MINUTES OF THE

July 22-23, 2002

BASIC ENERGY SCIENCES ADVISORY COMMITTEE

MEETING

Gaithersburg Marriott Washingtonian Center
Gaithersburg, MD

Geraldine Richmond
Chairperson

http://www.sc.doe.gov/production/bes/BESAC/Meetings.html

BASIC ENERGY SCIENCES ADVISORY COMMITTEE

Meeting Minutes
July 22-23, 2002
Gaithersburg Marriott Washingtonian Center
Gaithersburg, MD

I hereby certify that these minutes constitute a reasonably comprehensive and accurate record of the meeting of the Basic Energy Sciences Advisory Committee held on July 22-23, 2002.

Geraldine Richmond, Chairperson

Minutes are available on the BESAC website at:
http://www.sc.doe.gov/production/bes/BESAC/Meetings.html

Minutes for the
Basic Energy Sciences Advisory Committee Meeting
July 22-23, 2002
Gaithersburg Marriott Washingtonian Center, Gaithersburg, Maryland

BESAC members present:

Nora Berrah
Collin Broholm (Monday only)
Philip Bucksbaum
George Flynn
Wayne Goodman
Laura H. Greene
Eric Isaacs
John Hemminger
Anthony Johnson
Gabrielle Long
Anne Mayes
William McCurdy, Jr.
Bradley Moore, Vice Chair (Monday only)
Daniel Morse
Martin Moskovits
Ward Plummer
John Richards
Geraldine Richmond, Chair
Richard Smalley
Joachim Stohr
Samuel Stupp
Kathleen Taylor

BESAC members absent:

Patricia Dove
Mostafa El-Sayed
Walter Kohn
Cherry Murray
Rudolf Tromp
Stanley Williams
Mary Wirth

Also participating:

Altaf H. Carim, Office of Basic Energy Sciences, DOE
Peter Cummings, The University of Tennessee
James Decker, Principal Deputy Director, Office of Science, DOE (Monday only)
Patricia Dehmer, Director, Office of Basic Energy Sciences, DOE
Steve Dierker, Chair, National Synchrotron Light Source, Brookhaven National Laboratory
John N. Galayda, LCLS Project Director, Stanford Linear Accelerator Center
Paul W. Lisowski, Director, LANSCE Division, Los Alamos National Laboratory
Thom E. Mason, Director, Spallation Neutron Source, Oak Ridge National Laboratory
Terry Michalske, Head, Surface and Interface Science Dept., Sandia National Laboratories
Frederick M. O'Hara, Jr., BESAC Recording Secretary
William Oosterhuis, Materials Science and Engineering, OBES, DOE
James Roberto, Associate Director, Oak Ridge National Laboratory (Tuesday only)
Walter Stevens, Office of Basic Energy Sciences, DOE
Iran Thomas, Associate Director, Office of Basic Energy Sciences; Director, Division of Materials Science, Office of Basic Energy Sciences, DOE
J. Michael White, University of Texas, Austin

About 60 others were in attendance in the course of the two-day meeting.

Monday, July 22, 2002

Chairwoman **Geraldine Richmond** called the meeting to order at 8:32 a.m. and had the members introduce themselves. She welcomed the new members of the Committee and introduced **James Decker**, Principal Deputy Director of the Office of Science (SC), to present an update on the operations of the Office.

Last October, DOE started looking at restructuring SC. The restructuring project supports the *President's Agenda for Management Reform*. It is an effort to streamline and integrate SC at every level, in both headquarters and field. The objectives are to

- move decision authority to the lowest responsible management level while holding decision makers accountable for results,
- reduce layers of management,
- streamline the decision-making processes,
- clarify lines of authority,
- eliminate overlapping roles, and
- re-engineer management systems to eliminate inappropriate or redundant requirements.

This reorganization will affect the operations side but not the program side of the office's business. A major objective is to remove a thick layer of management out of the operations offices and make those offices into service centers.

Another restructuring is also going on for the creation of the Department of Homeland Security. DOE and SC have been affected in a major way. The Administration is proposing to transfer to the Department of Homeland Security $20 million of Biological and Environmental Research program funds (DNA sequencing of pathogenic microbes, technology development to compare gene sequences, and computational tools and databases); and $3 million of Advanced Scientific Computing Research program funds (applied mathematics and computer science research to achieve optimal efficiencies from large-scale computing systems). The DOE national laboratories will play an important role in performing R&D for the new department.

The SC mission has been re-affirmed. On June 14, 2002, at a speech at Brookhaven National Laboratory (BNL), the Secretary provided his commitment to SC. He said, "Our mission here at DOE ... is national security. And in my view, a serious commitment to national security demands a serious commitment to science, including basic research. This commitment strengthens our energy security, international competitiveness, economic growth and intellectual leadership." The Secretary is very supportive of both basic and applied research.

The Earth Simulator in Japan has gotten a lot of press. It runs certain scientific problems very efficiently. By some measures, performance is 50 times better that the best machines in the United States. It became operational in April 2002. It is the new No. 1 on the Top 500 list, based on a set of benchmarks called Linpack. (See www.top500.org.) Based on this benchmark, the Earth Simulator achieved a performance of 35.9 teraflops, or 90% of peak. It ran a benchmark global atmospheric simulation model at 13.4 teraflops on half of the machine (i.e., it performed at over 60% of peak). The total peak capability of all DOE computers is 27.6 teraflops. The Earth Simulator is applicable to a number of other disciplines, such as fusion and geophysics, as well.

Orbach has been publishing Occasional Papers that will become pieces of the new Strategic Plan of SC. These papers illustrate the cutting-edge science sponsored by SC and performed in universities, national laboratories, and the private sector. They give direction to scientific areas that need further exploration. Current papers, available at www.science.doe.gov, are:

- The Beauty of Nanoscale Science
- Biotechnology for Energy Security
- Dark Energy: The Mystery that Dominates the Universe
- Reasserting U.S. Leadership in Scientific Computation
- Building a 21st Century Workforce
- Scientific Foundations for Countering Terrorism
- Bringing a Star to Earth
- Using Nature's Own Tool Kit to Clean up the Environment

On the nanoscience front, the Secretary announced on June 14, 2002, the approval to begin the Conceptual Design of the $85 million Center for Functional Nanomaterials at BNL. Nanotechnology is one of the major scientific initiatives of the Bush Administration. The House Energy and Water Development Subcommittee provided requested FY03 funding:

- $11 million for further project engineering and design for the Nanoscale Science Research Centers (NSRCs) at Oak Ridge National Laboratory (ORNL), Lawrence Berkeley National Laboratory LBNL, and Sandia and
- $24 million to initiate construction at ORNL.

The only progress of the FY03 budget request so far is the markup by the House Appropriations' Energy and Water Development Subcommittee. That markup left unchanged the requested amounts for High-Energy Physics, Nuclear Physics, Biological and Environmental Research, Basic Energy Sciences, and Workforce (science education). It recommended increases in the budgets of Advanced Scientific Computing ($5 million), Infrastructure ($4.945 million), and Safeguards and Security ($4.383 million). And it recommended cutting the allocations to Fusion Energy Sciences (by $8.815 million), Program Direction (federal employees' salaries; by $5.169 million), Energy Research and Analysis (by $1.02 million; this amount was actually moved elsewhere), and a general reduction (of $18.639 million) that DOE and SC will have to spread around.

Richmond asked about the turnaround in Workforce funding. Decker responded that this funding was once 10 times this amount but had been zeroed out. It is a very effective program, and it is starting to grow in size again.

DOE is self-regulating; it is not subject to regulation by the Nuclear Regulatory Commission (NRC) or the Occupational Safety and Health Administration (OSHA). This self-regulation has been expensive. The House Energy and Water Development Subcommittee has been pushing DOE toward external regulation. The FY 2003 conference report accompanying the Energy and Water Appropriations Bill directs DOE to prepare an implementation plan for transitioning to external regulation at DOE's nondefense science laboratories. DOE is to assume that the NRC would have regulatory responsibility for nuclear safety and that OSHA would assume regulatory responsibility for worker safety. The underlying assumption is that external regulation will result in the same level of safety and performance for fewer resources expended. The conference report requests that by September 30, 2003, a detailed estimate be prepared on the cost of bringing all SC laboratories under external regulation. The Department is worried that it may end up with dual regulation; this course of action will have a significant effect on the national laboratories.

McCurdy noted that the programs to be transferred to the proposed Department of Homeland Security included basic mathematics and SciDAC mathematicians at Lawrence Livermore National Laboratory (LLNL) and asked if these people will be allowed to continue their basic mathematics. Decker said that they will need to respond to near-term development and will be diverted from long-term research. He went on to note that a Science Committee hearing will be held in Congress this week, which will be an opportunity for SC to get some visibility.

Richmond introduced **Patricia Dehmer** to present what was new from the Office of Basic Energy Sciences (BES).

The President's budget request for BES is currently before Congress. Of the $1019.6 million requested, $407.8 million (about 40%) would go to research, $244.6 million to the operation of user facilities, $251.6 to construction [largely the Spallation Neutron Source (SNS)], and $76.2 million to capital equipment. This budget request reflects significant increases for science at the nanoscale; other BES core activities; facility operations, upgrades, and construction; and major instrumentation. The budget request for the Office of Advanced Scientific Computing (ASCR) holds an increase for computational nanosciences, which prompted the recent joint BES-ASCR workshop on theory and modeling in nanoscience. Overall, this is an excellent budget for BES. The budgets for all the facilities are up except for those for the High-Flux Isotope Reactor (HFIR) and the SNS, both of which are completing major construction activities and therefore require less funding. An analysis of the budget request is on the Web at www.sc.doe.gov/bes/budget.html.

In response to the Nanoscale Science, Engineering, and Technology (NSET) solicitation, about 400 full proposals were received, and 56 awards were made (60% to universities and 40% to national laboratories), totaling $18 million. In April 2002, the first major review of the Nanoscale Science Research Centers (NSRCs) was conducted, and three centers were vetted to move forward in their designs. The two centers that did not get vetted redid their proposals and have been reviewed with good results. The BNL center was approved for conceptual design. The Argonne National Laboratory (ANL) proposal is still being reviewed.

At the BNL center's announcement, Spencer Abraham, Secretary of Energy, gave one of his most important speeches on basic science. In it, he said:

"What is so exciting about the work we do is that we produce benefits to America and the world that go well beyond the original scope of our mission.

Researchers probably never anticipated when they started smashing atoms and protons in our large accelerators that their science their very basic research on matter would eventually give us remarkable life-saving technology. One of every three hospital patients in the U.S. benefits from nuclear medicine. About 10,000 cancer patients are treated every day with electron beams from linear accelerators.

Superconductors developed for high energy accelerators now provide the strong and stable magnetic fields needed for the sharpest Magnetic Resonance Imaging. And accelerators invented for high energy and nuclear physics research now provide intense sources of synchrotron light that is used for structural biology, chemistry, and material research.

High energy physicists, looking to share information, invented and helped establish the World Wide Web: a profound advance in human civilization -- if only because it occupies the free time of our teenagers.

The practical value of basic research is often disguised. And those engaged in it often seek only to follow their curiosity, rather than to find an every day use for their work. But, as I hope I have shown, the connection of basic research to our missions here at DOE couldn't be stronger.

I think it's clear. A nation that embraces basic research embraces a brighter future."

Each of the NSRCs was asked to hold a workshop for potential users. They were astonished at how many people attended these workshops: more than 1000 unique users, reflecting an overwhelming interest by the scientific community. Such interest in planning workshops has never before been seen. A major theme that came out of these workshops was a desire to jump-start the activities of the NSRCs.

The February report of the Committee of Visitors (COV) provided recommendations in two main categories: program-specific recommendations and general recommendations. The latter observations were that (1) both university and laboratory activities (i.e., documentation) would benefit from standardization and better archiving and (2) national-laboratory new initiatives were generally well documented but continuing-program documentation was less complete. During the past six months, the processes for review have been reexamined; new, standardized processes will be implemented beginning in FY 2003. The merit-review procedures for laboratory proposals and grant applications were presented in a table that clearly displays the steps in each process, as well as the analogies. This process will be used as a template for doing the entire award process. A standard letter to reviewers was developed for both national laboratories and universities. A BES *Guide for Preparation of Review Documents* was developed that will be used for laboratory activities based on the university review process. After the foundation documents have been beta tested for clarity by external readers, they will be placed on the BES website. The new procedures will go into effect at the beginning of FY 2003. The details will be presented to the next COV in 2003. Standard document-archiving procedures were developed for laboratory activities, and a list of laboratory activities that will be reviewed in FY 2003 was prepared. The COV has had a significant impact on the operations of the Office; some of the new documents have gone through 20 iterations.

She reviewed (1) the operation of BESAC and its role in advising SC on science policy and (2) BESAC activities since 1996. She noted that all BESAC members are invited to attend and participate in all BESAC-sponsored meetings and workshops.

The next BESAC activities will be a COV for the Materials Sciences and Engineering Division of BES and an assessment of the short-pulse, short-wavelength, high-intensity light sources. Such assessments originated with the Birgeneau panel. This assessment should include a survey of the types of sources currently being proposed, the projected scientific impact of each, and the relative importance of each for the scientific programs of BES. This assessment will provide the foundation for establishing a roadmap for X-ray science. A number of techniques are being proposed around the globe to produce short-pulse, short-wavelength, high-intensity sources. BES would like BESAC's advice on how to proceed in this area. She asked for nominations for panel participation for both of these future activities.

She identified new staffing in SC and introduced the new BESAC members. She announced that Geraldine Richmond will continue as Chair for the next year and that Bradley Moore will serve as Vice Chair.

Goodman asked what the ultimate goal was in the standardization of the award process and how far it will go. Dehmer responded that BES has not gone to the extent that the National Science Foundation (NSF) has, which limits solicitations to one or two times a year, but the review process for universities and national laboratories will be as similar as possible. Richmond noted that the COV was very important in validating the review process, and Dehmer added that she was very happy with the COV.

Richmond declared a break at 9:53 a.m. The Committee was called back into session at 10:20 a.m. with the introduction of **William McCurdy** to report on the Workshop on Theory and Modeling in Nanoscience.

He had “volunteered” to lead the workshop and with Ellen Stechel of the Advanced Scientific Computing Advisory Committee (ASCAC) recruited an organizing committee. The purposes of the workshop were to identify the challenges and opportunities for theory, modeling, and simulation in nanoscience and nanotechnology and to investigate the role of applied mathematics and computer science in meeting those challenges. The 55 attendees represented a fairly even split between representatives from (1) nanoscience theory and modeling and (2) applied mathematics and computer science; 16 came from universities, 31 from national laboratories, 3 from industry, and 5 from DOE. All BESAC and ASCAC members were invited, and 20 additional invitations were issued, mostly to university researchers. Written contributions were solicited from all attendees, and responses were posted to a website together with the presentations (at www.nersc.gov/~hules/nano/).

The first day was devoted to topical presentations by Stanley Williams of Hewlett-Packard Laboratories, Uzi Landman of Georgia Institute of Technology, Steven Louie of the University of California at Berkeley, Dion Vlachos of the University of Delaware, Phil Colella of LBNL, Jerry Bernholc of North Carolina State University, Sharon Glotzer of the University of Michigan, Alex Zunger of the National Renewable Energy Laboratory, and Bernd Hamann of the University of California at Davis. Because a report had to be written, the second day was devoted to a panel discussion on the role of applied mathematics and computer science in the nanoscience initiative and to breakout sessions on

- Well-characterized nano building blocks;
- Complex nanostructures and interfaces;
- Dynamics, assembly, and growth of nanostructures;
- Crossing time and length scales;
- Fast algorithms; and
- Optimization and predictability.

It is not appreciated outside the theory community that nanoscience arose from the appearance of new experimental techniques over the past 15 years. No less revolutionary were the techniques of theory and modeling that emerged during the same period, such as

- Density functional theory for electronic structure,
- Ab initio molecular dynamics,
- Classical molecular dynamics with fast-multipole approaches,
- New methods for classical Monte Carlo simulation,
- New quantum Monte Carlo methods for electronic structure, and
- New mesoscale methods including dissipative particle dynamics and field-theoretic polymer simulation.

At the same time, advances in computational power have yielded an improvement of about 4 orders of magnitude since 1988.

The workshop identified some fundamental theoretical challenges:

- Bridging electronic through macroscopic length and time scales (this is the central problem);
- Determining the essential science of transport mechanisms at the nanoscale;
- Devising theoretical and simulation approaches for nano-interfaces;
- Simulating with reasonable accuracy the optical properties of nanoscale structures and modeling nanoscale opto-electronic devices;

- Simulating complex nanostructures involving "soft" biologically or organically based structures and hard inorganic ones as well as nano-interfaces between hard and soft matter;
- Simulating self-assembly and directed self-assembly;
- Devising theoretical and simulation approaches to quantum coherence, decoherence, and spintronics; and
- Developing self-validating and benchmarking methods.

The central challenge is to develop, within 5 to 10 years, robust tools for the quantitative understanding of structure and dynamics at the nanoscale, without which the scientific community will have missed many scientific opportunities as well as a broad range of nanotechnology applications. As one participant pointed out, before one manufactures and markets hundreds of millions of copies of a product, one must know a lot about not only the engineering but also the theory of how that product works. As has been shown time and again, a discovery of a theoretical principle can be responsible for the development of scientifically and economically important advances.

There is a strong, recent history of the impact of applied mathematics on theory and modeling of molecules and materials. In looking to the future, the mathematics of likely interest are not fully knowable at the present. But there are some candidates for improvement and invention in applied mathematics:

- in bridging length and time scales (e.g., mathematical homogenization, "space-sharing" methods, application of the "multigrid" and "proper orthogonal decomposition" paradigms, and formulation of bidirectional coupling between scale-adjacent models);
- in fast algorithms; and
- in optimization and predictability (e.g., multidimensional minimization algorithms, stochastic optimization methods, analytic techniques for propagating errors, and comprehensive error bounds).

People have very different feelings about what is important because nanoscience is not one discipline. This multidisciplinarianism is a challenge to SC, and it means that there is not an organized community of researchers. Theoretical efforts in separate disciplines are, however, converging on this intrinsically multidisciplinary field. But opportunities will be missed if new funding programs in theory, modeling, and simulation in nanoscience do not aggressively encourage highly speculative and risky research. Indeed, a new investment in theory, modeling, and simulation in nanoscience should facilitate the formation of such alliances and teams of theorists, computational scientists, applied mathematicians, and computer scientists.

Such alliances and teams face fundamental intellectual and computational challenges if they are to achieve the full potential of theory, modeling, and simulation in nanoscience. This is a wholly new science; the joining of hard and soft matter, for example, requires the development of new science. In addressing this new science, SC is in a unique position to build a new program in theory and modeling in nanoscience because much of the nation's experimental work in nanoscience is supported by DOE, new nanoscience facilities are being built at DOE national laboratories, and DOE supports the core portfolio of applied and numerical mathematics for the nation.

He introduced **Peter Cummings**, a member of the workshop steering committee, who said that the workshop was the most exciting one that he had ever been involved in. The techniques brought forward by the applied mathematicians will help solve a number of the problems faced in nanoscience.

Richards asked if there were any correlations of the methods used in nanoscience with other simulations and calculations. McCurdy responded that a lot of work in the Accelerated Strategic Computing Initiative (ASCI) Program is similar to the nanoscience work.

Stupp asked how the advances in computer power will proceed and how the right partnerships between theory and experiment will be struck in this area. McCurdy noted that computing power has been on track with Moore's Law (computing power doubles every 18 months) since 1988. That increase will continue for at least two or three more terms. But central processing units (CPUs) are facing a fundamental limit in communication. The Earth Simulator computer in Japan has demonstrated that one can do considerably better by designing a machine for specific scientific problems. The United States stopped designing computers for specific uses years ago. If that policy is changed back, the answer in terms of computing power could be more optimistic.

Cummings said that the answer to the second question is that advances in hardware can be dwarfed by advances in theory, algorithms, and techniques. Of the focus areas of nanoscience, some are theory based, and all have theory needs. It is remarkable how quickly theory, modeling, and simulation have come to play a major role in nanoscience. Often, one sees a theorist participating in the research team from day one of the research effort. McCurdy added that, if one embeds a materials science program in a theory and modeling program, the theory and modeling will suffer in the competition for funding.

Plummer asked how a return on investment was going to be obtained. McCurdy said that the amount of money spent by SC on theory is tiny; the return on investment is huge. Experimental techniques have brought science to a place in which theory has not yet been developed. That imbalance speaks volumes. Cummings observed that a new type of investment is being talked about here: collaboration between theorists and experimentalists.

Moskovits noted that, in 1988, it used to be called science or something else, and theory could easily be applied to an experimental situation. Today, complexity and advances are great, making it difficult for the theoretical community to pass on insights to the experimental community. McCurdy noted that that point is not reflected in the report. When some theoretical advance is passed on to the experimentalists to use *themselves*, it changes the experimental efforts fundamentally. That transfer is doable, but it is not what the nanoscience research centers are set up to do.

Richmond commented that this is a great report and said that the team that produced it is to be congratulated. She suggested that the Committee accept the report. McCurdy pointed out that the report is the result of many people's contributions and, as such, is necessarily incomplete because of the complexity of the subject matter. Moreover, another committee (the Advanced Scientific Computing Advisory Committee, or ASCAC) has to approve it as well as BESAC. Taylor suggested that the caveats of McCurdy be included in the acceptance. With those qualifications, the report was accepted unanimously.

Richmond introduced **Michael White** to present the report of the catalysis workshop.

DOE is a major supporter of catalysis science, which has a $500 billion value attached to it and is depended on by 80% of the chemical industry. The United States has no other organization funded for and focused on catalysis. Today, advances in nanoscience understanding offer new approaches to establishing a firm scientific basis for advancing our understanding and ability to predict catalytic phenomena. A recent report of the National Academies' Committee on Science Engineering and Public Policy concluded that catalysis is a subfield in which the United States is among the world leaders but is broadly expected to lose its current international position because of the refocusing of investments in the industrial sector without transfer of this expertise to the educational sector.

A workshop was held that built on a workshop held in Berkeley a year earlier. It drew national-laboratory, industrial, and university participants from across the nation and from foreign countries who were both young and old and reflected a broad range of catalysis.

The workshop had ten breakout sessions from which two common themes emerged:

- Catalysts are complex materials and involve massively interdisciplinary research requiring the long-term organized cooperation, collaboration, and funding of experts from many fields of science and engineering, and calling for the use of our specialized national facilities to their fullest potential.
- Advances have been emerging that enable tailoring, tuning, and designing nanostructured catalytic materials.

The workshop recommended establishing two to three National Catalysis Research Institutes (NCRIs), which would be competitively selected and located in the national laboratories or universities, as appropriate, and would be by charter collaboratively networked to other national laboratories, universities, and industry. Each NCRI would have a well-defined, long-term basic research theme, selected for its scientific importance and potential societal impact, and would consist of a closely integrated group of appropriately expert collaborators to address the interdisciplinary research theme. Each center would be evaluated periodically. To encourage and strengthen university (particularly student) involvement and increase participation of industrial users from throughout the country, each institute should include a prominent virtual component for those outside the center but in the research network.

Wherever possible and appropriate, institutes should include or be closely aligned with special research facilities, including state-of-the-art microscopes, light sources, neutron sources, terascale computers, and/or nanoscience institutes, in order to capitalize on their unique capabilities.

The workshop sought commonalities from the fields of homogeneous, heterogeneous, and biological catalysis. The common concepts that emerged were that

- The electrons drive catalysis (with occasional help from protons);
- Both structure and dynamics are important;
- Sites are central but so are more subtle features; and
- Catalysts should be efficient, effective, and robust.

Experiment, simulation/computation, and theory are highly linked through the size and time scale that can be handled. Calculations can become larger and longer with high accuracy. Experiments can become smaller and shorter. Calculations and experiment have the potential to meet at nanoscale lengths and subpicosecond times.

Assessments of catalyst efficiency, effectiveness, and robustness are based on the principles that faster is typically better (although often there is a selectivity penalty) and that, integrated over time, minor side reactions can become a major problem. The opportunity here is to tune heterogeneous catalysts using nanoscience methods to realize the selectivity of biocatalysts and the single-site characteristics of homogeneous catalysts without overly compromising the turnover number and the catalyst lifetime.

In much of heterogeneous catalysis, nanoscale particles are key. Nanoscale particles are unique. They have neither bulk nor atomic properties. There is the opportunity to design and build nanoscale materials from the bottom up. Addressing many grand challenges for catalysis in the age of nanoscience requires new funding for coherently managed focused experimental and theoretical basic research goals.

A number of foreign governments have either begun or continued to pursue catalysis as a matter of policy linked to their economic development. Breakthroughs, rather than incremental improvements, are needed in many of these complex systems areas. NCRI(s) can facilitate such breakthroughs in a basic research environment that brings together and maintains long-term support for capable, productive, and collaborative individuals.

The central goals for new catalysts include high turnover number at low temperatures, nearly 100% selectivity, and catalyst stability. Relevant intermediate-term targets include selective oxidation, alkane activation, by-product and waste minimization, stereoselective synthesis, functional olefin polymerization, alkylation, living polymerization, and alternative feedstocks and renewables. The relevant longer-term targets include photocatalytic water splitting, low-cost oxidants, NO_x decomposition, methane conversion to useful products, clean transportation fuels, low-cost fuel cells, and replacement of the platinum-group metals.

The ultimate goal of theory is to develop ways to reliably predict new reactions and catalysts and, thus, guide rational design of novel materials and processes. Powerful theoretical tools exist and are now being used. Theoretical work should put structure and dynamics on an equal footing; in catalysis, both are critical. Theory, experiment, and computation should be coherently linked.

Homogeneous catalysts are potentially highly selective, in part because the catalysts are well-defined molecules (i.e., single sites, with highly tunable structural and dynamical characteristics). But, the emerging ability to tailor and control solid structure at the nanoscale combined with ability to control molecular structure brings the exciting possibility of building novel catalytic materials that combine the best features of homogeneous and heterogeneous catalysts.

Biocatalytic conversion of renewable feedstocks derived from cellulose, hemicellulose, starch and plant oils into desirable products, including transportation fuels, is an important economic target needing long-term interdisciplinary basic research. The goals for biocatalysts do not differ from those for homogeneous and heterogeneous catalysts of petroleum feedstocks; efficiency and selectivity are central. Development, deployment, and application of high-throughput analytical techniques in an NCRI would be an enormous help.

Synthesis played an important role in the workshop. Advances in synthetic methodology, coupled with advances in temporally and spatially resolved characterization, provide a unique opportunity to construct nanostructured solid catalysts designed for high turnover numbers, superb selectivity, and minimal waste. Sufficient complexity must be incorporated in the nanostructured material to block undesirable paths and to keep open a low-energy catalyzed path to the target molecule. The potential exists to bring heterogeneous and biological catalysis into this research by attaching enzymes and homogeneous catalysts to these tailored structures.

An important and demanding goal for catalysis is to develop a tunable catalyst design from first principles. Combining nano and molecular science, synthetic chemists working with catalysis and materials scientists can develop new nanocatalysts based on numerous strategies. A concerted effort should be made to identify defect structures in nanocatalysts and, on a single-site basis, synthesize and characterize them structurally, electronically, and catalytically.

Dynamics provides the molecular-level basis for determining kinetic parameters (i.e., reaction-rate constants and diffusion coefficients) for each step in a reaction mechanism that describes an operating catalytic process. The dynamics of catalyzed reactions must, of necessity, involve the atomic motion and energy flow in the catalyst as well as the reactant. Biological, homogeneous, and heterogeneous catalysis share common dynamical issues.

Understanding the nonuniformity of reactions in situ is one key to unraveling the complexities. Transmission electron microscopy continues to advance as electron-beam sources and detectors improve, theoretical approaches expand, and in situ environmental accessories are developed. Experimental characterization of nanostructured catalysts often goes hand-in-hand with theory.

How should the national photon and neutron facilities be used to advance catalysis? Beamlines should be outfitted for and dedicated to catalysis research. Concurrent, in situ measurements of spatial, chemical, and temporal properties can be made available on one beamline. Amplified use would result if dedicated beamlines and end stations were built to accommodate the unique requirements of catalysis research, although ancillary instrumentation would be required. Onsite expertise in catalysis would be needed.

He showed a number of research results pertaining to catalysis that have been produced at the current state-of-the-art facilities.

A human-resources problem is unfolding. Academic catalysis researchers (and students being trained) are declining in numbers. Such personnel are needed if a well-developed basic understanding that is radically different from the situation five or ten years ago is to be achieved.

Stohr commented that the science needs to be coupled with those that use it in practice. In Europe, there was a good link between the companies that use catalysts with those that make catalysts. He asked how that was going to be done in the United States. White responded that the United States has many researchers who are developing catalysts and who understand the intellectual property issues. Industry money is going into Berkeley, Northwestern, and many other university centers of research. Alex Bell commented that this is an appropriate question to raise. Good science has to be coupled with industry. Mechanisms are needed to make these catalysts available without problems of intellectual property. Taylor asked how one identifies mechanisms to do that on a long-term basis. Richards noted that the report makes a very specific recommendation to establish research centers as an answer to that question and went on to ask whether, if the Committee accepted this report, it would be accepting the call for the creation of these centers. Richmond said that that was the case.

Plummer stated that this is an extremely important area. It needs to be formalized in a broad context, and the Committee has to do it right. He was disappointed in the Executive Summary of the report. The report is not suitable for acceptance as currently written. It does not address key questions:

- What are the opportunities and challenges? There is no great vision of the future in this report.
- What great discoveries are going to result from funding this program?
- Why now? What has changed in the last 10 years that will make this work?
- What are the key barriers that this program can overcome?
- What is the return on investment? How will this increased funding have a nonlinear effect on the advancement of catalysis?
- What is the cost of not doing this?

- Why DOE? (The rationale presented in the theory and modeling report was excellent, but the catalysis report should be able to include an even stronger section.)
- How does DOE accomplish your identified needs? A catalysis institute is not going to develop the advanced instrumentation needed nor is it going to push the frontiers of theory and modeling.
- Is a catalysis institute at a university going to take the place of a research program in industrial companies? How?

As written, he said, the document does not answer these concerns and tell how they are to be addressed or how any response to the problem is going to be integrated into a package that will have a payoff.

Goodman disagreed. He believed that the report includes the targets of opportunity. The key issues are there. The United States is behind in this area, and a proposed way of catching up is offered. If the United States is to get on with this enterprise, it is clearly a DOE issue. The country does not have a top institute in catalysis like that in Berlin, and that situation is not acceptable.

Moore asked what connection there would be between these centers and the nanoscience centers. White replied that one application of nanoscience is catalysis, and some of the work of the catalysis centers would be embedded in the nanoscience centers.

Taylor noted that the body of the report was devoted to the science and that she liked the gap between that and the recommendations for the future.. This is basically a workshop report; it is background rather than how things should be done by SC.

Richmond suggested accepting it as a report to BESAC and that several BESAC members use it to develop ideas on how to use it to develop recommendations to SC on a time line of about a month. She suggested Taylor, Hemminger, Plummer, and others use the report as a template and work up a series of recommendations. The Committee would be accepting it only as a report from the workshop, not as a BESAC report. Moskovits offered that the Subcommittee might like a second shot at writing the report. Catalysis is an incredibly important area. The report's problem is that the recommendations do not logically follow from the rest of the report. The Subcommittee should take advice from this Committee and rewrite the report accordingly.

Richards concurred. He said that two or three people from this Committee cannot fix this report in 24 hours. The Subcommittee should have the opportunity to fix it themselves.

Goodman pointed out that part of the charter of the Subcommittee was to address the issue of establishing the centers and to come forward with a recommendation.

Berrah said that it would be appropriate for the Subcommittee to rewrite the report themselves. Greene noted that the data are there in the report but are not presented in the right manner. Richards proposed circulating the Executive Summary to the BESAC members suggested by Richmond for review. Richmond commented that the Committee could do anything that will result in the best report and noted that it is such an important topic that several members want to ensure that it is done right. Isaacs commented that this rewrite cannot be done overnight; it requires a broader approach. Richards suggested that the identified BESAC members get together with White at this meeting and pinpoint what needs to be improved in the report and how it is to be done. Plummer pointed out that the report contains a good table on the international centers and said that he would like to see a similar table for all of the U.S. institutes. He suggested taking the references out of the report; they are not needed. The report should sell the science, not the people.

Richards suggested that the Committee should tell the Subcommittee what its concerns are and how they can be fixed. Richmond responded affirmatively and said that she would like to have the Committee develop by the next morning a strong sense of what is going to be done with this report. A break for lunch was declared at 12:17 p.m.

The meeting was called back to order at 1:32 p.m. Richmond called upon **Walter Stevens** to speak about SC's counterterrorism activities. The proposed Department of Homeland Security would like to have an in-house R&D capability, a DARPA-like agency [Defense Advanced Research Projects Agency], and a set of standards.

Stevens started with an overview of SC activities related to counterterrorism, including

- BES Workshop on Basic Research Needs to Counter Terrorism (February 28 to March 1, 2002);
- BES survey of national laboratory research and core research activities relevant to counter terrorism;
- SC/BES occasional paper on research to support counterterrorism;
- Counterterrorism added to national laboratory onsite review agendas;
- Development of a vision for future SC support of the proposed Department of Homeland Security;
- A High-Energy Neutron Physics (HENP) workshop on the Role of the Nuclear Physics Research Community in Combating Terrorism (July 11-12, 2002); and
- Office of Biological and Environmental Research (OBER) participation on an ad hoc panel for sequencing of pathogenic organisms [with the National Institutes of Health (NIH), NSF, Centers for Disease Control and Prevention (CDC), Central Intelligence Agency (CIA), etc.] to counter bioterrorism.

To get started to see how BES could fit in, the BES core research activities were mapped against five of the seven areas that the Department of Homeland Security believes it should be active in. A high overlap was observed, particularly in "Detection" and in "Response and Recovery."

A BES (not BESAC) Workshop on Basic Research Needs to Counter Terrorism was held February 28 to March 1, 2002 in Gaithersburg, Md. The objective was to identify critical science issues and opportunities in research areas supported by BES that will be important to our nation's ability to detect, prevent, protect against, and respond to future terrorist threats. The major outcome of the workshop is a report that summarizes the presentations and discussions and includes recommendations for future basic research investment needs. It has been posted on the BES website (www.science.doe.gov/production/bes/counterterrorism.html).

The workshop was divided into three parts: radiological and nuclear threats, chemical threats, and biological threats. It started with plenary presentations: a keynote speech by Jay Davis and overview talks on radiological/nuclear threats by Michael R. Anastasio, chemical threats by Michael J. Sailor, and biological threats by David R. Franz. These presentations put things in perspective and pointed at how basic research can contribute to real situations. They were followed by breakout groups on the three basic topics.

The workshop report was organized in the same fashion as the President's report (*Securing the Homeland; Strengthening the Nation*), covering detection, preparedness, prevention, protection, and response and recovery.

In radiologic and nuclear threats, the report focuses on (1) heavy element chemistry (fundamental research on the chemistry of the actinides and fission products, a field in which BES is the sole supporter of basic research); (2) radiation chemistry (in which BES investigates the fundamental chemical effects produced by the absorption of energy from ionizing radiation); and (3) separations and analysis (research on basic science issues related to chemical detection and separations of particular ions from other chemical species). Opportunities and needs that were identified for dealing with radiologic and nuclear threats include

- Reliable, simple-to-operate, inexpensive “yes or no” radiation detectors;
- Remote detection of radioactive material;
- Maintaining critical infrastructure and appropriately trained personnel;
- Readiness to contain contamination caused by a terrorist act;
- Therapies and treatment for victims of radioactive contamination
- Better stabilization of nuclear materials against dispersion (e.g., storage forms for plutonium);
- Alternate separations technologies to detect the chemical signatures of clandestine nuclear-material reprocessing; and
- Methods for the identification of chemical and physical form of radioactive contaminants.

In chemical threats, it focused on chemical-warfare agents (e.g., blister, nerve, choking, and blood agents) and on toxic industrial materials (e.g., methyl isocyanate, chlorine, and hydrogen fluoride) as well as on explosives (e.g., TNT, RDX, TATP). Opportunities and needs that were identified for dealing with chemical threats include

- New sensor concepts using one-molecule-based interactions,
- Improved materials for sample collection and transport,
- New gas-phase processes for selectivity and ion-trapping size limitations,
- Improved synthetic reactions with milder processing conditions,
- New catalysts and adsorbents to mitigate and protect against chemical threats,
- New polymers with designed nanostructures, and
- New separations and analysis schemes that use biomarkers for low-level chemical exposure.

In biological threats, it focused on human pathogens (e.g., smallpox, cholera, shigellosis), zoonoses (not highly contagious), animal pathogens, and plant pathogens. Opportunities and needs that were identified for dealing with biological threats include simple, inexpensive triggers that alert the need for detailed biohazard analysis and other processes and devices.

Many of the identified needs are dual use; that is, they would also be very helpful to the advance of science. And they can draw on extant coordinated research within SC programs in BES, BER, and ASCR, such as the Genomes to Life initiative.

SC has also been involved in the interagency coordination for characterization of biothreat agents to develop a list of potential biothreat agents, prioritize needed research, and determine security issues on data release. It also is involved in the National Nuclear Security Administration (NNSA) Chemical and Biological National Security Program. At the present time, SC does not know what its role will be in homeland security, but it definitely has a role to play. It would be effective to use a national-laboratory approach because the national laboratories provide significant infrastructure, research expertise, and links to the university community. They conduct strong, multidisciplinary science with many components relevant to counterterrorism. They have significant resources and infrastructure already in place. They have a history of successful contributions to national security. And they can bridge unclassified outside-the-fence research and sensitive behind-the-fence technology development. As a prelude to participation, Orbach has appointed a contact on homeland security at each of the SC national laboratories.

Bucksbaum noted that the report recommends that the number of people training for this field should be increased and asked how that could be accomplished. Stevens said that the report does, indeed, recommend that but does not say how it could be accomplished. The answer is offering fellowships and increasing the funding and employment opportunities available to the workforce.

Moore asked what DOE's overall strategy will be in marketing its capabilities to the homeland-security community, noting that, if it is too aggressive, it may lose a large part of SC. Stevens answered that there is not a focus on that topic because the government does not know how it is going to deal with the issue. DOE would like to contribute through the activities of its national laboratories and programs. At this point, it is unknown who will have the lead.

Flynn said that, in preparing the workforce, teachers are needed, not just students, so a longer lead time is needed.

Richmond called upon **Iran Thomas** to speak about the upcoming workshop on assuring a secure energy future. The charge is for "BESAC to oversee a small number of workshops (perhaps 2 or 3) that articulate 21st century discovery potential in DOE mission areas. Defining the role and challenges of basic research is particularly timely given the recent release of the President's National Energy Policy." The primary customer is BES (as opposed to SC). The advice will be used to develop a research portfolio.

When DOE was formed (and until recently), the major issues were increasing and ensuring the supply of oil and gas, finding ways to use coal cleanly and with fewer effects on the environment, and increasing efficiency (primarily to reduce imports). Then, energy sources were abundant and cheap. That situation is now changing. Climate-change predictions have had a profound effect. About 85% of the nation's energy comes from fossil fuels. If the country cannot continue to depend on them, other ways will have to be found to provide energy.

The focus of the workshop should be on the technical issues, such as the fact that currently there is no viable alternative for gasoline. Social issues should only be considered to the extent that science may affect those issues, such as the development of safer nuclear reactors. The basic research community has focused on many of the known problems in energy technologies for many years. The workshop should not rehash these areas. The workshop should focus on new, revolutionary, basic research opportunities.

The workshop will be held October 22-25, 2002, at the Gaithersburg Marriott Washington Center. The Chair will be John Stringer; the Vice Chair will be Linda Horton. The workshop will bring together representatives from national laboratories, universities, industry, DOE staff, etc. BESAC members are invited and will get a letter soon. About 150 attendees are expected.

A number of small topical panels will be used to make a preliminary assessment of the basic research opportunities in eight areas:

- Fossil [Fossil Energy (FE)]
- Nuclear fission [Nuclear Energy Research]
- Solar and other renewable energy [Energy Efficiency and Renewable Energy (EERE)]
- Nuclear fusion (Fusion Energy Sciences)
- Hydrogen (EERE)
- Distributed generation: transmission, storage, fuel cells, etc. (EERE, FE)
- Transportation (EERE)

- Industrial/residential/commercial (EERE)

A resource document is being prepared that will give facts and figures describing the world energy situation. The primary source of this information is the Energy Information Agency. It will include such data as regional population and gross domestic product, energy consumption and production, and energy reserves.

Isaacs asked what effect this workshop will have on SC programs. Thomas responded that that depends on how revolutionary the processes are that are identified in the workshop.

Bucksbaum noted that there were a number of other influences on the formation of DOE than just solving the energy-source problem and asked Thomas if he saw this workshop changing the organization and operation of DOE dramatically. Thomas responded, no.

Morse asked to whom Committee members should send their suggestions for speakers. Thomas said to send them to himself or Sharon Long.

Moore said that the presentation did not mention energy conservation and asked why the workshop does not look at that topic. Thomas replied that energy efficiency is built into all the topics and that transportation is probably the main one. Moore went on to point out that biotransformation (like an enzymatic hydrogen fuel cell) is not on the list of topics and asked if this is because BES does not believe that those devices are going to work. Thomas pointed out that fuel cells are terribly inefficient. A catalyst that would overcome that inefficiency would be welcome.

McCurdy said that the labeling of each topic with a DOE office (in the slide) makes it look like an attempt to market BES to other offices of DOE. Thomas responded that supporting the other offices is one of BES's core missions: not doing their work, but supporting it. McCurdy commented that carbon sequestration does not seem to fall under any topic listed. Thomas stated that it falls under "fossil" because the origin of the carbon dioxide is a fossil fuel.

Richmond introduced **Thom Mason** to report on the progress of the SNS. He briefly described the SNS as designed and under construction. The overall philosophy of the SNS is that it will provide high availability, high reliability operation of the world's most powerful pulsed neutron source. It will operate as a user facility to support peer-reviewed research on a best-in-class suite of instruments. Research conducted at the SNS will be at the forefront of biology, chemistry, condensed matter physics, materials science, and engineering. The SNS will have the capability to advance the state of the art in spallation neutron source technology, including (1) R&D in accelerators, targets, and instruments to keep SNS at the forefront for its 40-year operating life and (2) planned enhancement of SNS performance through upgrades of the complex and ongoing instrument development as part of the normal operating life of the facility.

The project's FY 2002 request of $291 million, was fully funded. The FY 2003 request is $225 million, as anticipated. The overall project design is 80% complete. Overall, the project is 44% complete (through May 2002) and within budget and schedule constraints ($1.4 billion and June 2006 completion). There is good progress on all of the technical components: front end, superconducting linac, ring, target, and instruments. More than 800,000 construction-site work hours have been completed without a lost workday injury. The post-handoff memoranda of agreement (MOAs) have been signed with LBNL and BNL; the LANL MOA is in draft form; others will follow. Relations are good with the partner laboratories. LBNL has now finished its portion of the project, and the performance of the instruments produced is excellent.

Since the outset, the project has been consulting with the user community. Out of 24 possible beamlines, 12 have been identified for instrumentation, 8 have been funded, and 5 are under construction. Two of the other three funded beamlines are BES funded; the other is Canadian funded.

The high-resolution backscattering spectrometer achieves a 2.2- eV resolution at the elastic position. It can operate up to an 18-MeV energy transfer with 10- eV resolution. The performance gains over comparable reactor backscattering instruments is more that a factor of 100 (depending on the bandwidth needed). The various inelastic instruments being deployed allow very good resolution over a wide energy range.

Twenty-four instruments will be positioned on 16 beamlines by having two reflectometers share a single beamport and installing new multichannel shutters in the target station. This setup will allow both vertical-sample (magnetism) and horizontal-sample (liquids) studies. Novel beam-bender optics allows multiplexing and reduces background. A small-angle neutron scattering (SANS) instrument will be used for time-of-flight measurements; it will be able to get data from a wide spectrum in one shot.

With the elastic instruments (the reflectometers, SANS, and a powder diffractometer) different types of science can be performed at different regimes of resolution.

The project is now shifting to higher interaction with the instrument development teams (IDTs). There are currently two funded IDTs with additional teams in various stages of maturity. A proposal for a high-pressure diffractometer (to BES) is imminent, and a German team is carrying out R&D for a spin-echo spectrometer. Guidelines governing IDTs have been issued (see www.sns.gov under users) incorporating input from advisory committees, the user-group executive committee, workshops, and user meetings. These guidelines are being used to implement agreements with the two funded IDTs. The guidelines will be updated once this is done with the use of a template modeled after MOUs developed with the Austrian Research Centers Seibersdorf (ARCS) and the Center for Nonlinear and Complex Systems (CNCS).

A white paper has been drafted to describe the expected operational mode in the early years of operation following project completion (CD-4; June 2006). It covers planning; decisions on spares, designs, budget, etc. that impact reliability; and setting user expectations. It sets the time frame of the evolution from a construction project to a fully operational facility. And it sets goals for the user mode in terms of reliability with respect to schedule (>90%) with the power level and availability as variables to be maximized.

What is wanted is to optimize the scientific performance, which depends on power, reliability, availability, number and performance of instruments, quality of staff, etc. in a nonlinear way. The first six months following CD-4 the facility is under regulatory constraint to stay below Hazard Category 3 inventory threshold [until the operations readiness report (ORR) is complete]. This constraint implies a low power (<10 kW) and duty factor. These conditions are suitable for accelerator commissioning and instrument tests with a beam. Following completion of the ORR, the facility will be able to proceed toward higher-power operation.

In the second mode, operation should be seen at a power level sufficient to test all operational modes of instruments (including inelastic scattering) and to debug control and analysis software. It will not accommodate external users. The facility will try to achieve 75% reliability at about 50 kW for about 500 hours. By the end of year two, the power level should be world class with improving reliability (85% reliability at about 300 kW for about 1000 hours).

In summary, the SNS is well positioned to deliver the world's leading facility for studies of the structure and dynamics of materials. Contingency is adequate (21%), and the early-finish schedule has 6 months of float. The current baseline reflects the results of a recent Estimate to

Complete analysis. The performance of the baseline facility meets the needs and expectations of the scientific community and exceeds the initial conceptual design report goals:

- It is capable of >1-MW beam power (1.4 MW +),
- It includes five best-in-class instruments with room for an eventual suite of 24 instruments (versus 18 in the CDR),
- It has sufficient laboratory and office space to support world-class-facility operations and user needs, and
- The superconducting linac is flexible and ungradable.

Greene asked if the other neutron-scattering facilities will be able to provide the necessary staff. Mason said that they would, that a lot of the operating staff is being pulled out of the other DOE laboratories. The SNS is doing quite well in getting personnel, pulling in the best and the brightest from around the world.

A break was declared at 3:03 p.m., and the Committee was called back into session at 3:34 p.m. **John Galayda** was introduced to report on the progress of the Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center (SLAC).

In the LCLS, an electron beam travels through an undulator magnet (actually, a series of close-packed magnets of alternating polarities), which causes the electrons to emit synchrotron radiation that, in turn, causes the electron beam to form into microbunches that act as if they were coherent single particles, each with a very large charge. The beam is not entirely coherent, but is much more coherent than shock noise. The fundamental free-electron-laser wavelength will be 1.5 to 15 angstroms; the bunch pulse length will be 230 femtoseconds; these conditions require a high power.

The LCLS is a joint effort by several laboratories: ANL, LLNL, and SLAC. The SLAC linac will be modified. A photocathode gun will produce a beam with the requisite brightness, which will then be accelerated through bunch compressors. Spurious microbunches produced will be removed with a wiggler. A 121-m undulator channel is housed in the extended Final Focus Test Facility at BNL.

The LCLS front end will include attenuators, shutters, primary diagnostics, and optics. The facility will also have computer facilities for experiments, a laser for pump/probe experiments, and detectors matched to the LCLS requirements. The project also hopes to include the essential infrastructure for the LCLS experimental program.

The specifications of the device include focusing of 0.1 to 1 m over the full energy range, a ratio of higher harmonics to fundamental of less than 10^{-6}, and split and delay over the range 1 ps to 500 ps.

With regard to the optics, there are major technical challenges: Extreme fluences make it difficult to maintain the optics for more than one pulse. Extremely small temporal and spatial characteristics make it difficult to maintain coherence during beam transport and manipulation and to carry out high-resolution diagnostics. Parameters may vary from pulse to pulse; data are needed on every pulse on a shot-by-shot basis. Windowless operation is required at 0.8 keV. The focusing, imaging, data acquisition, spectroscopy, etc. push the state of the art.

The fluence poses the primary challenge. To deal with the fluences, the following strategies are being adopted:

- A far-field experimental hall to reduce energy densities by natural divergence,
- A gas-absorption cell and solid attenuator to attenuate by up to 10^4,
- Low-Z optics that are least prone to damage, and

- Grazing-incidence optics that increase the optical footprint and reflect most of the incident power.

The LCLS science program is based on the Stanford Synchrotron Radiation Laboratory (SSRL) model. Experiment proposals will be developed by leading research teams with SSRL involvement. Proposals will be reviewed by the LCLS Science Advisory Committee (SAC). Research teams will secure outside funding with SSRL participation and sponsorship, as appropriate. SSRL will manage construction, cost and schedule control, and rationalized design and will establish the maintenance and support infrastructure. SSRL will partner with research teams to commission endstations. In the general-user mode, the beam-time allocation will be based on SAC recommendations.

A cost estimate was performed at the Level 6 of the work breakdown structure; costs were collected in base-year dollars (FY 2002) and did not include inflation. That cost was spread over the schedule to get final project cost. Beam generation was the largest cost (about $100 million or 52% of the whole project). Counting the building, 61% of the costs accrued to SLAC, 25% to ANL, and 14% to LLNL. (Not counting the building, SLAC accrued 48% of the costs.)

The DOE review of the conceptual design at the end of April found that

- The conceptual design is sound and is likely to meet the technical performance requirements.
- The project's scope and specifications are sufficiently defined to support the preliminary cost and schedule estimates.
- The cost and schedule estimates are credible and realistic for this stage of the project.
- The project is being managed as needed to begin Title I design.

In summary, the review found that the CDR is superb, the cost estimate is credible, and the project is on track for approval of its CD-1 in the summer of 2002.

The construction strategy has the project engineering design beginning in 2003 with a $6 million budget to prepare for long-lead procurements (the undulator, gun laser, and injector linac systems) in 2005. In spring of 2003, plans for long-lead procurements would be reviewed. The preliminary design of the LCLS would be completed in spring 2004. Long-lead procurements would begin in October 2004. Critical Decision 3 (approval of the start of construction) would be sought in summer 2005. Free-electron-laser (FEL) commissioning would begin in winter 2007, and the project would be completed in October 2008.

Currently, the R&D of the gun design, undulator prototype, optics-fabrication techniques, and cost-effective magnet fabrication are in good shape. A planning workshop for the LCLS experiment program will be held October 7-8, 2003, to plan for early use of the LCLS. It will define areas for R&D leading to experiment proposals and will kick off the preproposal-preparation process. An international XFEL [X-ray FEL] collaboration workshop will be held in late October to define areas of common interest and collaborative activity. Other opportunities for US-Europe-Asia collaboration will be explored.

In other news, the German Science Council has endorsed the TeV-Energy Superconducting Linear Accelerator (TESLA), giving very strong support of the TESLA XFEL and collider and endorsing the physical separation of the collider and XFEL. The endorsement calls for a technical design report and a faster-track, scaled-down (by about one-half) XFEL. And the first scientific use of a self-amplified, spontaneous-emission (SASE) FEL to do an atomic physics experiment was published on photoionization in xenon clusters.

Johnson asked if there were any issues related to the lifetime and fidelity of the photocathode under these extreme conditions. Galayda replied that they had been using a copper cathode; it gives a good lifetime. Semiconductor cathodes have been used at the Jefferson Laboratory and elsewhere, but they have to be kept under a very high vacuum.

McCurdy asked what the pulse length was and if there were any other parameters that are limiting that the Committee should be worried about. Galayda responded that the target pulse length is still at 230 femtoseconds. However one might not get lasing at that compression. Shorter X-ray pulses can be bred; certain techniques are in the offing to do this. They also intend to look into seeding techniques.

Bucksbaum asked if there was a design goal for the synchronization. Galayda replied that it is a picosecond. Bucksbaum asked if the scaled-down version at TESLA is closer to the LCLS (not a multibeamline version). Galayda answered that they are now talking about having five beamlines at reduced energy.

Richmond called upon **James Roberto** to give an update on the High-Flux Isotope Reactor (HFIR). A major refurbishment has been completed at that facility. A new reflector, cage, shroud, cooling tower, waste line, and larger beam tubes have been installed. Improvements were made to the electrical, mechanical, and control systems. The safety analysis report (SAR) and technical safety requirements (TSR) updates were completed and approved, and the Operational Readiness Review was completed. Operations resumed in December 2001.

The neutron-scattering upgrades included a new guide hall with new and upgraded instruments and with 15 cold and thermal beams, a cold-source intensity comparable to the world's best, increased thermal-neutron intensities, and the establishment of a formal user program (the same as the SNS's). Larger beam tubes were fabricated and installed for increased intensity with vertical focusing. A shielding tunnel was constructed at HB-2 to support multiple beams and instruments. New shutter assemblies and monochromator drums were installed to replace the 30-year-old equipment and to support the larger, more intense beams. The refrigerator plant and moderator vessel were completed and tested. The neutron guides are currently being fabricated in Europe, and the new SANS I and II instruments are also in fabrication. The SANS hall is under construction and includes increased user-support space. After these upgrades, the instrument suite will have improved optics, monochromators, and software. The thermal-neutron intensities will be increased 2 to 10 times at the sample position, and cold-neutron intensities will be increased 100 times for SANS.

There are four thermal-neutron triple-axis spectrometers at HFIR, making the facility world class for investigating magnetic structures (HB-1A); for conducting polarized inelastic studies (HB-1); for studying medium-energy excitations in small or weakly scattering samples (HB-2); and for exploring medium- and high-resolution inelastic scattering at thermal energies (HB-3). It is a very powerful suite for inelastic scattering.

The HB-1 triple-axis spectrometer upgrade has been installed and is operating in commissioning mode. It includes a new monochromator drum, instrument shutter, software, display, motor configuration, analyzer wedge system, and vertically focused monochromator. The typical intensities at the sample are 3 times higher than before the upgrade. Similar improvements are expected at HB-2 and HB-3.

The neutron powder diffractometer is also being upgraded with the addition of 12 new detectors (bringing the total to 44) and a vertically focusing monochromator that uses individually deformed germanium wafers. It also has software, a diffractometer control, and sample environments that are new, producing a factor-of-10 performance improvement for most experiments. This instrument is world class for structural studies, magnetic structures, texture, and phase analysis.

The wide-angle neutron diffractometer that is being upgraded is one of the instruments in the U.S./Japan program. It is getting overhauled to produce a gain in intensity by a factor of 5 to 10. The four-circle diffractometer is getting a new monochromator, diffractometer control system, and software for more efficient peak searching. These changes will produce a performance improvement that is higher by a factor of 2 to 4. It will be world class for small unit-cell crystal structural studies.

There is another US/Japan instrument currently at BNL, the cold triple-axis spectrometer. It is world class for high-resolution measurements of excitations in single crystals, and it will be very complementary to the time-of-flight instruments done at the SNS. Cold-neutron triple-axis spectrometry is very good for high-resolution measurements of excitations. Many frontier problems in condensed matter and other areas demand these instruments.

The cold-neutron spectrometers are being upgraded for large-scale structures, and a 40-m high-resolution SANS spectrometer and a medium-resolution (Biology) SANS are being built for studies of weakly scattering biomaterials, small samples, and pharmaceuticals.

The reflectometer upgrade is moving it to a cold beam line in the guide hall. The upgrade will increase the flux by a factor of 10 and will decrease the background by a factor of 10, making it 100 times more sensitive for

- protein adsorption and biofilm structure at surfaces,
- semiconductor and metallic multilayers,
- polymeric segregation and biomolecular diffusion,
- complex fluid structure at surfaces, and
- time evolution of these surface structures.

In SANS, flux is being increased by two orders of magnitude. Larger-area detectors will make it possible to explore new directions in soft materials; study weakly scattering biological materials; use much smaller samples; and use polarized neutrons to explore magnetic materials, super-paramagnetism, spin-glasses, etc.

Comparing the upgraded HFIR to Institute Laue Langevin (ILL) shows that the pre-sample flightpath, wavelength range, collimator area, and flux at sample are comparable.

The facility is starting to return to full use. It is still a construction site, but experienced people can currently use the equipment. Planning for the formal user program is under way in conjunction with the SNS. A general call will be made in the fall (the formal user program starts at the end of the calendar year). Instruments will be phased into the user program as they are commissioned (with five to six instruments by early 2003 and 10 to 12 in early 2004).

The HFIR user-program guiding principles include:

- Reliable, predictable operation (before the shutdown, it achieved >220 days/year at >90% schedule predictability),
- The provision of world-class instrumentation,
- The provision of fully staffed user support,
- A formal proposal-review system with external committees,
- An integrated HFIR/SNS user program, and
- A joint HFIR/SNS users group (to provide input for instrumentation and user operation).

Plummer noted that increased support would be necessary to operate ten to twelve beamlines in 2004 as planned and asked how that will be possible with a decreased budget. Roberto responded that there is another budget line that covers the operations staff.

Richmond introduced **Altaf Carim** to speak on the transmission electron, aberration-free microscope (TEAM) project. A workshop was held on this topic the week before this BESAC meeting.

When used as a probe of matter, energetic electrons give strong (Coulombic) interactions with both electrons and nuclei. They have very short wavelengths, having been accelerated to ~ 2.5 pm at 200 kV. A high source brightness (~ 1032 s^{-1} m^{-2} $ster^{-1}$) is available today. Such electron beams are readily focused, and there is exceptional spatial resolution. (They can exceed 0.1 nm for imaging.) The main tools for high-energy electron scattering are transmission electron microscopy (TEM) and scanning transmission electron microscopy (STEM).

TEAM is a collaborative development project among four DOE-BES electron-microscopy centers to design, build, and operate the next-generation electron microscopes that take advantage of the correction of limiting lens aberrations and other technologies. The basis is to define a common base instrument platform with a modular approach to tailoring instruments for specific purposes. The focus is on enabling new, fundamental science via quantitative in situ microscopy, to achieve synchrotron spectral resolution at atomic spatial resolution, and to push the resolution to subangstrom resolution in real time and in three dimensions.

They are developing modular experimental stations (e.g., of the sample chamber) for in situ work. Another area that might be modular is a sample holder that uses microelectromechanical systems (MEMS) techniques for in situ studies.

Spherical aberration and chromatic aberration are unavoidable and limiting. With spherical aberration, rays that go through the center of the lens focus differently than those that go through the outer portion of the lens. Chromatic aberration is produced by the angle at which electrons strike the lens; it limits the signal (control) .

Johnson asked if there would be a Coulombic aberration because of charge interaction. Carim answered that there would be, but there is only a very little refraction and it is well understood and corrected for.

Lenses that maintain a large, field-free volume at the sample avoid the high contrast produced by a Lorentz lens. Spherical aberration correction provides a much higher current at a given probe size for quantitative STEM. Improvement in spherical aberration provides a much improved signal in smaller probe sizes. And reducing chromatic aberration enhances resolution and contrast for imaging with electrons undergoing energy losses; through filtering, one can get a chemically specific image.

The principles of aberration correction have been known for 30 years, but it is not easy. A quadrupole-sextupole set can be used to correct aberrations in a Gatan imaging filter (enhanced energy-loss spectrometer). In another design, hexapoles and transfer doublets correct spherical aberration in the current Jülich instrument, but getting all the settings and alignments correct is very difficult. Another way of doing it is to employ quadrupole septuplets and many octupoles.

The impact of aberration correction on microscopy is not known yet, but could be very large. The resolution of current-day corrected electron microscopy is not much different from that of traditional electron microscopes, but it is definitely off the historic curve for those traditional machines.

TEAM aims at enabling new fundamental science, such as:

- Nanoscale tomography, including 3-dimensional determination of glass structure and possibly location of individual point defects;
- Direct observation of atomic-level microstructure during controlled, quantifiable deformation;
- In situ control of electric and magnetic fields for direct observations of interfacial structure, segregation, and defects in active devices and changes induced by fields; and
- Single-column microanalysis, including chemical state information available by improved energy resolution.

Recent breakthroughs and opportunities include the imaging of individual dopant atoms of antimony in silicon by annular dark-field (ADF) STEM; the determination of the ribosome structure to 1 nm by TEM (it could be determined to 0.1 nm with aberration correction); the quantization of conductance in nanowires made up of a single-atom chain of gold; and the real-time observation of the growth of islands of germaniun on silicon (001), which is dominated by coarsening, and the development of a bimodal distribution, in which the small clusters of germanium disappear.

The promise of aberration correction in in situ TEM is to allow more-sophisticated experiments to take place, including those involving vapor-phase processes and liquid-phase processes. The TEAM Project has prepared a vision document, which has been reviewed by a BESAC subpanel. The subpanel recommended favorable consideration of such an effort. A second workshop was held at Berkeley and drew more than 100 attendees. They expressed a very strong interest in, and expressions of support for, the program. A scientific advisory board has been established to provide guidance. A full proposal, involving at least the four electron-beam microcharacterization centers, with possible participation from other parties, is expected by the end of the year. Rough estimates of cost are in the neighborhood of $70 million over five years.

Hemminger asked where the United States stands in this field. Carim responded that there are several aberration-corrected devices in Japan and one in Europe. No science performed with such a machine has come out of Japan; all of the science is coming from Jülich. There are none of these devices in the United States. Some are on order. One has to redesign the whole column.

Moskovits asked why this is a scientific rather than just a technological challenge. Carim replied that there are a couple of problems. First, if one has spherically symmetric lenses, one would *always* have spherical aberration. Second, part of the problem is that an electron beam is a different beast; one cannot make a correcting lense.

Stupp asked what was in the electron microscopy pipeline for soft matter. Carim said that soft matter gets less attention because it is outside the comfort zone. Some techniques (like helium-cooling stations) were discussed at the workshop. It all depends on the size of the sample holder. The problem of doing very short exposures is also being looked at.

Stohr asked what is preventing the commercial sector from producing the advanced designs and why a government program is necessary. Carim said that the commercial sector would probably produce machines with these capabilities eventually in the normal course of business, but it would not happen in the coordinated manner that a DOE project would: setting the baseline and doing acquisition and analysis. The problem is getting bigger all the time.

Isaacs asked if a microscope with perfect aberration correction would be brightness limited. Carim said, no, there would be other, lesser aberrations. The problem ends up being stability.

Richmond called for public comment. There being none, she adjourned the meeting for the day at 5:16 p.m.

Tuesday, February 26, 2002

Richmond called the Committee to order at 8:05 a.m. and initiated a discussion of the catalysis-workshop report. A group of BESAC members and Michael White had met on Monday evening to devise a strategy for moving forward. **John Hemminger** presented the findings of that group. The group agrees with the sense of the outcome of the workshop, including agreement with the specific recommendations of the report. The problems are that (1) the report needs to be livened up and (2) there is a perception that no results have come from the funded catalysis research in the United States (that statement is proven wrong by every car with a catalytic converter). There has been a fundamental revolution in catalysis because of

- nanostructure characterization
- nanostructure synthesis
- controlled models of oxide supports
- fundamentals of reaction dynamics on complex surfaces
- theory of complex systems

As a result, the time is ripe for a new investment in fundamental catalysis research that builds on this fundamental revolution.

For the current version of the report, the group proposed a new statement of the recommendations and called for a statement of why the time is right for new funding. It also suggested that the report recommend the issuance of a call for proposals that focus on the creation of new and innovative approaches to research in catalysis and that specifically address modes of interaction with the NSRCs and other DOE user facilities. Richmond polled the members of the reviewing group, and all of them agreed with the assertions put forward in the presentation.

Long suggested holding a workshop to bring together basic researchers with industrial users. Hemminger said that BES should not be funding work for industry, but one *does* need to find ways to couple the research done with potential users.

Bucksbaum noted that the call for the establishment of national centers seemed to have vanished. Hemminger acknowledged that there had not been a lot of discussion of the centers versus principal investigators (PIs). It is important that the research done integrate the advances of the past decades; therefore, it must adopt a multi-individual, multidisciplinary, multi-institutional approach. That approach may or may not involve centers.

Johnson called attention to the fact that the nanoscience report made it clear that, if the United States did not support theory and modeling in nanoscience, opportunities would be lost. He did not hear the same level of convincingness from the catalysis report. Hemminger said that it is hoped that the rewritten report will address that problem. One of the primary revolutions is theory and modeling of catalytic designs.

Richmond suggested that the Committee accept the ideas put forward in the report but not accept the report as written. Rather, it should request that the report be rewritten according to the suggestions of the reviewing group. BESAC should then review the revised report at the November meeting. Plummer added that a cogent executive summary be written for the report. The suggestion was accepted unanimously.

Dehmer introduced **James Roberto** to speak about a workshop for the DOE Nanoscale Research Centers to be held in Washington, D.C., Feb. 26-28, 2003. The purposes of the workshop are to roll out DOE's NSRCs to the scientific community; communicate the NSRC concept to policymakers and the scientific community; hold the first national NSRC users meeting (on the second day of the workshop); announce a program to initiate user operations; and provide a forum for communication on nanoscience and the NSRCs among agencies, policymakers, and the scientific community.

The preliminary program includes poster presentations and booths for each NSRC. A science session will cover four topics:

- What is nanoscience
- Carbon-based nanostructures
- Catalysis and nanoscience
- Integrated view of NSRC science

An industry session will take a venture-capitalist view of nanoscience and look at nanoscience in information technology and in the chemical (or auto) industry. A follow-on session will discuss the report of the NRC study on the National Nanotechnology Initiative (NNI) and what the agency roles are in that initiative (agency by agency). The workshop will conclude with a NSRC users meeting that gives an overview of the program, presentations from each center, and a panel discussion by the center scientific directors.

Stupp noted that an earlier workshop on nanoscience attracted representatives from the Department of Commerce and the Central Intelligence Agency.

McCurdy commented that, if the planning committee wanted to influence policymakers, this method of presenting the agencies seems inefficient and asked what types of people did they have in mind as industry types. Roberto responded that no invitation list had been drawn up yet, but people like Paul Horn came to mind.

Greene said that they need to address users and let them know about the existence and capabilities of the centers and how they can use them. Roberto responded that that is what the second day is devoted to. Greene said that she would suggest having some university speakers. She would like to hear some success stories out of the new centers, projecting a new science and a new perspective. Then she would tell how other researchers can get involved, telling them what they can and cannot do. Stupp suggested that they tell what these centers are right up front. Then, through the rest of the workshop, get feedback from the attendees about how they would and would not use the centers. Regarding the agency presentations, he urged them not to miss the NIH while promoting DOE.

McCurdy said that it was not clear if this is a multiagency or strictly DOE workshop. Smalley commented that one of the wonderful things of the NNI is that it *is* multiagency and that he found DOE’s intent to be inclusive to be very attractive.

Flynn called attention to the fact that this workshop is addressed at a variety of audiences. The policy meeting should be one entity, and the science meeting another. Roberto noted that the different days are largely aimed at different audiences. Perhaps Friday’s schedule could be expanded to better meet the needs of the scientific audience. Berrah asked if they could have a session on Friday for the scientific community to talk about what they need and would like to do. Roberto replied that they have the time and space to do that.

Dehmer asked **Terry Michalske** to talk about the NSRC rollout campaign. It includes the kickoff workshop described by Roberto, connecting with the professional societies, announcements in journals and bulletins, a Web page, briefing materials, educational outreach, and NSRC-sponsored symposia. Some action items have been identified for each of these categories and assigned to personnel:

- Briefing materials:
  - One-page fact sheets (Parkin)
  - A view-graph package (Alivisatos)
- Website:
  - BES website for the NSRCs (Carim)
  - Consistent content and terminology for the centers (Dierker)
- Connection to professional societies:
  - Collect input (Michalske)

Richmond then called upon **Paul Lisowski** for an update on the Los Alamos Neutron Science Center (LANSCE). He reviewed the physical plant and general operations of the LANSCE. The Lujan Center had a highly successful run cycle in 2001. It delivered 2499 hours, or 131% of its goal of 2735 hours at 75% availability. It delivered an integrated charge of 83% of its goal with a 54- A average current. It performed 113 user experiments with a 91% reliability of beam delivery and more than 95% instrument availability. It supported 270 user visits, representing 150 unique users. It commissioned five new scattering instruments [SMARTS, HIPPO, PROTEIN, PHAROS (rebuilt), and ASTERIX] and one nuclear-science instrument (DANCE). It developed and implemented a new generation of data-acquisition and chopper-control systems. It also obtained approval for actinide experiments and doing experiments with plutonium.

Major milestones for LANSCE's CY 2002 schedule are

December 24, 2001	Cease CY 2001 operations
January 2, 2002	Begin CY 2002 outage (17 weeks)
April 22-23	Materials Program Advisory Committee Review Meeting
May 1, 2002	Begin CY 2002-2003 user-facility turn-on (37 days)
May 27, 2002	Begin proton radiography operations
June 1	Schedule of operations published on Web
June 3, 2002	Begin proton storage ring operations
June 19, 2002	Begin Weapons Neutron Research facility low-power operations
July 7, 2002	Begin Lujan Center tune-up
July 26, 2002	Begin scheduled user-facility operations
January 26, 2003	Cease CY 2002-2003 operations

The facility plans to run longer next year.

The Lujan outage schedule in CY 2002 was aggressive and completed in time to start the user program. The old Lujan target was removed and placed in storage as a low-current spare, and a new target was installed and is operational at 100 A). The integrated-shielding package was installed on flight paths 11, 12, and 13. A new, redundant personnel-protection system was installed on all flight paths (a major effort). New mercury shutter reservoirs were installed for older flight paths with upgraded piping and sensor systems (for fire safety). Computerized control of all shutters was implemented, and data are now available in the Central Control Room. The data-acquisition conversion of user-program instruments was completed. The ASTERIX instrument was rebuilt. The NPDF (formerly the Neutron Powder Diffractometer) upgrade is under way.

The size and quality of the user program is being expanded as rapidly as possible, consistent with the strategic plan and previous BESAC recommendations. The goal is to increase the user base by 15%. The facility plans to deliver beam at 100 A with >75% availability for 2616 hours for the user program, supplemented by 336 hours for instrument tune-up and 384 hours of

contingency time. The beam downtimes longer than 8 hours are being limited to <10% of scheduled time. As a result, 95% instrument reliability will be delivered. Money is being put into an increase in sample-environment support (an 11-T magnet, a cryofurnace, and more staff support).
The rotation model for CY 2002-2003 user program in neutron scattering maximizes the number of instruments.

LANSCE will continue a predictable, repetitive 28-day operating cycle with contingency in CY 2002-2003. Beam delivery to the Lujan Center will increase 25% after installation of a switchyard kicker magnet during the CY 2003 outage. It is also aggressively implementing the December 2000 BESAC recommendations in its operations and governance:

- Stewardship responsibility was assigned to NNSA, and an Executive Council was established.
- An externally and internally peer-reviewed, bottom-up cost estimate was completed for LANSCE.
- A ramp-up schedule for full functional status was completed as part of the cost estimate. There is a funding increment of $10 million in 2003 LANSCE operations budget. The facility began the process with a successful CY 2001 operating cycle with 270 user visits and 150 unique users.

In summary, in 2001 LANSCE completed an excellent scientific program at all facilities with the largest number of users to date. Proposals for LANSCE use in 2002 were evaluated, and an operations schedule was developed with the lessons learned from 2001. LANSCE completed an aggressive, well-managed outage on schedule and is operational. The Mark-I Lujan target-moderator-reflector system has been moved to storage and is available as a 55- A backup. The Mark-II Lujan target-moderator-reflector system has been installed and is operational at 100 A. The switchyard-kicker project is proceeding well, and the equipment will be installed and commissioned in 2003. The Lujan Center user program will start on July 26, 2002, and run until January 26, 2002.

Morse asked what the annual budget of the Lujan Center was. Lisowski responded that it is $9 million to support the user program out of a total budget of $50 million.

A break was declared at 9:32 a.m. The Committee was called back into session at 10:01 a.m., and Richmond called upon **William Oosterhuis** to talk about the operating light and neutron sources. Four light sources have been reviewed during the past year. Reviews of the light sources are performed by BES every three years. The objectives of these reviews are

- to produce the best science possible at our facilities,
- to ensure that the user community has access to the light sources through a proposal-evaluation system that is fair and competitive and that stimulates the performance of high-quality research, and
- to make sure that the resources provided to the facilities are used to optimize its utilization and to develop new and better techniques for synchrotron radiation applications.

The topics covered in the review include

- Facility performance in terms of schedules, user participation, number of proposals, etc.;
- Selected presentations of the most outstanding research performed at the facility during the previous two years;
- R&D plans and future scientific directions that are possible with the facility; and

- Laboratory plans that may affect the facility.

The schedule of the review should include time for the reviewers to meet individually with the facility scientific staff in their focus areas and additional areas of interest. Reviewers would like to have a focus session with representatives of the users community (i.e., the User Executive Committee) and participating research team (PRT) spokespersons (not affiliated to the facility) without the laboratory management present. The agenda and logistics for the review should be coordinated with BES.

Information Requested from the Facility	
Facility	Brief description Breakdown of all staff and their assignments Description of ongoing R&D
Beamlines	Floor plan with a brief description of each beamline's capabilities and use Beamlines available to users and percentage of time allocated to outside users Beamlines operational and percentage of time allocated to outside users Communities served by each beamline
Support Facilities	What is available What is planned
Users	How beam time is allocated to outside user Beamtime allocations versus the number of groups receiving this allotment
Impact	Publications in refereed journals in the past two years Invited lectures and major awards The 20 most important publications of work performed at the facility during the past 2 years, including citation index
Cost Indicators	Cost per paper Cost per delivered beam day
Future	Plans for future beamlines and facility upgrades Potential impact of the phasing out of PRTs because of financial or scientific difficulties Budget estimate for keeping beamlines operating Potential problems Budget estimate for upgrading the beamlines' scientific instrumentation, motor controls, detectors, and associated electronics Expected trends in user demand

The reviewers receive a set of questions to consider, such as: What is the quality of the research performed at the facility in terms of number and impact of published research? What is the appropriateness and quality of the facility staff R&D program? What is the satisfaction of the user community with the facility support and staff? And each reviewer writes a separate review.

The reviews of the four BES synchrotron radiation facilities were completed by February 2002: SSRL on April 3-5, 2001; the National Synchrotron Light Source (NSLS) on July 11-13, 2001; the Advanced Photon Source (APS) on October 16-18, 2001; and the Advanced Light Source (ALS) on February 4-6, 2002. For those four facilities in FY 2001, the total number of users was 6568, the total number of general users was 4412, the total number of publications was 2061, and the total number of beamlines was 166.

BES will begin a review of the neutron sources this fall.

Plummer asked him how he knew that a grant, not a scientific thrust, is what has a lifetime of 7 years. Oosterhuis replied that the decision not to fund the project results from peer review by the funding agency's science advisory committee. Dehmer added that these reviews look at operations and the science. They are built on what Birgeneau did. These reviews are different from those that make funding recommendations.

Stohr asked what they did with the information they gather. Oosterhuis answered that the reviewers usually say that the facilities are operating very well. In some facilities, the reviewers have suggested significant changes in how those facilities allocate their funds. The process is moving toward the SSRL model. Stohr pointed out that, when a problem is found, that information does not get back to BESAC for discussion. Dehmer said that it is not appropriate to go into the details of operations reviews here; such reviews should be alternated with Birgeneau-type reviews conducted by BESAC. The two types of reviews have some overlap, but in some ways look at different aspects of the facilities. One or the other does not give the whole picture.

Plummer pointed out that one needs to know where the funding comes from. Dehmer responded that the staff could put together a high-level summary the next time, including some summary statistics. Oosterhuis noted that Steve Dierker would have a chart that shows such a summary for the NSLS in his presentation, which was to follow Oosterhuis's.

Berrah said that she would like to see some way for this Committee to address any issue that was raised in these reviews. Oosterhuis replied that the issues raised are, typically, personnel or funding. The review looks primarily at performance of the facilities.

Johnson commented that one role of the light sources is to train the next generation of users. Oosterhuis replied that Stanford certainly had a program to do that but acceded that not all facilities do that.

Richmond asked **Steve Dierker** to give the facilities' perspective on the review process.

The NSLS was the second facility reviewed by BES last year. It was a comprehensive look at a wide range of activities and it focused sharply on the user experience. The facility was notified five months in advance and was asked to prepare two full days of presentations, site visits, etc. and to touch on a variety of topics:

- Facility performance (schedules, user participation, etc.),
- Selected presentations of the most outstanding research performed at NSLS during the last two years (by field of research),
- R&D Plans and future scientific directions, and
- BNL plans that may affect NSLS.

The panel expressed a real desire to spend time with individual facility scientific staff and the user community, so focus sessions with user representatives and PRT spokespersons were arranged. Information was prepared on the facility, its beamlines, support facilities, users, beamtime allocations, user experiments, proposals, impact (in terms of publications, awards, etc.), costs, future plans, potential problems, and trends in user demand. All of this information was compiled ahead of the visit.

In addition, BES scientific facilities are required to complete surveys on

- User satisfaction,
- User demographics, and
- Budget and operations.

The major tasks involved in participating in the review are defining the agenda; choosing and scheduling speakers; responding to information requests; arranging the participation of users, the User Executive Committee, and PRTs; and arranging site visits.

The agenda for the review started with presentations of outstanding science arranged by scientific category. Lunch was used as an opportunity for reviewers to meet users. The review continued with an overview of operations and budget issues followed by beamline visits and breakout sessions with NSLS scientists. A second series of science-highlight presentations was held, followed by forward-looking presentations on programs, hardware, improvements, and other resource issues.

The demographics of the user community showed 2500 scientists being served each year. They were from more than 400 academic, industrial, and government institutions. This represents a 50% growth in the number of users during the past decade. A strong growth in the life sciences was noted. Two-thirds of the users were from northeastern states, one-sixth were foreign, and one-sixth came from the rest of the United States. The users included large numbers of graduate students and postdocs; most are young, early-career scientists. An increased number of academic and BNL users was apparent. Analysis showed that 47% of the beamtime is used for materials science, with the average experiment running 11 days; 16% is used for the life sciences, with the average experiment running 3 days. Looked at from a different perspective, the data show that 35% of the experiments are in materials science, and 35% are in the life sciences. More than 800 publications appear each year from the work done at the NSLS; more than 100 of them in premier journals. The staff has worked hard to ensure that operations are reliable and the facility is well maintained. For the vacuum ultraviolet (VUV) ring, availability last year was 103.7% of what was planned; for the X-ray ring it was 107.4%.

The overall DOE report was that

- Research is outstanding, as reflected in large number of publications and the high index of citations.
- There was a notable, continued improvement in performance, especially in efforts in digital orbit feedback and the development of in-vacuum undulators.
- The infrared research program is very important, a unique feature.
- The scientific/technical staff is doing outstanding job.
- NSLS is a mature and stable facility, and there was a concern that staffing levels would not reflect this.

The DOE report raised several issues:

- Beamline staff is too small to deal with users, upgrade beamlines, and maintain a viable scientific program.

- There is an imbalance in full-time equivalents (FTEs) in machine physics versus beamline staff.
- There are significant operating problems with some PRTs.
- Several beamlines show signs of neglect from benign to serious.
- The X13 insertion device should accept external users.
- The U5 insertion device scientific program has underachieved and should be modified.
- There is a need to focus accelerator research on projects relevant to the operational improvement of the NSLS.

The DOE report recommendations flowed from these issues and called for

- An increase in beamline scientific staff;
- A plan to optimize beamline utilization and to eliminate the operation of beamlines that are not scientifically productive and/or do not have upgrading capabilities;
- A plan for facility control, or at least participation, in the management and operation of PRTs that are having financial and staffing problems;
- A redefinition of the U5 scientific program;
- Facilitation of general-user access to X13 on a peer-review basis;
- A reduction in accelerator-physics staff; and
- A plan for accelerator research at the NSLS.

One subsequent response to the review was the reorganization of NSLS into four divisions: ES&H, User Science, Operations, and Accelerator. In accelerator physics, the Accelerator Test Facility (ATF) was transferred from the NSLS to the Physics Department, where it will be better aligned with High-Energy Physics and BNL programs. That move also allowed the redirection of more than $500,000 to user program support. The mission of the Accelerator Division was declared to include

- Maintenance and upgrading of the existing storage rings,
- Provision of X-ray digital feedback for beam position stabilization,
- Development of new insertion devices,
- Investigation of NSLS upgrade options, and
- Basic studies of beam physics.

To increase the beamline scientific staff, the user-program support is being increased by 13 FTEs, including 8 new hires and the redirecting of 5 current FTEs. User support is being improved through three levels of support: routine maintenance of beamlines by NSLS, routine beamline operation and user support by NSLS, and support of scientific programs jointly by NSLS and the user community.

In conclusion, the review is very thorough and comprehensive. The facility staff must prepare well in advance. A strong involvement of user community is crucial. The results have weight and can be useful in helping to enable change.

Flynn noted that Dierker's slides had shown the number of undergraduate and graduate students to be 900 and the number of participants who were 20 to 30 years old to be 600 and asked why. Dierker did not know why. Flynn asked what the costs were that were cited. Dierker responded that they were the facility operating costs. Bucksbaum asked if the members of PRTs were added into the users. Dierker said that the operation of beamlines and maintenance are the responsibility of the PRTs. If an instrument is of interest to a specific group, they are responsible for its funding. This approach is evolving.

Isaacs asked whether DOE has given any thought to how to partner more effectively with NIH, given the growth of that agency. Thomas responded that BES is concerned that, given that most of the beamtime is devoted to the physical sciences, too much of the floor may be allocated to the biological sciences. That floor usage must be monitored very carefully. If NIH wants to increase that usage to accomplish the research that they must perform, DOE would have to think very carefully about how to do that and would have to consider the impact on other programs. Dehmer added that this topic has been considered time and time again and was revisited recently by a committee of the National Academies. That committee was very thoughtful and experienced and knew firsthand the instability in operations that can be produced when the operation of a facility was multiply funded by different agencies or by different parts of the same agency. A very strong recommendation came out: that all major user facilities be coordinated by a steward agency and that there be a number of partner agencies (representing all other users) that support the facility, beamlines, users, upgrades, and specialized operations. The Office of Science and Technology Policy also held committee hearings on the subject with participation by all the agencies that are in play here. Those hearings discussed the appropriate roles of the agencies and showed that NIH has made significant investment in its own beamlines. They also identified roles that the steward agencies were performing.

Berrah asked if BES provides financial support for undergraduate and graduate students. Dierker responded that it provides some modest support for travel. After one year, they have to have their own support.

Hemminger noted that the data that the light sources pulled together for the reviewers are data that the management should be looking at continually and asked if those data are continuously maintained and referred to. Dierker agreed that these data were important to the management of the facilities and stated that the NSLS was putting in place means to keep them up to date.

Oosterhuis noted that Marberger was on these reviews and now, as Presidential Science Advisor, is very knowledgeable about light sources and mentions them often in his public presentations.

Richmond called for general comments from the Committee; there being none, she opened the floor for public comment. There being no public comment, she thanked the BES staff for organizing the meeting and announced that the next meeting will be Nov. 4-5, 2002. The meeting was adjourned at 11:21 a.m.

Repsectfully submitted by
Frederick M. O’Hara, Jr.
Recording Secretary
Aug. 5, 2002