron Light Source (ESRF) in Grenoble, France, ESRF is counted once for each country. Industrially operated rings are not included.

[4] Costs were provided by facilities in each country. If necessary, figures were converted to US$ at current (September 1997) exchange rates. No data were received from facilities in India, The People's Republic of China, or the Former Soviet Union (Russia, Ukraine, and Armenia). Projected operations expenses for the Siam Photon Source in Nakhon Ratchasima, Thailand, were not available.

Total operations costs for each country include facility expenditures for operations and, for European countries, national contributions to the ESRF. Operations costs variously cover accelerator improvements, accelerator operations/maintenance, improvements to existing beamlines, beamline/experimental station operation/maintenance, in-house research, in-house research on future facilities, user support, proposal review, personnel, facility administration, and overhead, but not every facility provided costs for all categories. Operations costs do not include new beamline and experimental station construction.

Total ESRF operations and improvements expenses for 1997 are $62.8 million. Percentage contributions toward ESRF operations are: France 27.5%, Germany 25.5%, Italy 15%, UK 14%, Benelux (Belgium and the Netherlands) 6%, Spain 4%, Switzerland 4%, and Nordsynch (Sweden , Denmark, Finland, and Norway) 4%. The Benelux contribution is split equally between the two countries. The Nordsynch contribution is split 41.5%, 28.5%, 16%, and 14% in the order listed.

Costs in cases where a new facility is under construction and will replace or partially replace an older one are explained in subsequent notes.

[5] The total includes the four DOE-funded facilities (ALS, APS, NSLS, and SSRL), two NSF-funded facilities [University of Wisconsin Synchrotron Radiation Center (Aladdin) and Cornell High Energy Synchrotron Source (CHESS)], the CAMD facility at Louisiana State University, and the SURF facility at the National Institute of Standards and Technology (NIST).

[6] The total includes the Photon Factory in Tsukuba, Spring-8 in Kamigori, and UVSOR in Okazaki. No operations costs were available for facilities at the Electrotechnical Laboratory (NIJI II, NIJI IV, and Teras) in Tsukuba, HISOR in Hiroshima, and Suburu in Himeji. Costs for industrially operated facilities (Sumitomo, NTT, Mitsubishi, IHH) are not included.

[7] The total includes DELTA at the University of Dortmund and HASYLAB at Hamburg, projected costs of ANKA at Karlsruhe (estimated to be operational in 2000) and BESSY II in Berlin (estimated to be operational in 1999), and the ESRF contribution. It does not include expenses for BESSY I in Berlin, which will be replaced by BESSY II. It also does not include the synchrotron at the University of Bonn. HASYLAB is an integral part of the DESY laboratory, which is primarily a high-energy physics laboratory; the HASYLAB costs were estimated as a percentage of total DESY operations.

TABLE D.I. FOOTNOTES (CONTINUED)

[8]The total includes operations/improvement expenses for the LURE source at Orsay and the ESRF contribution. It does not include expenses for the Soleil source (projected to become operational in 2003 but site not yet determined), which will largely, but not completely, replace LURE. The Soleil operations costs are expected to exceed those of LURE somewhat.

[9]The total includes the Sincrotrone Trieste (ELETTRA) and the ESRF contribution. Costs for the synchrotron radiation operations at the Daphne facility at the Frascati laboratory in Rome, from whom no data were received, are not included.

[10]The total includes the Synchrotron Radiation Source (SRS) at the Daresbury Laboratory and the ESRF contribution.

[11]The total includes projected costs of the Canadian Light Source (CLS) at Saskatoon, Saskatchewan. Additional costs for Canadian beamlines at the University of Wisconsin Synchrotron Radiation Center (Aladdin) at Stoughton and at the APS at Argonne are not included.

[12]The total includes projected costs of the Barcelona Light Source (LSB) and the ESRF contribution.

[13]The total includes only the ESRF contribution.

[14]The total includes projected costs of the Swiss Light Source (SLS) at the Paul Scherrer Institute in Villigen (estimated to begin operations in 2007) and the ESRF contribution.

[15]The total includes the Max Laboratory (which has two storage rings Max I and Max II) at the University of Lund and the ESRF contribution.

[16]The total includes only the ESRF contribution.

[17]The total includes the Institute for Storage Ring Facilities (ISA) at the University of Aarhus and the ESRF contribution.

[18]The total includes only the ESRF contribution.

[19]The total includes only the ESRF contribution .

[20]Operations expenses for the Pohang Light Source in Pohang.

[21]Operations expenses for the Synchrotron Radiation Research Center (SRRC) in Hsinchu.

[22]Operations expenses for the National Synchrotron Light Laboratory (LNLS) in Campinas.

OBSERVATIONS

We offer several observations based largely on the statistics presented in Table 1. We consider the most meaningful comparisons to be those among the G7 countries, and have emphasized those below.

(a) The annual synchrotron facilities operating costs normalized to the GNP for the G7 countries are remarkably constant, averaging 28 x 10^{-6} for all countries except the UK and Canada. The normalized cost for the UK is higher (40 x 10^{-6}), whereas it is lower for Canada (15 x 10^{-6}).

(b) The annual synchrotron facilities operating costs normalized to the population for each G7 country ranges from a low of \$0.30 per capita (Canada) to a high of \$1.01 per capita (Japan), with an average value of \$0.75 per capita per annum. The annual per capita operating costs, or projected operating costs, for other countries considered in this survey range from \$0.03 for Brazil, which commissioned its first synchrotron facility (LNLS) in 1996, to a projected cost of \$2.54 per capita per annum for Switzerland, which recently approved the construction of a new synchrotron facility (SLS). The average per capita cost per annum for non-G7 countries that have or plan to construct major synchrotron facilities is \$0.26, which is three times less than the G7 countries spend per capita per annum.

(c) The U.S.A. annual synchrotron operating cost relative to the GNP or per capita is roughly the same as the average of the G7 countries; our per capita expenditures are below that of Japan and comparable to the average of the European G7 countries (\$170.9M annual operating costs, 254M people, \$0.67 per capita).

(d) The number of synchrotron radiation facilities in the G7 countries ranges from nine for Japan and the U.S.A. to one projected for Canada. Not included in the number for Japan are NIJI-IV at the Electrotechnical Laboratory, which is primarily used for FEL R&D, the AR Ring at KEK in Tsukuba, which may be rebuilt as a dedicated light source, and four or more rings operated by industry. Not included in the U.S. number are the FELL ring at Durham, which is primarily used for FEL R&D, and one ring operated by industry.

(e) The number of primarily hard x-ray synchrotron facilities in operation and under construction (those operating at an energy ≥ 2.5 GeV) is -13, whereas the number of primarily soft x-ray facilities in operation or under construction (< 2.5 GeV) is -20, including all countries considered in this survey. The modifier “primarily” is used above because many soft x-ray sources in the energy range around 2 GeV also generate useful hard x-rays (e.g., DCI at Orsay, SRS at Daresbury, and PLS in Korea). Similarly, hard x-ray sources such as SSRL and HASYLAB, operating at 3 GeV or above, have many soft x-ray/VUV experimental stations. All of the primarily hard x-ray sources are located in G7 countries. The fact that non-G7 countries have constructed only lower energy, primarily soft x-ray sources is undoubtedly related to the significantly lower construction cost of such facilities (≈\$36M to ≈\$106M for third-generation facilities such as Max II and SLS). In contrast, the present third-generation hard x-ray facilities (ESRF, APS, and SPring-8) had construction costs ranging from ≈\$800M to ≈\$1B.

(f) Our observations indicate that the hard x-ray user base in most countries is generally larger than the soft x-ray user base. Thus, although most of the smaller countries have opted for less expensive soft x-ray sources, they have subsequently pushed them to higher operating energies to generate harder x-rays. For example, the SRRC facility in Hsinchu, Taiwan, the PLS in Pohang, Korea, and ELETTRA in Trieste, Italy, all operate mostly at the highest achievable electron energies, although they were originally optimized for lower energy operation. It is also interesting to note that the ALS facility at LBNL, optimized at 1.5 GeV, now operates about two-thirds of the time at 1.9 GeV. The improved lifetime at higher operating energy is also a factor in these changes in operating conditions.

TABLE D.2. STORAGE RING SYNCHROTRON RADIATION SOURCES
(Sept., 1997)

LOCATION	RING (INST.)	ELECTRON ENERGY (GeV)	NOTES
BRAZIL			
Campinas	LNLS- 1	1.35	Dedicated
	LNLS -2	2.0	Design/Dedicated
CANADA			
Saskatoon	CLS (Canadian Light Source)	2.5-2.9	Design/Dedicated
CHINA (PRC)			
Beijing	BEPC (Inst. High En. Phys.)	1 S-2.8	Partly Dedicated
	BLS (Inst. High En. Phys.)	2.2-2.5	Design/Dedicated
Hefei	NSRL (Univ.Sci.Tech.of China)	0.8	Dedicated
Shanghai	SSRF (Inst. Nucl. Res.)	2.0-2.5	Design/Dedicated
CHINA (ROC-TAIWAN)			
Hsinchu	SRRC (Synch.Rad.Res.Ctr.)	1.3-1.5	Dedicated
DENMARK			
Aarhus	ASTRID (ISA)	0.6	Partly Dedicated
	ASTRID II (ISA)	1.4	Design/Dedicated
ENGLAND			
Daresbury	SRS (Daresbury)	2.0	Dedicated
	DIAMOND (Daresbury)	3.0	Design/Dedicated
	SINBAD (Daresbury)	0.6	Design/Dedicated
FRANCE			
Grenoble	ESRF	6	Dedicated
Orsay	DCI (LURE)	1.8	Dedicated
	SuperACO (LURE)	0.8	Dedicated
	SOLEIL (LURE)	2.15	Design/Dedicated
GERMANY			
Berlin	BESSY I	0.8	Dedicated
	BESSY II	1.7-1.9	Dedicated*
Bonn	ELSA (Bonn Univ.)	1.5-3.5	Partly Dedicated
Dortmund	DELTA (Dortmund Univ.)	1.5	Dedicated/FEL Use
Hamburg	DORIS III (HASYLAB/DESY)	4.5-5.3	Dedicated
	PETRA II (HASYLAB/DESY)	7-14	Partly Dedicated
Karlsruhe	ANKA	2.5	Dedicated*
INDIA			
Indore	INDUS-I (Ctr. Adv. Tech.)	0.45	Dedicated*
	INDUS-II (Ctr. Adv. Tech.)	2.0-2.5	Design/Dedicated
ITALY			
Frascati	DAΦNE	0.51	Parasitic*
Trieste	ELETTRA (Synch. Trieste)	1.5-2.0	Dedicated

* Under construction as of 9/97

TABLE D.2. STORAGE RING SYNCHROTRON RADIATION SOURCES

LOCATION	RING (INST.)	ELECTRON ENERGY (GeV)	NOTES
JAPAN			
Hiroshima	HISOR (Hiroshima Univ.)	0.7	Dedicated
Ichihara	Nano-hana (Japan SOR Inc.)	1.5-2.0	Design/Dedicated
Kashiwa	VSX (Univ. of Tokyo-ISSP)	2.0-2.5	Design/Dedicated
Kusatsu	AURORA (Ritsumaiken Univ.)	0.6	Dedicated
Kyoto	KSR (Kyoto University)	0.3	Dedicated*
Nishi Harima	SPring-8 (Sci.Tech.Agency)	8	Dedicated
	Subaru (Himeji Inst.Tech.)	1.0-1.5	Dedicated*
Okasaki	UVSOR (Inst. Mol. Science)	0.75	Dedicated
	UVSOR-II (Inst. Mol. Science)	1.0	Design/Dedicated
Sendai	TLS (Tohoku Univ.)	1.5	Design/Dedicated
Tokyo	SOR-Ring (U of Tokyo-ISSP)	0.5	Shut down in 97
Tsukuba	TERAS (ElectroTech. Lab.)	0.8	Dedicated
	NIJI II (ElectroTech. Lab.)	0.6	Dedicated
	NIJI IV (ElectroTech. Lab.)	0.5	Dedicated/FEL Use
	Photon Factory (KEK)	2.5	Dedicated
	Accumulator Ring (KEK)	6	Planned rebuilding
	Tristan Main Ring (KEK)	8-12	Brief Use in 1995
KOREA			
Pohang	Pohang Light Source	2	Dedicated
Seoul	CESS (Seoul Nat. Univ.)	0.1	Dedicated*
NETHERLANDS			
Amsterdam	AmPS	0.9	Planned Use
Eindhoven	EUTERPE (Tech. Univ. Eind.)	0.4	Planned Use
RUSSIA			
Moscow	Siberia I (Kurchatov Inst)	0.45	Dedicated
	Siberia II (Kurchatov Inst)	2.5	Dedicated
Novosibirsk	VEPP-2M (BINP)	0.7	Partly Dedicated
	VEPP-3 (BINP)	2.2	Partly Dedicated
	VEPP4 (BINP)	5-7	Partly Dedicated
	Siberia-SM (BINP)	0.8	Dedicated*
Zelenograd	TNK (F.V. Lukin Inst.)	1.2-1.6	Dedicated*
SPAIN			
Barcelona	Catalonia SR Lab	2.5	Design/Dedicated
SWEDEN			
Lund	MAX (Univ. of Lund)	0.55	Dedicated
	MAX II (Univ. of Lund)	1.5	Dedicated
SWITZERLAND			
Villigen	SLS (Paul Scherrer Inst.)	2.1	Dedicated*
THAILAND			
Nakhon Ratchasima			
	SIAM(Suranaree Univ. of Tech.)	1.0-1.3	Dedicated*

* Under construction as of 9/97

TABLE D2. STORAGE RING SYNCHROTRON RADIATION SOURCES

LOCATION	RING (INST.)	ELECTRON ENERGY (GeV)	NOTES
UKRAINE			
Kharkov	Pulse Stretcher/Synch. Rad.	0.75-2.0	Partly Dedicated
Kiev	ISI-800 (UNSC)	0.70-1.0	Design/Dedicated
USA			
Argonne	APS (Argonne Nat. Lab.)	7.0	Dedicated
Baton Rouge	CAMD (Louisiana State Univ)	1.4	Dedicated
Berkeley	ALS (Lawrence Berkeley Lab.)	1.5-1.9	Dedicated
Durham	FELL (Duke University)	1.0-1.3	Dedicated/FEL Use
Gaithersburg	SURF II (NIST)	0.28	Dedicated
Ithaca	CESR (CHESS/Cornell Univ.)	5.5	Partly Dedicated
Stanford	SPEAR (SSRL/SLAC)	3.0-3.5	Dedicated
Stoughton	Aladdin (Synch. Rad. Center)	0.8-l	Dedicated
Upton	NSLS I (Brookhaven Nat.Lab.)	0.80	Dedicated
	NSLS II (BNL)	2.5-2.8	Dedicated

Appendix E

Evironmental Safety and Health Issues

Note that the subsections in Appendix E Environmental Safety and Health Issues were provided by the individual facilities and were incorporated as received into this report.

Environmental Safety and Health Programs at SSRL

The SSRL Safety Office and Environmental, Safety and Health programs are in place to ensure that both accelerator and experimental research programs are conducted in a manner that will ensure the safety and health of its employees, its users, the public and the environment. Achieving this is carried out by implementation of the SLAC site-wide safety program as well as through the development and implementation of programs specific to SSRL. SSRL's User Safety Program covers conditions or practices that may be unique to specific experiments, non-routine in nature, or new to the facility.

Three fundamental features are inherent in the ability to provide a safe and healthful workplace: 1) identifying hazards; 2) developing engineering solutions to mitigate or eliminate the hazards; and 3) implementing the solutions with emphasis on educating the end user. The User Safety Program in place at SSRL covers all three facets.

The first step in the User Safety Program is the review of new proposals with the intention of identifying possible hazards and the level of risk associated with the hazards. The level of risk ultimately dictates what further safety analysis work will be required before the proposed experiments can be run. The Safety Office and the users work together to determine what safety measures need to be implemented to run the proposed experiments safely. The majority of hazards can be controlled with relative simplicity, however, some experiments may need in-depth analysis, and may need engineering and administrative controls that take months to develop and require multiple layers of approval. The Safety Office must be satisfied that users are trained to handle the specific hazards their experiments present, and that oversight staff who monitor the experiments are knowledgeable concerning the controls being used and can respond to any incident appropriately.

As an example of this process, preparation for actinide experiments took about 18 months from proposal submittal to implementation of the first experiments. During this time, SSRL, in cooperation with the users, Los Alamos National Laboratory (LANL), performed an in-depth safety analysis. The Safety Office investigated the hazards, modeled effects of an accidental release, and quantified the risk of release. A "no release philosophy" was established and based on this, containment systems were developed for sample handling at the beam line and a real time monitoring system was installed. SSRL, SLAC, LANL, and DOE (as well as the local community) were provided with assurances that the experiments would be managed in a manner consistent with the nature of the hazard.

In the case of materials where the risk and consequences of a spill are very well known (such as bio-hazardous samples), the time frame from proposal submittal to actual beam time is considerably shorter. These samples can be fitted under a standard model, and a graded approach, based on the classification of the biohazard, can be used to implement required safeguards. Overall, the most important part of a proactive and dependable safety program is the capability of identifying hazards early in the proposal scheduling process and provide users with solutions that enable them to run experiments efficiently and safely.

Communication and training are major factors in SSRL's User Safety Program. SLAC provides training in basic safety principles and safety awareness for all employees, as well as appropriate specialized in-depth training for individuals with work assignments in hazardous areas. Safety stand-downs are performed annually, affording all personnel time to discuss their safety

safety issues in a small group setting. The combination of targeted training programs and open communications has been the cornerstone of making SSRL a safe and healthy workplace.

To summarize, the SSRL Safety Office provides users and staff with a comprehensive safety program that can analyze hazards, determine risk, and provide engineered and administrative solutions. The Safety Office provides the training, analysis and technical support required to ensure that SSRL's activities and experiments are conducted in a manner consistent with SLAC and DOE ES&H goals. These programs have contributed to the overall excellent safety record of SSRL.

Environment, Safety and Health at the National Synchrotron Light Source

The NSLS commitment has always been to provide the safest possible working environment for the users and staff at the NSLS, consistent with efficient and productive utilization of the facility for scientific research. The basic philosophy which this system embraces is that the staff and users must take ownership of their own safety.

The primary guiding principles of the ESH program are 1) line management from the Chairman to the Associate chairman for ESH, to the staff and users, 2) passive safety provided by radiation interlock systems, 3) administrative controls for configuration control of shielding and other safe working conditions such as lock-out tag-out rules, work permits, and experimental safety approval forms, 4) training of all staff and users at levels commensurate with need based on the workplace hazards, 5) functional testing of all interlocks as a routine part of operations, 6) safety review of all beamline and accelerator physics experiments prior to commencement of work to provide proper planning and work control procedures, 7) formal standing safety committees in the areas of ALARA, Beamline Safety Review, QA, Training, Operations, Interlocks and ESH.

The personnel efforts associated with the ESH program are integrated and allow coordination of: the NSLS Safety Officer responsible for day-to-day operations; the NSLS ESH Coordinator responsible for administrative, regulatory, and coordinating activities of personnel monitoring and facility ESH documentation; the NSLS Safety Engineers responsible for Safety Approval Form reviews and documentation, safety inspections such as Tier I, radiation monitoring, industrial hygiene and hazardous waste programs; and the interactions with the NSLS Operations Section where the Operations Coordinators are directly supervised. The Operations Coordinators provide constant coverage of the experimental areas whenever the machines are operational. They provide the primary safety interactions between the experimental users and the NSLS on all operational safety issues. There are also permanent personnel assigned to the NSLS from the Safety and Environmental Protection Division. They provide coverage of the personnel monitoring system, contact points for industrial hygiene efforts, chemical tracking, hazardous waste removal, etc.

The hardware systems which provide radiation safety are tightly controlled by maintaining strict configuration controls on the shielding, beamlines and accelerators. In addition, all interlock systems are tested on a bi-annual basis. The Interlock Working Group oversees and approves any changes to the safety systems. New beamlines or changes in a beamline configuration or operational parameters are reviewed by the Beamline Review Committee.

Other industrial hazards such as the presence of electrical hardware, chemical toxins and noxious gases, hazardous waste materials, cryogens, high pressures, and biological materials are dealt with on a case by case basis through the reviews of programs and the individual safety approval forms. Whenever a hazard is present in a scientific or accelerator physics experiment, it is reviewed and work control procedures invoked by direct interactions between the NSLS staff and users to assure safety of the experimenters and others at the facility.

Training of the users and staff in safe conduct of work is a continual effort. For the staff the NSLS follows BNL/DOE guidelines for training on radiation and industrial hygiene practices. The users are treated as two categories: those who intend to be at the NSLS longer than 2 weeks are treated as BNL personnel and get all appropriate training; the rest receive NSLS training consisting of some reading, and a safety video followed by an examination. All users of any beamline receive Beam Line Operations and Safety Awareness training. The NSLS Training Coordinator and the Users Administration Office track the training of the users. No personal radiation monitoring badges or NSLS User Identification and Access card is issued unless the basic training has been completed.

Communications on safety issues to users and staff are accomplished through: the weekly NSLS X-ray and VUV user meetings; the ìNSLS Newsletteri; the ìESH Highlightsi whenever issues of immediate concern are learned or lessons learned need distribution; supervisor meetings; NSLS staff meetings and ESH stand-downs; Tier I safety inspections. The NSLS Tier I inspections are designed to evaluate safe operations on the experimental floor, laboratories and office space. Findings and corrections are tracked in a database which will soon be expanded laboratory wide. In addition, the NSLS does yearly ESH self-assessments (Tier II safety assessments) and the findings of those efforts are also tracked.

EH&S POLICY AND PRACTICES AT THE ALS

EH&S administration at the ALS takes place within the LBNL EH&S structure in which all levels of management are delegated the responsibility and authority necessary to implement LBNL's health, safety, and emergency preparedness policies.

The Director has established an ALS EH&S Policy which states that the Advanced Light Source basic EH&S policy is to ensure that all activities are planned and performed in a manner which ensures that every reasonable precaution is taken to protect the health and safety of employees and the public, and to prevent damage to property and the environment. Operations activities are specifically in compliance with DOE Order 5480.19 (Conduct of Operations), DOE Order 5480.25 (Safety of Accelerator Facilities), DOE Order 5700.6C (Quality Assurance), and DOE Order 4330.4A (Maintenance Management Program) with formal documentation of all procedures. Development and updating of requirements, training procedures, and documentation for controlled access to the accelerator areas and experimental areas, operation of the protective interlock systems, operation of experimental end stations, monitoring of radiation levels, and use, storage, and disposal of hazardous, toxic, and carcinogenic chemicals, biologically active and infectious materials, and radioactive materials is emphasized.

The ALS Director has overall EH&S responsibility for the facility and its operations. The primary source of EH&S expertise within the ALS is the EH&S Group, which acts in accordance with applicable DOE orders and the LBNL Health and Safety Manual and coordinates with the LBNL Environment, Health, and Safety Division. There is also an ALS EH&S Committee, whose responsibilities include eliminating threats to the environment and workplace safety and health hazards . The Technical Safety Subcommittee meets as directed by the EH&S Committee to consider EH&S-related matters that require specific technical expertise.

Radiation generated by the accelerators (gamma rays, and neutrons) is confined inside the accelerator tunnels. The radiation around the interlocked high-radiation areas is regularly surveyed. The radiation shielding is highly effective, reducing the radiation fields to safe levels at the outside surface of the shield wall. In the experimental area, the radiation level is well within the levels that are considered safe. The radiation level in the accelerator building is re-measured every time a change in equipment or procedures had the potential to affect the radiation. The Beamline Review Committee reviews all proposed beamlines according to the guidelines contained in the ALS

Beamline Requirements document containing the technical and safety requirements for both facility- and user-constructed beamlines.

As part of the user support and safety documentation and training requirements, an ALS Safety Handbook and a Users Handbook are produced by the Program Support Section and the ES&H Group. An Experimental Form identifies, in advance, all ES&H issues associated with a proposed experiment and to ensure that all ES&H requirements are complied with. All users are required to take safety training before being permitted to perform experiments.

Environmental, Health and Safety at the APS

Since its inception, the APS has given highest priority to assuring the health and safety of employees, users, and visitors, as well as to protecting the environment. The results achieved during the 5-year construction period (September 1991 through September 1996) speak for themselves. During that time, the APS project experienced an average lost-workday accident rate of 1.2 accidents per 200,000 hours worked. During a comparable 5-year period, the average lost-workday accident rate for all DOE-funded construction was 2.9, and that for the U.S. construction industry as a whole was 5.6. From a statistical viewpoint, the construction of a project the size of the APS is expected to involve at least one fatality; the APS had none.

To create and sustain a safe working environment for APS users, the APS treats safety as a line management responsibility that is shared by the CATs. The following are the basic elements of the APS user safety program:

1. The APS reviews both preliminary and final beamline designs, and proposed modifications, to ensure that the CATs incorporate appropriate engineered safeguards into their APS facilities. APS approval is required before installation can begin.

2. Each CAT conducts its activities at the APS in accordance with a written safety plan developed by the CAT and approved by the APS. The CAT safety plan supplements the ANL Environment, Safety and Health (ESH) Manual, which is incorporated by reference, and relevant safety manuals of the CAT member institutions. It describes the CAT's safety policies, organization, and management practices; identifies the hazards to which its users, and other individuals in or near its facilities, may be exposed; and describes how the CAT will control these hazards. The APS has provided a model plan that can be tailored to reflect each CAT's activities and organizational structure. All 14 of the CATS that are currently active at the APS have APS-approved safety plans in place.

3. Users receive appropriate safety training for their activities at the APS. The CATs and the APS share responsibility for this training. "Core" training, required for all APS users, is delivered in a computer-based format by the APS User Office. As of July 22, 1997,423 APS users have completed the core training program. "Sector-specific" training, also required for all APS users, is administered by the CATs; it focuses on communicating specific information needed to implement the CAT's safety plan. In addition, the CATs identify "task-specific" training needs for their personnel and users in accordance with their CAT safety plans. Qualified CAT staff members may perform some of this training themselves; other task-specific training needs are met through courses offered by ANL's Environment, Safety and Health (ESH) Division.

4. Each CAT reviews the safety aspects of all proposed experiments at its beamlines and ensures that appropriate controls are in place before any experiment begins. The APS is developing a Web-based approval process based on a standard Experiment Safety Approval Form, which all the CATs will use.

5. The APS, ANL, and the CATs themselves perform safety oversight of user activities. The APS Floor Coordinators provide informal day-to-day safety oversight, and periodic walk throughs are conducted by the XFD ES&H Coordinator with invited participation by safety specialists from the ANL ESH Division. The CATs receive written recommendations for addressing any concerns that are identified. APS oversight is also an integral part of the above-mentioned experiment safety review process. Finally, the APS has created three “mutual safety assessment groups,” each consisting of representatives from four or five CATs who have agreed to review each other’s safety programs on a rotating basis. The APS has provided these groups with model assessment criteria which they can modify as appropriate. Each CAT is reviewed annually in this fashion and receives a written report (which is copied to the APS) identifying action items and a schedule for completing these actions.