

**Basic Energy Sciences Advisory Committee**

**Subpanel Review of the Advanced Light Source  
at Lawrence Berkeley National Laboratory**

**February 2000**

**U.S. Department of Energy**

**Office of Science**

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# UNIVERSITY OF OREGON

10 March 2000

Dr. James Decker  
Acting Director  
Office of Science  
U.S. Department of Energy  
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Dear Dr. Decker,

I would like to express my appreciation for your attendance and presentation at our Basic Energy Science Advisory Committee (BESAC) meeting last week. It is encouraging to see the proposed budget increases for the Office of Science and Basic Energy Sciences (BES). As a Committee we are committed to helping to make the proposed budget a reality.

At our meeting three Subpanel reports were presented addressing the recent charges given to us by former Director of Science, Martha Krebs. The three reports submitted by the Subpanels pertained to Neutron Scattering in light of the recent shutdown of the High Flux Beam Reactor (HFBR) at Brookhaven National Laboratory (BNL), a review of the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory (LBNL), and a review of the Electron Beam Microcharacterization Centers at Oak Ridge National Laboratory (ORNL), University of Illinois, Argonne National Laboratory, (ANL), and LBNL. The purpose of this letter is to forward to you the reports of these Subpanels and the response of BESAC to these reports. Overall, the BESAC members are supportive of the recommendations of the Subpanels. We are appreciative of the tremendous amount of work that Panelists and BES staff contributed to these important planning and review exercises.

## **Neutron Scattering Research Capabilities**

The purpose of this Subpanel, chaired by Dr. Martin Blume, was to recommend steps to provide the best possible neutron scattering research capabilities in the United States in the near term. Subpanel deliberations took into account the shutdown of the High Flux Beam Reactor at BNL and assumed that the Spallation Neutron Source at ORNL would be operational in a timely manner. The Subpanel was also asked to provide advice on how to properly accommodate the neutron scattering groups at BNL, conditional on their submitting satisfactory long-term plans for programs to be funded by BES.

Neutron scattering is a critical tool in the arsenal of experimental techniques for studying condensed matter systems. It will be particularly valuable for studies in nanotechnology and nanoscience. BESAC is committed to assuring that neutron scattering science in this country retains its world-class standing and to supporting facilities that allow

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scientists to conduct first-rate science in this area. BESAC commends the Subpanel for the high quality of the submitted report, recognizing the short time constraints imposed by the need to assure continuity in the field in light of the HFBR shutdown. BESAC supports the general recommendations of the report that is provided with this letter. However, with respect to the funding recommendations, first BESAC regards these numbers as estimates requiring detailed review. Second, several factors need to be considered before funding decisions are made, including determination of what costs are currently in the FY 2001 budget, the shutdown costs of HFBR, and the anticipated growth in the number of users over the next few years as the other neutron scattering facilities increase their operations. BESAC however felt strongly that any increase for the existing facilities should not come at the expense of core BES programs. The funding for research and instrumentation should be competitive with the core program.

### **Review of the Electron Beam Microcharacterization Centers**

BESAC's charge was to help assess the scientific impact of the nation's need for the Electron Beam Microcharacterization Centers operated by BES. To this end a Subpanel of experts was assembled and chaired by Dr. John Stringer. The four centers considered were the Shared Research Equipment Program at ORNL, the Center for Microanalysis of Materials Research Laboratory at the University of Illinois Frederick Seitz Materials Research Laboratory, the Electron Microscopy Center for Materials Research at ANL, and the National Center for Electron Microscopy at Lawrence Berkeley National Laboratory. The Subpanel visited each of the four centers and met with members of their management, staff and user communities. The recommendations of this group are summarized in the enclosed report. The Subpanel's review was a monumental effort and BESAC expresses its appreciation for the efforts of the committee, the chair and the BES staff.

In general these facilities were found to operate well and produce excellent science. BESAC is supportive of the recommendations found in the report. The recommendations have been carefully derived and attention has been paid to the unique nature of different facilities. BESAC accepted the recommendations provided that any additional funds allocated to these centers as a result of the review be competitive with the core BES program.

### **Review of the Advanced Light Source**

BESAC was charged in August 1999 with reviewing the Advanced Light Source (ALS) at LBNL. The purpose of the review was to examine those issues that were raised by the BESAC report on "DOE Synchrotron Radiation Sources and Science," known as the Birgeneau Report. In particular, BESAC was asked to explore ALS's vision for the future, the quality and diversity of the science program at the facility, the user demand, and the interaction and relationship with the user committee. The Subpanel charged with this study was chaired by Dr. Yves Petroff and consisted of expert scientists from a broad spectrum of scientific areas.

The Subpanel gave an enthusiastic review of the ALS. The response of the management of the ALS to criticism in the Birgeneau Report has led to a restructuring of LBNL to raise the ALS to the divisional level. The user hours have dramatically increased, and the user participation in the ALS decision making process has been welcomed by the users. Most important is the high quality of the science being generated at the ALS. LBNL Director Chuck Shank and ALS Director Daniel Chemla are commended for this impressive turn around. BESAC accepted the recommendations of the subpanel provided that any increase in funding to the ALS as a result of this positive review not come at the expense of the BES core program. Increases in funding for beamlines should be competitive with the core program.

Thank you again for attending our BESAC meeting and giving us your insights into the FY 2001 budget process.

Enclosures  
Sincerely,

/s/ by

Geraldine L. Richmond, Chair  
Basic Energy Sciences Advisory Committee

cc. Iran Thomas, Acting Director of Basic Energy Sciences  
Patricia Dehmer, Acting Deputy Director of the Office of Science  
Sharon Long, BES



# Subpanel Review of the Advanced Light Source (ALS)

Lawrence Berkeley National Laboratory

February 2000

## Subpanel Members:

Yves Petroff, European Synchrotron Radiation Facility (Chair)

Massimo Altarelli, Elettra Synchrotron Light Source

Chris Greene, University of Colorado

Janos Kirz, State University of New York

Richard Smalley, Rice University (BESAC Member)

John Carruthers, Intel Corporation

Doug Rees, California Institute of Technology

Ted Madey, Rutgers University

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## **1.0 Introduction**

The meeting of the Advanced Light Source (ALS) review committee took place at the ALS on February 3-4, 2000. In preparation of the meeting the members of the panel received the Birgeneau Report, the ALS Annual Report, the list of publications ... plus, on the day of the meeting, the photocopies of the transparencies of the presentations.

The goals of the review panel were clearly stated by Pat Dehmer (DOE):

- to check on the quality of the science carried out
- to verify that the management has been able to respond to the criticisms of the Birgeneau committee
- to see if the user demand is fulfilled and if the interaction with the user community has improved
- to explore the scientific vision

During the two days of scientific presentations followed by a tour of the facility and presentation of posters by young scientists, the committee had the opportunity to judge the scientific output of the facility. In addition we met the ALS SAC and the Users Executive Committee.

It is obvious that the LBNL management has reacted very quickly to the criticisms of the Birgeneau report (we will see later that some of these were only partly justified).

The appointment of D. Chemla as Director, the changes made in the management, the elevation of the ALS to divisional status, the increase of links with the University, the interaction with the users and the SAC have dramatically changed the scientific output of the facility.

The outstanding success of the macromolecular crystallography at the ALS (not expected at all for a UV soft x-ray machine) is a nice illustration but we will see later that remarkable science has been produced in many other areas.

## **2.0 Scientific Presentations**

The scientific presentations focused on some recent highlights, but represented only a fraction of the work done at ALS. Here we summarize our impressions of the presentation.



## 2.1 Macromolecular Crystallography at the ALS

Over the past two years, an outstanding program in macromolecular crystallography has been developed on beamline 5.0.2. This beamline has capabilities for rapid data collection at tunable wavelengths for MAD (multiwavelength anomalous dispersion) data collection, and can successfully accommodate small crystals and crystals with large unit cells ( $> 800 \text{ \AA}$ ). To date, over 318 users from 62 research groups have collected data at this facility, resulting in  $> 120$  structures solved, with  $> 40$  determined by MAD phasing methods. A number of these structures have been published in high profile journals. Two of the most significant structures have been the 70S ribosome and the high resolution structure of bacteriorhodopsin, which showcase the capabilities of this beamline. The 70S ribosome work has been conducted by H. Noller's group at UC Santa Cruz in collaboration with T. Earnest at ALS, and these efforts have resulted in structure determinations of the entire bacterial ribosome complexed with mRNA and tRNAs, at resolutions up to 7.8Å. Since publication, the resolution of the data has been extended to 6.3Å. The unit cell dimensions of the crystals used in this study (space group I422) are 507Å x 507Å x 805Å, with one complex (molecular weight  $\sim 2.6 \times 10^6$ ) in the asymmetric unit. It is unquestionably a tremendous technical accomplishment both to collect this data and to use MAD and isomorphous replacement methods for phasing. In the bacteriorhodopsin work, H. Luecke and colleagues at UC Irvine determined the structure of this membrane protein at high resolution (1.55Å) using very small crystals (30-50 microns) and subsequently have obtained detailed structures for intermediates that occur during the mechanism of this light-driven, proton pump.

The capabilities of macromolecular crystallography program at ALS have been quickly appreciated by the structural biology community, as evidenced by both the high demand from users to use this beamline for data collection, and by the surge of interest from outside groups to develop superbend beamlines as PRTs. This interest is fueling a period of substantial growth in macromolecular crystallography at ALS, with eight new beamlines planned, including five that have already been funded. To manage this growth, G. Fleming described the organization of a Berkeley Center for Structural Biology that will be headed by a Division Deputy for Structural Biology who will coordinate these activities, including user support and interactions with associated programs. The proposal to coordinate beamline development to ensure compatibility and standardization is to be strongly encouraged, as are the initiatives to develop both the robotic approaches to crystallization and the computational systems for automated structure determination that will be at the foundation of the high-throughput demands of present day structural biology. The proposal to develop virtual beamlines with SSRL will ensure year-round access to beamtime at West Coast crystallographic facilities, and also represents a potential mechanism for streamlining applications and proposal review for general user beamtime at both facilities that is to be strongly encouraged. One

consequence of the increased activity on structural biology beamlines will be increased demands on user facilities, including both sample preparation and computational facilities, that strongly support the construction of the new ALS users building.

The present beamline for macromolecular crystallography has been outstandingly successful. With the development of the superbend beamlines, ALS is positioned to make continuing and significant contributions in macromolecular crystallography in the areas of large macromolecular complexes and high-throughput structure determination that define the frontiers of macromolecular crystallography.

## **2.2 Magnetic Nanostructures**

The committee was quite impressed by the science reported on by Z.Q. Qiu. The investigation of oscillatory exchange coupling in magnetic-nonmagnetic multilayer systems effectively combines Angle-Resolved Photoemission (ARPES) and Magnetic Linear X-ray Dichroism (MLXD) techniques with a clever use of the growth possibilities offered by MBE technology. This allows a detailed understanding of the role of quantum confinement in the nonmagnetic quantum wells in this important phenomenon. Although each of the techniques has been known and used in multilayers for some time, this example shows how the combined use can open new perspectives. This is a good start for an ambitious program of “spin engineering”, which is undoubtedly risky, but well worth trying.

J. Stohr described spectromicroscopy work with polarized light on the interface between a ferromagnetic and an antiferromagnetic material. He has been one of the leaders in the field of dichroism imaging of magnetic domains and a long time user of SSRL; his current activity at the ALS is a good example of the successful attraction of outstanding users to this facility. His work is promising and is especially interesting for the connections it could open up with the magnetic recording industry. It should develop further when the new spectromicroscope (PEEM 3) becomes operational.

Altogether, the activity in magnetic nanostructures appears vigorous, of consistently high quality, very suited to a third-generation source and with a clear road to the future. It can be ranked excellent.

## **2.3 Strongly correlated materials**

Today ALS has an angular photoemission set-up allowing very high angle and energy resolution (that was obviously missing at the time of the Birgeneau report). Z.X. Shen of Stanford University presented recent data on the electronic structure of the charge ordered states in  $(\text{La, Sr})_2\text{CuO}_4$ : the main goal being to find out if it is related to superconductivity. There are very nice and exciting experimental results. The interpretation is preliminary,

especially concerning the role of the stripes in the superconductivity. However it illustrated the capacity of UV science to obtain important information on the electronic properties of materials.

## **2.4 Dynamics of Liquid Crystals and Magnets**

Transverse coherence is one of the outstanding features of undulator radiation, which grows rapidly with the wavelength. It is therefore particularly important for VUV and soft x-ray sources. Dynamic light scattering and “speckle” scattering are well known techniques for the study of fluctuations in the spatial and temporal domains, well tested in the visible, where lasers are available, and more recently with hard x-rays at NSLS, ESRF and APS. Since the accessible length scale is related to the wavelength used, and the temporal scale to the time required to acquire a diffraction intensity, each spectral region has its own interest and field of application. The ALS users group must be credited for trying the experiment with soft x-rays, which can explore much faster time scales than hard x-rays, but of course only length scales much larger than interatomic distances. It is a straightforward idea, but it probably took some boldness to try it out, because most people would be intimidated by the technical difficulties as well as by the small scattering volume available in the soft x-ray domain, where photoelectric absorption dominates the cross section. The success of the experiment and its applicability to a variety of systems with interesting dynamical properties (among which magnetic systems are especially significant) opens up a new research direction for which the ALS is extremely well suited. It is an activity to be ranked outstanding/excellent.

## **2.5 Microscopy**

### **2.5.1 Polymers and soft matter**

The ALS is an ideal source for studies in spectromicroscopy. The high brightness available can be translated to rapid data collection at high spatial resolution and high energy resolution at the same time. Much of the work in the recent past has concentrated on NEXAFS studies of polymer systems. Both with the Scanning Transmission X-ray Microscope (STXM) on BL 7, and using PEEM II, excellent results have been obtained which illustrate the powerful capabilities of the techniques for the identification of isolated structures, and the observation of pattern formation in confined systems. The lack of beam time on the heavily oversubscribed BL 7 has limited the rate of progress both in instrument development and in scientific investigation. A much more powerful instrument is ready to be installed in this location, and an additional bending magnet beamline dedicated to polymer work is under construction. The new instruments are designed to provide higher spatial resolution and -at least on the undulator line - more rapid data collection. Plans to upgrade PEEM II and to install it at an elliptically polarizing undulator will provide higher spatial resolution and the ability to extend the capability for the study of molecular alignment. With these additional

capabilities and with the scientific talent assembled, this area of investigation should yield a rich harvest of results in the future.

### 2.5.2 Cell biology

The zone plate microscope XM1 has been used for a variety of studies in cell biology. It has unique capabilities in correlating and pre-aligning specimens with a light microscope, and tiling together arbitrary sized specimen fields. With the use of silver enhanced gold labels it can identify the location of structures of biochemical interest. The instrument has been upgraded recently with zone plates, which provide spatial resolution on the order of 25 nm, and the ability to observe cells in a frozen hydrated form without the need for fixation or staining. These improvements make this microscope a very powerful instrument for the study of biological systems. There is now an impressive list of biological investigators lining up to make use of this instrument, which appears poised to make important contributions. As the transverse resolution continues to improve, the need for depth resolution becomes more important. Stereo imaging has already been demonstrated.

## 2.6 Chemical Dynamics and Spectroscopy

The Chemical Dynamics Beamline (9.0.2) presents a number of opportunities that are being successfully pursued by a talented set of users. In molecular photoionization and photodissociation, the VUV generally constitutes *the most* interesting energy range of the spectrum. It is in this range that electrons efficiently absorb light. This is also a range in which the resulting excitation energy can be transferred efficiently into nuclear motions that produce chemical reactions and rearrangements. The research to date clearly has been carried out at an excellent level, and has effectively utilized the unique capabilities of this source.

One arm of the chemical dynamics effort uses the synchrotron radiation to analyze the state distributions and angular distributions of reaction fragments produced by a chemical reaction carried out in a beam-beam collision geometry. Here the high brightness of ALS plays a crucial role in making such experiments viable, because reactants are produced in small numbers. T. Baer's presentation described an experiment on the formation of HCl in collisions between Cl and n-pentane, which capitalizes on the power of this technique. This experiment demonstrated that abstraction processes that remove the H atom from the periphery of the target molecule result in forward scattering of the HCl products. In contrast, head-on collisions that remove an H atom from the molecular end generally result in backward scattering of the resulting HCl.

The high photon flux permits molecular spectroscopic analyses to be carried out with world-record resolution. The resulting gains are clear in the photoionization of free radicals, for instance. One innovative tool that has been implemented to great effectiveness is a harmonic

filter that diminishes the unwanted harmonics by a factor of 10,000. The implementation of pulsed-field ionization or ZEKE techniques has produced beautiful rotationally-resolved spectra in the VUV for a number of species. These techniques have also demonstrated the ability to provide high accuracy information on chemically-critical properties like the hydrogen bond energy in small hydrocarbons.

Among the appealing directions for future ALS studies in this field, the characterization and spectroscopy of clusters seems particularly timely. An expanded presence in the field of combustion and flame diagnostics also makes sense for this facility and deserves continuous effort over the long term. The reactivity of highly-excited molecular ions with other atmospheric diatomics is a difficult but potentially important challenge which occupies a naturally-important part of the future scientific agenda.

## **2.7 Atomic and Molecular Physics**

In atomic and molecular physics, ALS experiments have already capitalized on the high resolution and high brightness of the source to reveal unexpectedly rich dynamics in the photoionization of supposedly simple species like helium, lithium, neon, and argon. The VUV portion of the spectrum remains an exciting challenge for many-body theory. It is an important and fundamental testbed for modern ideas in intellectually challenging subfields like “quantum chaos” in systems with few degrees of freedom. When two or more degrees of freedom are coupled nonperturbatively, as in multiply-excited atomic states, or even single-electron processes in an external field, the theory becomes extremely challenging. Guidance from well-considered experiments still has a crucial role to play in this field. Data needs still drive portions of this field, including the need to provide benchmark tests of modern theoretical descriptions of fundamental atomic and molecular photoionization processes. The experiments in this area have already demonstrated innovation and excellence, and future experiments are eagerly anticipated.

The development of a beamline for photon-ion interactions constitutes one of the most impressive applications of this high-intensity photon source. It is difficult to imagine any other synchrotron radiation facility where high-resolution spectra could now be measured for such a dilute sample of ions. As R. Phaneuf described in his presentation, this beamline has only recently become operational. Initial applications are rightfully aimed at providing benchmark tests of theory in the photoionization of positive ions. To date, theory has been relied upon almost exclusively to determine photoionization cross sections that are needed to model astrophysical environments or terrestrial fusion plasmas. Until now, there have been almost no experimental tests of theory for positive ions. Already, ALS experiments have demonstrated that theoretical methods can successfully treat light elements such as  $O^+$  and  $Ne^+$ , while showing occasionally significant discrepancies that point to where theory requires

improvement. The future planned measurements of negative ions will test nonperturbative theoretical methods far more stringently.

Core-hole spectroscopy in molecular photoionization still is an important in reconstructing and interpreting complex photochemical dynamics. Level shifts reveal the specific chemical environment where an absorption process occurs. Analogous but complementary information is seen in the distortions of the intensity patterns.

Another promising area has been the study of how angular momentum is distributed between an escaping photoelectron and a residual ion. Prior to work carried out at the ALS, the number of experiments that measured orientation of residual photofragments could be counted on one hand. Now the ALS permits such experiments to be carried out continuously as a function of photon energy at high resolution, which expands dramatically the amount of dynamical information that emerges concerning the fragmentation process.

Still on the agenda for the future are a number of promising directions, such as pump-probe experiments that combine the power and flexibility of lasers and the synchrotron source. Other benchmark work continues to be performed on the limit of validity of key approximations that have been almost universally applied, in some cases uncritically in the past. These include the electric dipole approximation and the independent electron approximation, for instance, at keV and higher energies. Finally, we note that as activities grow in the arena of magnetism of transition metal atoms in solids or surfaces, it is important to understand the behavior of these atoms when isolated in the gas phase, e.g. through spin-polarization or dichroism studies.

## **2.8 Chemical Bonding at Surfaces**

### **2.8.1 X-ray emission spectroscopy**

A. Nilsson reported on an innovative program to probe the local electronic structure in chemical bonds at surfaces and interfaces using X-ray emission spectroscopy (XES). Despite the considerable advances in electronic structure at surfaces in recent years, an atom-specific

view of chemical bonding at surfaces has not, in general, been possible. The problem is that the dominance of d-states in electronic spectra has made it difficult to extract chemically-specific information in most cases. Nilsson demonstrated elegantly in a number of examples that the use of atom-specific XES was the equivalent of photoemission spectroscopy from a single atom! He showed further that for adsorption of a homonuclear diatomic molecule, N<sub>2</sub>, adsorbed molecularly on Ni(100), there is a “compensation effect” in the bonding: Whereas the bonding to the surface is relatively weak, there is a surprising amount of charge redistribution between “inner” and “outer” nitrogen atoms. In a more complex example,

glycine on Cu(110), he showed that one can use the polarization characteristics of the synchrotron radiation to probe atom-specific orbital symmetries. These demanding experiments are an outstanding example of the value of synchrotron radiation in the VUV and soft X-ray range for electronic structure determination. The high brightness of an undulator beamline is *sine qua non* for such measurements, in which fewer than 1% of core holes decay by X-ray fluorescence.

Many other seminal experiments are underway in surface and interface science at ALS, with exciting new results in photoelectron diffraction, magnetism, multi-atom resonant photoemission, and detection of vibrational fine structure in core level photoemission.

### **2.8.2 X-ray absorption spectroscopy**

Another exciting application of X-ray methods is in X-ray absorption spectroscopy (XAS) of the local electronic structure of atoms that participate in hydrogen bonding: these are issues of critical importance in biology and environmental science. The experiments at ALS run the gamut from model ultrahigh vacuum studies of adsorbed water and glycine, to measurements in ambient atmospheres of water vapor. The ALS group has found evidence for unique hydrogen bonding in water, and their measured spectra are supported by a theory that indicates fewer than four hydrogen bonds in liquid water. This is a remarkable demonstration that there is much to be learned about one of the most widely studied (and most important) substances in the world.

### **2.9 Femtosecond x-ray Research - Time-Resolved x-ray diffraction**

Perhaps the most innovative, unique capability being developed at the ALS is the femtosecond spectroscopy and diffraction work discussed by R. Falcone and R.W. Schoenlein. For the study of ultrafast chemical reactions, phase transition, surface dynamics and a wide variety of critical biological processes operating on the sub picosecond timescale, direct x-ray experiments have long been a dream. Impressive first steps along these lines have now been done at the ALS using femtosecond laser excitation of the sample, monitoring the evolving phenomena by xray diffraction with a streak camera (R. Falcone et. al.). As this capability is advanced there will clearly be many interesting measurements that will be enabled. By far the most intriguing, however, are the successes reported by R.W. Schoenlein et. al. in production of 100 fs x-rays by scattering of a femtosecond laser off of the electron beam packet in the synchrotron itself (femtosecond slicing). Used in pump/probe schemes with another femtosecond laser on the sample there are a vast number of experiments that will be possible for the first time. In this development the ALS is poised to be the world leader for many years to come. The panel feels that development of the new undulator beamline for femtosecond x-ray science now being discussed should receive top

priority. There is no comparable effort in any other synchrotron light source in the world (except for Free Electron Laser projects, that will take much more time).

## **2.10 Applied Research - EUV Lithography and Metrology**

The extensive optical and defect measurement program in support of the national program in EUV lithography was described by J. Bokor. The ALS carries out three major metrology elements: reflectivity/scattering of the multilayer resonant reflective optics, at-wavelength (13.4nm) phase shifting point diffraction interferometry of the optical elements and projection optics systems, and mask defect identification in the multilayer-coated mask substrates. These experiments are supported by the EUV LLC, an industrial consortium (Intel, Motorola, AMD), in cooperation with the Virtual National Laboratory (LBNL, LLNL, SLNL).

The reflectivity/scattering program has served as the main measurement mainstay for the development of advanced multilayer resonant reflection films which have now almost achieved theoretical reflectivity. Due to the multiple reflections in the lithography systems, small reflectivity improvements have a very large impact on increasing the photon throughput of the systems.

The interferometry research program has been the major measurement capability which has permitted assembly of the reflective optics into projection systems with unprecedented levels of alignment accuracy (accuracy of 0.04nm and measured wavefront aberrations of 0.6-1.1nm in the 4-mirror projection optics camera).

This ALS capability is truly at the leading edge and represents outstanding, world class, optical research. Both European and Japanese EUVL programs are starting to build equivalent capabilities and are expected to be heavy users of the ALS capability in their emerging efforts. The students graduating from this program are in extremely high demand in the semiconductor industry because of their knowledge and scientific contributions and leadership. The 3 beamlines also support non-LLC-funded research in new areas of optical

science at the diffraction limit and will be the basis for possible new technology directions in the future. The ALS will continue to be the leader in EUV optics measurement technology and will be the source of much new research and thinking in this emerging area of technology.



### **3.0 Conclusion**

#### **3.1 The Machine**

Today the ALS source has the lowest horizontal emittance in the world for machines having an energy lower than 2 GeV. It is very reliable (95% of availability). There has been a continuous improvement in the stability and lifetime: this is clearly shown by the quality of the data obtained in MAD experiments (structural biology). The installation of superconducting superbends for higher energy x-rays will enhance considerably the capacity of the facility.

#### **3.2 Organization**

The reorganization of the laboratory, the elevation of ALS to Division level, the appointment of D. Chemla as Director, have produced remarkable results. We believe that D. Chemla and the staff have done an outstanding job.

#### **3.3 Areas of excellence**

It is very clear today that ALS has established areas of excellence in

- structural biology
- femtosecond and picosecond dynamics in condensed matter and in gas phase
- electronic processes and many body effects in highly correlated systems, magnetic nanostructures and correlation in small systems
- surface science, thin films and microscopy
- ultra high-resolution spectroscopy of gas phase atoms, ions and molecules
- chemistry and catalysis (wet, heterogeneous, nanoscale chemistry and biochemistry, radicals dynamics, catalytic interfaces at atmospheric pressure)
- Analytical sciences and metrology

#### **3.4 Future developments**

During the meeting D. Chemla presented a list of important projects for the near future, by order of priority

- (a) Molecular Environment Science (already funded for a large fraction)
- (b) Magnetic and Polymer Nanostructure Research (PEEM3 photoemission microscope)
- (c) Femtosecond Spectroscopy and Diffraction

In addition there is a strong development in structural biology (eight new crystallography beamlines are being developed with varying research and technological demands).

We support strongly the program on structural biology (non DOE money) and the 3 topics discussed above.

- we believe that in the area of femtosecond spectroscopy and diffraction ALS is in a unique position: it is the only center in the world able to produce 100 fsec pulses (by

slicing the electron bunch with a laser). In addition, in the neighborhood there are very strong groups in the fields of pico and femtosecond research (R. Falcone, C. Shank, ...).

Achieving  $10^{12}$  ph/s/mm<sup>2</sup>/mrad<sup>2</sup>/0.1% should open a lot of new possibilities. This development will be very important to prepare a possible free electron laser in the x-ray range.

- the development of the PEEM3 photoemission microscope for magnetic and polymer and nanostructure research is also very important. There is a strong competition within Europe (a very ambitious project is underway at Bessy II in Berlin).
  
- Environmental Science  
The goal is to provide an understanding of chemistry in natural systems, and in particular the chemistry associated with toxic and radioactive contamination, in order to underpin long-term solutions to environmental problems. We believe that this program is important and that the financing should be completed.

### **3.5 Interaction with the users representatives and SAC member**

The first thing to notice is that the number of users has been increased by a factor three since the Birgeneau report.

The users were very pleased with the appointment of D. Chemla as Director of the ALS in June 1998, appreciating his openness and approachability.

The ALS management and the user community have established productive, respectful and direct two-way communication.

The ALS has made significant improvements in both the User Services group and the Scientific Support group. Administrative procedures have been streamlined and low-cost accommodation for users has been arranged near to the campus.

The main recommendations are:

- to increase the size of the Scientific Support group
- to obtain funds for post-doctoral associates
- to support the ALS plan to have a new building adjacent to the machine to have more office space for the users and laboratories for sample preparation and experiment staging.

### **3.6 Comparison with other U.S. facilities**

This is a very difficult exercise. What we have done is to select the three highest ranked journals in Structural Biology and Solid State Physics and Chemistry. This is only an indication: a lot of very good papers are not published in those journals and some of those published can even be wrong! But this is the same for every facility.

The results are presented in both tables of Appendix 1. We also present the number of experimental stations. In structural biology the production of ALS for one experiment is outstanding. In solid state physics and chemistry again the situation is remarkable for the ALS. We would like to point out that APS is still in a construction phase, as was ALS at the time of the Birgeneau report.

### **3.7 Scientific issues requiring UV radiation**

In the Birgeneau report there was a very surprising sentence: "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."

Obviously this is difficult to understand. If you study a new material you need to know the electronic properties (obtained mostly by UV and soft x-rays) and the structural properties (obtained mostly with hard x-rays or neutrons). But you need both. In the case of the high  $T_C$  superconductors the results obtained using UV are much more fundamental than those using x-rays.

A study of the publications in Table 1 shows that in the case of solid state physics and chemistry out of 80 publications in the 6 facilities 36 have been obtained in the IR, UV or soft x-ray region and 44 in the hard x-ray region. Considering that there are about 20% more beamlines for hard x-rays, one can conclude that the number of publications is the same for both.

### **3.8 Superbend beamlines**

For the superbend beamlines, the management should be careful to maintain a good balance between structural biology and the other fields.

## **4.0 Recommendations**

It is clear that ALS is doing an outstanding job in many areas. None of the criticisms of the Birgeneau report are still valid. The committee recommends unanimously that the penalty imposed on the ALS in light of the Birgeneau report be lifted.

Finally, we think that the ALS should be left without a review for some months at least.



**APPENDIX 1 - Study of Journal Publications**

**Structural Biology**

Journal	APS	ALS	CHESS <sup>+</sup>	NSLS	SSRL
CELL	5	4	10	16	6
NATURE	3	3	5	8	3
SCIENCE	1	9	6	10	6
Total	9	16	21	34	15
Number of experiments working simultaneously	7*	1	3	7	4

Only counted here are the publications related to work carried out at the facilities

\*2 beamlines built for industrial purposes

<sup>+</sup>CHESS has been partially down during the year for new construction

**Solid State Physics and Chemistry**

Journal	APS	ALS	CHESS	NSLS	SSRL	SRC
NATURE		1		3		
SCIENCE		3		5	3	1
P.R.L.	10	13	6	24	3	8
Total	10	17	6	32	6	9
Number of experiments working simultaneously	18	20	6	72	21	27

**1999 publications in high ranked journals  
for six American synchrotron radiation centers**

*The BESAC Subpanel Review of the Advanced Light Source -- February 2000*  
**Department of Energy**  
**Washington, DC 20585**

August 10, 1999

Professor Geraldine L. Richmond  
Chair, Department of Chemistry  
University of Oregon  
Eugene, OR 97403-1253

Dear Geri:

I very much appreciate your willingness to serve a second term as Chair of the Basic Energy Sciences Advisory Committee (BESAC). I believe that the continuity in leadership that you will provide will be critical during the coming year as BESAC completes its study of the electron beam microcharacterization centers and begins its new activities. Under your leadership during the past year, BESAC activities have produced extraordinary results that already have - and will continue to have -- broad impacts in the Basic Energy Sciences program. I especially want to acknowledge BESAC's help in the review of the programs and operations of the High Flux Isotope Reactor at Oak Ridge National Laboratory; the determination of the appropriate five-year R&D agenda for novel, coherent light sources ("4th generation" light sources); and the identification of the forefront of the physical and biophysical sciences in the area of complex systems through BESAC's help with the organization of and the participation in the workshop at Lawrence Berkeley National Laboratory.

During the coming year, I would like BESAC to advise me on the current status of the Advanced Light Source and to take on a new and continuing charge to oversee Committees of Visitors for the Basic Energy Science (BES) Program. I have provided an overview of each activity below. You should develop the detailed charges through discussions with the chair of the panel, committee, or workshop and the Associate Director of BES.

The first activity is a renewal of the Advanced Light Source to examine those issues that were raised by the BESAC Report on "DOE Synchrotron Radiation Sources and Science," known as the Birgeneau Report. In particular, BESAC should explore ALS's vision for the future, the quality and diversity of science programs at the facility, the user demand and the interactions and relationship with the user community.

The second activity is the establishment Committees of Visitors (COVs) through which BESAC can provide an assessment on a regular basis of matters pertaining to program decisions. COVs should review program management every three to four years on a rotating basis for major elements of the BES program selected by the Associate Director for BES. The COVs should provide an assessment of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs. You should work with the Associate Director for BES to establish the processes and procedure for the first COV to occur in 2000.

I appreciate BESAC's willingness to take on these important activities, and I look forward to meeting with you and learning of your progress throughout the coming year.

Sincerely  
/s/ by  
Martha A. Krebs  
Director  
Office of Science

24 November, 1999

Professor Yves Petroff, Director  
European Synchrotron Radiation Facility  
B. P. 220, Building Central, Room 519  
Grenoble Cedex  
France, F-38043

Dear Professor Petroff:

The Basic Energy Sciences Advisory Committee (BESAC) has been asked by Dr. Martha Krebs, Director, Office of Science, to review activities of the Advanced Light Source (ALS) at the Lawrence Berkeley National Laboratory. I am very grateful that you have agreed to chair this panel.

The panel should consider the issues raised by the BESAC Report on "DOE Synchrotron Radiation Sources and Science," known as the Birgeneau Report. In particular, the panel should explore the vision for ALS in the future, the quality and diversity of science programs at the facility, the user demand, and the interactions and relationship with the user community.

I anticipate that you will want to assemble a panel of 6-10 members who will make a site visit to the ALS. Professor Daniel Chemla, Dr. Patricia Dehmer, and I each will provide you with names of suggested panel members. You should make the final selection, and you should feel free to add other names to the list of suggested names. In addition, you should work directly with Professor Chemla to arrange the date, time and agenda for the visit. I realize that you have already been in contact with him about this review.

I am hopeful that the review can take place within the next few months and that your panel is able to present a final report to BESAC at its next meeting, which is scheduled for February 2000. You are invited to the February meeting to make the presentation of the panel's findings and recommendations. Alternatively, if you cannot attend the meeting, I ask that you designate a member of the panel to make the presentation.

Logistics for the meeting will be handled by Sharon Long of DOE's Office of Basic Energy Sciences in coordination with the ALS contacts and the panel members. She can be reached at (301) 903-5565 or [sharon.long@science.doe.gov](mailto:sharon.long@science.doe.gov). Travel expenses for you and non-Federal panel members will be reimbursed by DOE. Reimbursement for Federally employed panel members, including DOE laboratory staff, will be handled through their respective offices.

Thank you again for agreeing to chair this review panel, and I look forward to your report.

Sincerely,

/s/ by

Geraldine Richmond

Chair, Basic Energy Sciences Advisory Committee

cc:

J. Decker, - DOE/SC-2

P. Dehmer, DOE/SC-10

S. Long, DOE/SC-10

C. Shank, LBNL  
D. Chemla, LBNL