Minutes for the
Basic Energy Sciences Advisory Committee Meeting
February 26-27, 2001
Gaithersburg Marriott Washingtonian CenterGaithersburg, Maryland

BESAC members present:

Boris W. Batterman	Collin L. Broholm
Jack E. Crow	D. Wayne Goodman
Laura H. Greene	Anthony M. Johnson
Walter Kohn	Marsha I. Lester
Anne M. Mayes	C. William McCurdy, Jr.
Geraldine L. Richmond, Chair	Zhi-Xun Shen, Vice Chair
Sunil Sinha	Joachim Stohr
Samuel I. Stupp (arrived late Monday morning)	Edel Wasserman

BESAC members absent:

David D. Awschalom	Patricia M. Dove
James A. Dumesic	Mostafa A. El-Sayed
C. Bradley Moore	Robert B. Horsch
Cherry Murray	Richard E. Smalley
Kathleen C. Taylor	David E. Tirrell

BES Management present:
Patricia Dehmer, Director, Office of Basic Energy Sciences
Iran Thomas, Deputy Director, Office of Basic Energy Sciences

Also participating:
Bruce Brown, Director, Intense Pulsed Neutron Source, Argonne National Laboratory
John Browne, Director, Los Alamos National Laboratory
Steve Brueck, Director, Center for High Technology Materials, University of New Mexico
Daniel Chemla, Director, Advanced Light Source, Lawrence Berkeley National Laboratory
Massimo Cornacchia, Assistant Director, Stanford Linear Accelerator Center
Patricia Dehmer, Director, Office of Basic Energy Sciences, DOE
J. Murray Gibson, Argonne National Laboratory
J. B. Hastings, Center for Neutron Sciences, Brookhaven National Laboratory
Keith Hodgson, Director, Stanford Synchrotron Radiation Laboratory, Stanford University
Allen Hurd, Director, Manuel Lujan, Jr., Neutron Scattering Center, Los Alamos National Laboratory
Paul Lisowski, Director, LANSCE Division, Los Alamos National Laboratory
Thom Mason, Director, Spallation Neutron Source, Oak Ridge National Laboratory
Terry Michalske, Head, Surface and Interface Science Department, Sandia National Laboratory
Richard Osgood, Associate Director, Brookhaven National Laboratory
Don Parkin, Center for Materials Science, Los Alamos National Laboratory
James Roberto, Associate Director, Oak Ridge National Laboratory

In addition, about 60 others were in attendance as observers.

Monday, February 26, 2001

Chairwoman Geraldine Richmond called the meeting to order at 8:35 a.m. She noted changes in the agenda and had the committee members introduce themselves. She introduced **Patricia Dehmer** to review developments within the Office of Basic Energy Sciences (BES).

Since the previous meeting of the Basic Energy Sciences Advisory Committee (BESAC), George W. Bush became the 43rd president of the United States, and he has appointed Spencer Abraham as the new Secretary of Energy. Abraham represented Michigan in the United States Senate from 1995 to 2001, where he served on the Budget, Commerce, Science, Transportation, Judiciary, and Small Business committees. He is not trained as a scientist but has a strong interest in science and is a strong supporter of science. The offices of Deputy Secretary; Under Secretary for Energy, Science, and Environment; and Director of the Office of Science (SC) are vacant and may remain so for 6 to 8 months. The organization of SC was reviewed. Of particular note was the fact that Jim Decker is the Acting Director, Milton Johnson is the Acting Principal Deputy Director, and Leah Dever is the Acting Deputy Director for Operations. This situation puts people with a lot of experience in the front office.

The directions of the new administration are being revealed by what the members of the Executive Branch are saying. In conference hearings, Secretary Abraham spoke positively about the national laboratories: “The science and technology programs at the Department have been widely praised, and justly so. I cannot stress enough my desire to continue to move this Nation forward in this area.” Mitchell H. Daniels, Jr., Director of the Office of Management and Budget (OMB) said, “I no longer support this legislation [to break up DOE].” The first budget will focus on restraining the growth rate and implementing the President’s campaign promises. “Major programmatical changes in the main will be reserved for the future.” President Bush has indicated that he wants to slow the pace of government spending, seek Department of Energy cutbacks in the budget for the nuclear-weapon program, and make room for tax cuts and education by tightening the budgets for science agencies. The outlook is that the National Science Foundation (NSF) budget will be up 1% and those for other agencies will be flat; the National Institutes of Health (NIH) budget may be doubled by 2003.

In the House of Representatives, Sherwood Boehlert (R-NY), Chairman of the House Committee on Science, said that “any downturn in our science investment is cutting into our competitive edge and against our long-term interests. ... I want... a healthy, sustainable, and productive R&D establishment.”

In the Senate, Jeff Bingaman (D-NM), Senate Committee on Energy and Natural Resources, said, “I have been a strong proponent of the science and technology programs at DOE for many years. In the last year or two, I have been increasingly concerned about the stature and health of the DOE programs funded by the Office of Science.” He believes we need to revitalize DOE’s missions.

BES has established a Web page at http://www.sc.doe.gov/production/bes/congress.html, where one can find the membership of all Congressional committees as they are updated. This listing includes the House committees on Science, Energy and the Environment, Appropriations, and Energy and Water Development and the Senate committees on Energy and Natural

Resources; Energy Research, Development, Production, and Regulation; Appropriations; and Energy and Water Development.

Trends in federal research from FY 1970 to FY 2000 were analyzed by the NSF and distributed by the American Association for the Advancement of Science (AAAS). These graphs show that the physical sciences have had constant budgets or worse (in inflation-adjusted dollars) for nearly two decades. Funding for the life sciences has been increasing and will continue to do so. Funding for other disciplines is flat. At its recent meeting in California, the AAAS Council passed a resolution to encourage balanced support for all sciences, reflecting their importance in society.

The indicators that are important here are funding statistics and trends, workforce statistics and trends (especially international comparisons), the physical infrastructure, international scientific leadership, industrial leadership and innovation, and the public attitudes toward and understanding of basic physical sciences. These indicators are not linearly independent variables. Funding impacts the workforce and the physical infrastructure; the workforce drives scientific leadership; there is a link between scientific leadership and industrial leadership; and all of these attributes impact public attitudes. Those public attitudes, in turn, influence funding.

An analysis of normalized growth since 1980 shows that funding for NIH has quintupled, the gross domestic product (GDP) has increased by a factor of 3.6, funding for SC has about doubled, and funding for DOE has remained about the same. At the same time, inflation has caused a 20% decrease in buying power, construction of BES facilities has grown, and funding for basic research has grown (but does not match inflationary trends).

Workforce statistics at the DOE SC Labs in both high-energy physics and basic energy sciences have seen a decline. Statistics on undergraduate science degrees indicate that the United States is not training as many people as other countries are. In the population of 24-year olds, the percentage having scientific training increased from 4.0% to 5.5% in the United States between 1975 and 1997. In the United Kingdom, it increased from 2.9% to 9.3%. For the first time in 14 years, the total number of PhDs awarded in the United States has gone down, dropping 3.6% between 1998 and 1999. NSF statistics show that PhDs awarded in physics, chemistry, and geosciences all declined in 1999. Historical data indicate that the number of science and engineering doctoral degrees awarded in the United States flattened out in 1996 and 1997 and declined slightly since then.

The condition of the infrastructure at the DOE SC laboratories ranges from superb to downright ugly. The worst problems in the complex were illustrated with examples of deteriorating laboratory conditions at Oak Ridge National Laboratory (ORNL). World-class research cannot be conducted under the conditions in these facilities.

Scientific leadership is quantified by looking at the Nobel Prize research supported by BES during the 1990s, resulting in four Nobel Prizes: 1994 Physics, Clifford G. Shull; 1995 Chemistry, Frank Sherwood Rowland; 1996 Chemistry, Richard E. Smalley and Robert Curl; and 1997 Chemistry, Paul D. Boyer. The list of major prizes and awards received by BES researchers in FY 2000 is extensive. In this regard, the program is doing well. In chemical sciences, researchers in the catalysis program have won 60% of the awards given by the American Chemical Society for homogeneous or heterogeneous catalysis and for organometallic catalysis and 70% of the awards given by the North American Catalysis Society for heterogeneous catalysis. In materials sciences, the large DOE laboratory programs consistently rank among the top materials sciences programs worldwide. Of more than 1000 institutions surveyed, typically

Argonne National Laboratory (ANL), Lawrence Berkeley National Laboratory (LBNL), ORNL, and the University of Illinois materials-research laboratories rank among the top 25 institutions in the world based on citations of high-impact papers published.

Is there a problem? SC conducted international benchmarking studies of U.S. materials science and engineering research (biomaterials, ceramics, composites, magnetic materials, metals, electronic and optical-photon materials, superconducting materials, polymers, and catalysts) and concluded that the United States is currently among world leaders in all the subfields of materials science and engineering and currently enjoys a clear lead in biomaterials. The United States is expected to maintain its lead in metals and electronic-photonic materials because of its large industrial base. However, erosion of U.S. leadership is expected in the subfields of composites, catalysts, polymers, and biomaterials because of the high priority being given to these subfields by other countries. Current U.S. weakness in materials synthesis and processing relative to Europe and Japan is especially highlighted in the benchmarking panel's assessment. SC is going to do more of these international benchmarking studies.

Submissions to the American Physical Society (APS) journals *Physical Review* and *Physical Review Letters* is skyrocketing, but U.S. submissions are declining.

In R&D as a percentage of GDP in the G-8 countries, the United States is between Japan and Europe and is decreasing as the other countries are increasing.

A survey of the public's understanding of scientific terms and concepts in 1999 indicated that only 12% of those polled correctly understood the concept of a molecule. But the public attitude about science is positive; 75 to 80% believe that the benefits of scientific research outweigh any harmful results. The public has a lot of faith in science even though its members do not understand it.

During the past 25 years, public confidence in the leadership of medicine and science has remained constantly high while confidence in the leadership of other sectors has plummeted. However, these attitudes are volatile and tenuous because the respondents do not understand the institutions they are judging.

Asking how much science has advanced is instructive. The first X-ray was made public by Roentgen in a Jan. 23, 1896, lecture. Today, X-rays are used to produce images of complex molecules. The concept of ion channeling was introduced in the 1960s; only 30 years later, ion implantation was used to modify materials for use in artificial hip prostheses and to modify silicon to make chips. Tools for manipulating materials have advanced from crude handaxes about 1,000,000 years ago to a scanning electron microscope tip that can position individual atoms.

Fitting these bits and pieces together, one can assess the status of BES. The major funding components of BES (in millions of dollars) are: user facilities, 255.0; construction, 100.0; base research (universities), 131.3; and base research (laboratories), 198.6. This budget includes support for the world's largest collection of scientific user facilities for "materials sciences and related disciplines" supported by a single organization, serving nearly 8000 users annually. Notable among the facilities are four synchrotron-radiation light sources and three neutron-scattering facilities.

Synchrotron-light sources in the past two decades have shown a great increase in use. The number of researchers using the radiation synchrotron light sources is expected to reach nearly 11,000 annually when beamlines are fully instrumented. There will be a large growth in users at the Advanced Photon Source (APS) and the Advanced Light Source (ALS). BES provides the complete support for the operations of these facilities. Furthermore, BES continues as the dominant supporter of research in the physical sciences, providing as much as 85% of all federal funds for beamlines, instruments, and principal-investigator (PI) support. Many other agencies, industries, and private sponsors provide support for instrumentation and research in specialized areas, such as protein crystallography.

Under construction is the Spallation Neutron Source (SNS), which will be the world's most powerful accelerator-based pulsed-neutron source, producing 6 to 10 times more neutrons than any other such source. The $1.4 billion project at ORNL is the nation's largest civilian science project. It will be commissioned in FY 2006. Currently, the SNS is on schedule and within budget. It is 20% complete overall (design is 70% complete). Technical systems R&D, design, and procurements are all on track; notable technical achievements continue to be produced with no significant problems. The site is ready for building foundations, and utility work is being conducted this spring. The project is staffed at the planned level [more than 700 full-time-equivalent employees (FTEs) at all the participating laboratories]. It has an outstanding safety performance, and the project is on track to meet Level 0 (Secretarial) baseline goals.

BES supports a broad array of fundamental research in materials science and engineering, chemistry, physics, geosciences, and biosciences. In the past, BESAC has looked at a lot of the components of the BES science program and done an outstanding job assessing and guiding that program. BESAC is now going to look at the program through "visiting committees." The draft charge calls for the visiting committees to achieve several goals:

1. For both the DOE laboratory projects and the university projects, it will assess the efficacy and quality of the processes used to (1) solicit, review, recommend, and document proposal actions and (2) monitor active projects and programs.
2. Within the boundaries defined by DOE missions and available funding, it will comment on how the award process has affected the breadth and depth of portfolio elements and the national and international standing of the portfolio elements.
3. It will comment on future directions proposed by the Division and BES management and on opportunities that might not have been presented.
4. It will comment on how the process for these reviews might be improved.

Four new people have been added to the BES staff.

In the Nanoscale Science, Engineering, and Technology (NSET) initiative, $32 million in new funding has been received. A request for NSET solicitations was issued with preapplications from universities due Jan. 12, 2001, and formal applications due March 14, 2001; 745 preapplications were received, 313 encouragement letters were mailed, and 432 discouragement letters were mailed. Submissions by DOE laboratories were restricted to four proposals per laboratory; full proposals were due Jan. 24, 2001; 46 proposals were received. Proposals were received in the areas of experimental condensed matter physics, theoretical condensed matter physics, materials chemistry, engineering research, structure and composition of materials, mechanical behavior and radiation effects, physical behavior of materials, synthesis and processing, chemical energy and chemical engineering, catalysis and chemical transformations, separations and analysis, and geosciences.

The FY 2001 funding was not enough to pursue Nanoscale Science Research Centers, but funding for these centers will be pursued in the future. Such centers are designed to support research for the fundamental understanding of and control of materials at the nanoscale and to provide state-of-the-art nanofabrication and characterization facilities to in-house and visiting researchers at no cost. Proposals for such centers were received from ANL, Brookhaven National Laboratory (BNL), LBNL, ORNL, and Sandia National Laboratories (SNL)/Los Alamos National Laboratory (LANL). Funding for conceptual designs will be provided in FY 2001 from available funding. Funding for Title I (preliminary design) and Title II (final design) could begin as early as FY 2002. Title III (physical construction) could begin as early as FY 2003

In looking toward the future, BES sees its scientific user facilities as a national trust. It must provide for optimum utilization of the facilities, support excellent science, invest in beamline and instrument development, and invest in R&D for the next generation of facilities. Reinvestments in the laboratories is a small portion of the pie. With their roots in the Manhattan Project, the DOE laboratories today provide unique laboratory and research capabilities to the nation. Hosting scientific user facilities that serve 15,000 researchers annually and world-class research programs, which are often associated with the facilities, the laboratories play a significant role in the nation's science enterprise. It is incumbent on us to invest in them.

The SNS is a best-in-class facility for research in materials science, physics, chemistry, biology, and engineering. DOE is committed to construct the SNS on time and within budget and to strengthen neutron-science research in the United States.

Beyond the SNS, DOE would like to begin the Nanoscale Science Research Centers and the Linac Coherent Light Source in the near term. In the long term, DOE would like to (1) strengthen its core competencies, particularly those for which BES is the dominant or sole supporter of research in the United States; (2) investigate science and engineering at the nanoscale, which is expected to produce a revolution in materials design and synthesis; (3) study the control of chemical reactivity, the analogue to the control of material properties through nanoscale design and synthesis; (4) analyze the synergistic interaction of molecular biology with materials and chemistry to make full use of Mother Nature's machinery; and (5) cultivate an appreciation of vast assemblies of atoms and temporal scales from milliseconds to millennia through advanced computing.

Kohn asked if the attitude data could be stated as trends. Dehmer responded that, at the national level, very little change has occurred during the years but that she did not know about international comparisons. Kohn asked if there had been a reaction from DOE to BES's attempts at benchmarking, and Dehmer replied that BESAC was the first to see this presentation.

Wasserman asked if the public's information about science was obtained through formal schooling. Dehmer said that the data did not show that.

Sinha commented that this year's budget did get an increase with a lot of people's help and asked where that money went to. Dehmer responded that almost all of the core program facilities have gotten increases. Most increases went to nanoscale science, small increases for genomics, microbial cell, etc. across the board.

Hodgson noted that part of the success was produced by people's support for physical science and the unified effort among DOE, the societies, institutions, and individuals. Wasserman said that that support and cooperation have been critical in influencing Congress; the mathematics and physics societies have played a crucial role.

McCurdy called attention to the massive increases in the costs for construction and maintenance and noted that the costs of deferred maintenance along with cleanup costs have added greatly to the costs of doing business for the national laboratories. Dehmer responded that most costs go for FTEs. If you look at FTE costs, you will get a good idea of what the staffing level will be.

Richmond then introduced **Jack Crow** to review the activities of the Subpanel on the IPNS and LANSCE/Lujan Center. He pointed out that summaries of the activities of the Subpanel are available and reviewed (1) the charge that was put to BESAC to review the Intense Pulsed Neutron Source (IPNS) at ANL and the Manuel J. Lujan Neutron Scattering Center (MLNSC) at LANL and (2) the Subpanel membership. Several reports are available that underscore the important role neutrons play in the U.S. science agenda. Some investments have been made in neutron science, such as in the SNS and the High-Flux Isotope Reactor (HFIR) upgrade. The flagship of this endeavor will be the $1.41 billion SNS, which will be commissioned in the summer of 2006 and reach full power in 2008. But the user base in the United States (approximately 1000) is much smaller than Europe's base of 4000 to 5000 users.

The Subpanel held a meeting on Oct. 12-13, 2000, in Gaithersburg, Maryland. It issued a very extensive request for information from the directors of the facilities on Oct. 25, 2000. It then held site visits at LANL/LANSCE/Lujan Center on Nov. 14-15, 2000, and ANL/IPNS on Nov. 16-17, 2000. A report was prepared and presented to BESAC on Dec. 11, 2000. That report concluded that (1) the LANSCE source at 80 kW and 100 microamps at 20 Hz was very competitive internationally but that it has other clients that fed off the facility and (2) the IPNS source, a dedicated facility at 7 kW and 14 microamps at 20 Hz was much lower in power but modifications resulted in an effective power level of 15 kW for thermal or epithermal neutrons and 50 kW for cold neutrons.

The Subpanel evaluated each source's proton beam power, target effectiveness, moderator optimization, number and type of instruments, quality of instruments, reliability, facility support, and users. The Subpanel used a grading scale of Outstanding (++), Competitive (+), Needs Improvement to be Competitive ( ), and Unacceptable ( ). This scale was applied to each of nine categories. The results were

	LANSCE/MLNSC	IPNS
Source	+	-
Reliability	-	++
Instrumentation	-	-
Support facilities	-	-
Support staff	+	+
User community	+	+
Cost-effectiveness		
Operations	- -	++
Science	-	+
Stewardship/management	- -	+
Impact	-	+

A major problem is that LANSCE has no real champion. Users are slowly backing away from the source, and personnel decreases are taking a toll. There is evidence of commitment at all levels, but a lack of integration renders this ineffective. The IPNS is an outstanding value. It is impressively operated with a well-integrated team that keeps an outmoded source operational at the highest levels of efficiency; it can be sustained and enhanced with modest investments; plans for cost-effective upgrades have been identified; and it provides a window of opportunity to pass on expertise to a new generation (at the SNS). That point is important because the SNS user community, at approximately 1000 people, needs to increase if the SNS is to be fully exploited. It is imperative that every spallation source in the United States be utilized to its full potential to assure that a sufficiently large and well-trained user community exists when the SNS is fully operational in 2008. It is also essential to substantially increase the neutron-user community to fully exploit the SNS. This increase will not occur in a timely fashion without an active neutron-science program. This user community will play an important role after the completion of the SNS.

Stohr asked what insights the Subpanel had. Crow replied that, in Europe, there is a more significant crossover between light-source and spallation users that does not occur in the United States.

Kohn commented that the stories of IPNS and LANSCE were very different but were very much the same 10 years ago. Fortunately, the National Institute of Standards and Technology (NIST) has stepped in here; without it, neutron science in the United States would be desperate. IPNS is an outstanding example of what can be done with an antiquated facility. Stewardship and leadership are cited, but no solution is identified. The management-structure problem has caused the dysfunctionality at LANSCE. It is a shared facility (IPNS and NIST are not). *That* causes major problems (and did 10 years ago, also). The managers are outstanding. The root problem is the disparity in the funding sources. One needs an in-depth study of this root problem and the identification of a solution to that problem. The report does an excellent analysis but leaves us with the original problem. The facility needs a single stewardship.

Crow responded that the multiple groups that support LANSCE recognized that the success of the facility and its programs depend on the resolution of that problem. Batterman commented that, even in the early eighties, the Birgeneau Subcommittee was assured that that same problem would be resolved by the LANL management.

Richmond introduced **Iran Thomas** to review BES activities following the LANSCE and IPNS review. Members of BES met with John Browne, Director of LANL, and Steve Younger (who has control of the money that operates the LANSCE) to discuss the review. Based on this discussion, John Browne wrote BES on January 4, 2001, giving a very strong, positive commitment and response to the problems raised by the review, describing seven actions. Among those actions was a pause in the building of instruments so that LANSCE could focus on operating existing instruments; the first two spectrometers, HIPPO and SMARTS, are complete and being commissioned. Two impending instruments, VERTEX and SABER, were reviewed. The designs and plans for SABER and VERTEX were found to be adequate and to merit funding. Funding for the two instruments will be continued, but they will be designed for the SNS. Once LANSCE has addressed the concerns of the Committee, BES will continue building instruments at LANSCE. Even after the SNS is completed, the United States will very likely need the capacity at the LANSCE. BES wanted to increase funding for instruments for IPNS, but funding was not available for this year; it will be for next year.

Mayes asked if this turn of events will affect the SNS construction money. Thomas responded that it will, but in a complicated way, making the grants to universities for instrument development for the SNS earlier. A call for proposals will go out next year.

Kohn said that he was disappointed that no expanding or upgrading of the IPNS instruments would be done this year. The facility has an inspiring track record, and the Subpanel recommended it as the most-effective means of improving the situation of neutron science.

Thomas reiterated that it will happen, but next year. Greene commented that it is not known if the SNS will be in a position to proceed when it needs to and that holding back on the IPNS will not increase the chance of success for the SNS. Thomas responded that funding for LANSCE will be held until there is a response from LANL; BES will be providing instrument money for the IPNS. Lester asked if there will be another review then, and Thomas replied, yes, but that that review does not address the timing problems highlighted by Greene.

Crow said that he would like to see what went down in the budget, what went up, and what is expected to happen because coordinating the activities at IPNS and LANSCE with those at SNS is critical. Thomas said that an interagency working group (DOE, NIH, and NSF) on neutron science instruments has been set up. That working group will produce more activities from the other agencies. You cannot design an instrument in the abstract; where it is installed and what it is to be used for are important to the design. The request for proposals (RFP) that will go out will allow universities to participate in the SNS and will produce prototypes of instruments for other facilities. Crow said that he was trying to get a handle on the budget and the priorities reflected in it. Thomas responded that neutron scattering has not been cut. Unexpected demands have come in, but research opportunities and instrument funding have been increased.

A break was declared at 10:36 a.m., and the meeting was reconvened at 10:59 a.m. with the introduction of **John Browne**, LANL Director, and **Paul Lisowski**, LANSCE Division Director, to present the LANL response for exploiting the full potential of LANSCE. Browne started by stating that it was a good report and that LANL had no qualms with the content. The Laboratory only wants to address the issues.

Some things have changed since the eighties. The Lujan Center has developed and been made capable to host users. In 1993, the Nuclear Physics program stopped funding the Los Alamos Meson Physics Facility (LAMPF), and funding switched to Defense Programs (DP). From 1993 to 1997, the facility made good gains in availability, reliability, and instrumentation. In 1998 to 1999, attention was diverted from reliability and availability by other issues. A strong message in the report was that LANL has to straighten out the governance of LANSCE. In response, a letter was sent to Dehmer by the laboratory's management. In it, they said that LANL's primary goal is to deliver neutrons and protons safely and reliably for all LANSCE users. To ensure that that goal is met, LANL will (1) appoint a new LANSCE management team; (2) engage other scientific user facilities to benchmark and improve LANSCE performance; (3) develop and implement an effective governance model involving the National Nuclear Security Administration (NNSA); SC; the Office of Nuclear Energy, Science, and Technology Research (NE); LANL; and the user communities; (4) ensure appropriate support and oversight that is informed by an independent review of its operations, that includes a detailed bottom-up review of all costs, and that results in the adoption of a 5-year planning cycle for LANSCE; (5) initiate a pause in the development of new instruments at the Lujan Center in order to focus on the operation of the user program (with the two instruments now coming on line, the Center will have ten instruments, five of them in the user program); (6) increase the Laboratory-Directed Research and Development (LDRD) investment in the Lujan science program; and (7) maintain strong communication with the LANSCE User Group (LUG).

Lisowski said that the new management team is in place. (Alan Hurd is the new Lujan Center director and BES Neutron Scattering Program manager.) LANL has started the benchmarking of scientific user facilities and user programs. The Laboratory has developed and started implementing a governance model that incorporates the ideas and expertise of the LANSCE User

Group and of many at DOE, NNSA, and other organizations. Yet to be done are a LANSCE operations budget review (which is scheduled for completion and review in June 2001) and the establishment of a general awareness that the funding needed is likely to be larger than that currently provided. The major near-term focus is on completing the outage successfully and resuming operations with high reliability on July 1, 2001. The pause in BES spectrometer development will allow LANL to focus on the instruments that are in place and to use them more effectively. Spectrometer-development teams (SDTs) are focusing on instruments for SNS. LANL has proposed to meet the user demand for inelastic scattering by completing the chopper spectrometer PHAROS for introduction into the user program by 2002.

LANSCE has drafted a neutron-scattering plan based on user input. A LANSCE planning workshop involving the broader user community will be held in concert with the next LUG meeting in summer 2001. LANSCE will be integrated into the NNSA/DP 5-year planning process, giving a level of stability that has not been attained before. Additional LDRD investments in Lujan science have been secured for FY 2001.

LANL has worked intensively with DOE/NNSA and BES to develop a path forward and an improved governance system. It has identified the needs and expectations of customers. It has developed the elements of a functional governance for LANSCE that will meet its ultimate customer needs within the user community, for DOE/NNSA, and for Los Alamos. The governance plan will include deliverables and a schedule to implement the plan.

DOE has clarified its chain of command for LANSCE in a memorandum from the Deputy Secretary of Energy to General Gordon. In it, DOE states its intent to "assign ... Defense Programs as the Organizational entity with corporate responsibility and accountability for strategic integration of all three program offices using LANSCE. This approach applies both to the short-term objective of facilitating IPF [Isotope Production Facility] construction and the long-term goal of reliable accelerator operations." This governance plan will provide a single point of responsibility within DOE/NNSA, leading to single-point accountability, a single line of authority, participation of all stakeholders, and an authority and responsibility chain that includes accountability for those controlling the resources.

The proposed governance model provides a clearly defined steward in DP; clearly delineated responsibilities with respect to the facility and other sponsors; a single point of contact for all aspects of security, operations, and scientific output (the LANSCE Director); participation of all stakeholders at several levels to clarify priorities and resolve conflicts; and a triennial program review by DP, SC, NE, and advisors will assess performance and impact. Under this plan, the Director of LANL will be advised by a senior executive team, the Executive Secretary of which will be the LANSCE director. Over LANSCE will be an associate laboratory director, who will be advised by a Governance Committee made up of LANL division directors, program directors, and the LUG chair; it will be the first recourse to resolve conflicts. The LANSCE director will report to that associate laboratory director and be counseled by the LUG and a LANSCE Advisory Board

LANSCE's highest priority is to establish a long-term sustainable program serving all users safely and reliably. Multiple sponsors and programs make this difficult. The facility is currently in an outage. Proposals are due March 12, 2001, for Program Advisory Committee (PAC) review for the user program scheduled to start on July 1, 2001, and running through December 2001, when another outage is scheduled. The ultimate goal is to run safely and reliably for all users by implementing the governance, management, and science plans to realize the full potential of LANSCE and the Lujan Center.

Stohr said that LANL had addressed the problem of internal management and noted that, in the transition period, an outside advising group is very important. Browne said that the LANSCE Advisory Board and the LUG are being used for that purpose.

Kohn said that one must recognize the mistakes of the past and asked if they considered the failures of the past as a fluctuation or as a continuing underlying problem. Browne responded that, indeed, one must learn from the past. In the eighties, LANSCE did not have a solid commitment from any sponsor for the Lujan Center. In 1993, the mission change was a step in the right direction, limiting the focus of the facility. LANL is now trying to establish stable, long-term support and activities for the facility. Previously, the governance did not allow such stability and solution of problems. If LANL can get the 5-year plan in place, that stability can be achieved. Lisowski noted that LANL has had a lot of feedback of what went wrong in previous years.

Batterman asked what the difference is between customers and users, what the number of users/customers are, and what affiliations they have. Lisowski said there are approximately 126 external users and 200 internal and external customers. There are two other user facilities there that have fewer than 100 users. Batterman asked how many of these are from universities and independent laboratories. Lisowski said that the 126 are from universities and independent laboratories (including Sandia National Laboratories). Batterman asked what percentages of the neutrons and budget are weapons related. Lisowski replied that 30% of the neutrons and 85% of the budget of the whole facility are DP. Batterman asked what fraction of the user community is not related to weapons or the national laboratories. Lisowski responded: the 126 people, which is more than half of all users.

Kohn noted that the report refers to more outreach to universities. Browne said that LANL collaborates with a lot of universities. Approximately 150 students come to LANL each summer; the laboratory needs good ties to universities; it should have stronger ties to universities with programs in neutron science and nanoscience. As long as the laboratory is tied to a university, why not make use of that relationship?

Crow noted that ISIS is serving 1300 users a year and asked what the speakers saw as the potential for growth in users as we approach the SNS. Hurd said that there are several programs on the horizon; the LANSCE wants to run reliably and safely in the next operational cycle. With two new instruments on the floor; new users will be attracted. Lisowski said that, if LANSCE increases availability and reliability, the user community will come. If it does not, they will vote with their feet.

Crow asked what could be developed in the Lujan Center to bring up its standing against the benchmark institutions. Lisowski said that the Center will increase the number of postdocs from the Director's budget. Browne noted that the best people get the best funding, but those people have to be recruited.

Goodman commented that his institution, Texas A&M University, expects to have a long-term arrangement with LANSCE and has been a satisfied customer.

Broholm said that the Subpanel was concerned that the LANSCE director had to report to two entities and that it was not obvious that that concern had been addressed. Lisowski said that, looking at the diagram that details funding and authority, both funding and authority have to be together, and the only place they are together is the director's office, so that is where that question will be addressed.

Stupp joined the meeting.

Mayes stated that, in addition to a reliable beam, you must ensure adequate support for users; DOE is less good at that than NIST. Lisowski said that LANSCE should strive to provide support and the requisite amenities for users. The demographics at LANSCE will change as new young researchers join the research team.

Richmond thanked them for their rapid response to the Committee's report and asked **Bruce Brown** to comment on IPNS's response to the BESAC review. He noted that the Subpanel's recommendations say that IPNS must (1) invest to maintain the excellent reliability, (2) invest to enhance the IPNS source and instrumentation, (3) expand operation of the user program to 30 weeks per year, (4) strengthen the scientific programs at ANL that develop the user base and the scientific agenda for the SNS, and (5) explore the possibility of developing and operating first-class instruments at IPNS that can later be moved to the SNS. The estimated cost to do this is an additional $9 million per year.

The IPNS is committed to broadening and increasing the user community in preparation for the SNS. It presented a four-part plan (at $9 million per year) to the Subpanel that is the first recommendation in its report. Under that plan, IPNS would increase operation to 30 weeks per year, initiate a maintenance and upgrade plan for the accelerator system that will guarantee at least 10 years of reliable operation, significantly upgrade all scattering instruments, and greatly increase the ANL research program strongly coupled with instrument enhancements. The budget to do all this would include

Staff for additional operation, users, and maintenance	$3.1 million per year
Equipment: accelerator	$1.0
Equipment: instruments	$2.5
Research programs	$2.6
Total	$9.2

In addition, IPNS would establish a program to expand the university base for neutron scattering. The users are grown at the universities. In response to the Subpanel's third recommendation, IPNS has submitted a proposal to DOE for $2.5 million per year to enhance university research in the area of neutron scattering, including joint faculty appointments, faculty leaves, postdocs, and graduate students.

IPNS proposes increasing operation from 25 to 30 weeks per year, which will require additional accelerator staff, increases in scientific support for the user program, and some more expenditures [e.g., electricity, maintenance and surveillance (M&S), and spare parts]. Additional operation has the negative effect of decreasing the time available for maintenance, which requires additional staff increases.

IPNS's needs for ensuring at least 10 years of operation have been detailed in a white paper. The linac is 40 years old. The rapid-cycling synchrotron (RCS), built in 1979, has delivered 6 billion pulses, more than any proton synchrotron in the world except ISIS. Reliability has been very high (95%), but some systems must be replaced or upgraded to maintain this reliability. No machine runs forever. For a $100-million accelerator, the replacement value is approximately $80 million. But for many years, only about $140,000 per year of equipment funds have been available for all accelerator activities. The main operations issue is that there are no replacement parts available for many of the old systems, and our spares will not last forever. For comparison, ISIS has begun a similar project. It is costing approximately $18 million and 29 staff years over 7 years, including a shutdown for six months starting in December 2001. Along with increased operating hours with high reliability, IPNS plans to increase beam current by 30%, using the second harmonic on the RF.

IPNS has an instrument-enhancement plan (that assumes a $2.5 million per year increase in the equipment budget relative to FY 2000). A lot of the planned changes can get going early because IPNS has a lot of empty slots for detectors that were not funded. The motivations for these improvements are increased data rates, new scientific capabilities, and anticipation of the SNS needs. The plan was presented to the Subpanel, and that is what came out in its recommendations.

In increasing research programs, IPNS hopes to broaden and increase the user community for SNS by opening new areas of research, involving new people, and creating careers in neutron scattering by starting new Materials Sciences Division (MSD) research programs ($500,000 already received); involving university researchers ($100,000 already received); and increasing visiting professors, joint postdocs, and research students. These new areas of research will be closely coupled with the IPNS instrument upgrades

The budget for the ANL MSD Neutron Scattering Group shows a decrease from $1.65 million per year in 1989 to $1.2 million in 2001, all in 1999 constant dollars.

Potential new research programs that were highlighted were (1) the magnetic structure of soft and hard magnetic composites, with the objective of understanding and optimizing their performance by probing the behavior of nanoscopic hysteresis phenomena, and (2) magnetism in complex bulk systems with dilute magnetic constituents.

In terms of an IPNS-SNS synergy, the IPNS has access to neutron-scattering scientific and technical expertise for providing instrumentation ideas and training to the SNS staff. IPNS also has access to a pulsed spallation neutron source facility for testing prototypes and for scientific research. For the IPNS, this means an infusion of new ideas and SNS development activities that can lead to new IPNS capabilities. It also means that there will be skilled people available to "jump-start" solutions to IPNS enhancement or troubleshooting needs. Such interactions also provide valuable hands-on experience for SNS staff through shared staffing, where appropriate.

The Long Wavelength Target Station (LWTS) is proposed for funding by the NSF, but it is possible only because the SNS is already being constructed; it would greatly enhance the capabilities of the SNS. Also possible is the Cold Neutron Chopper Spectrometer, which was originally funded at LANL but was suspended because they are in their instrument-development pause. A joint university and national laboratory collaboration has proposed pursuing the first of two phases of this option at IPNS. The first phase would provide commissioning and testing in advance of SNS, development of analysis techniques, high involvement of the academic community, and development of new users in advance of the SNS. The second phase would be carried out at the SNS and include a full spectrometer and a true Day-1 instrument.

The IPNS is ready to move on the $9-million-per-year plan that will broaden and increase the user community in preparation for the SNS. MSD received an additional $600,000 in January and has begun its program. But, the present IPNS budget will permit no enhancements in FY 2001. During the past year, the operations budget increased 3.9%, and the equipment budget decreased 2.0%. During the past 5 years, the operations budget increased 17.9%, and the equipment budget decreased 7.1%.

The Subpanel's key findings were reiterated: (1) "It is imperative ... to assure that a sufficiently large and well-trained user community exists when SNS is fully operational in ~2008," and (2) "It is essential to substantially increase the user community ... [which] will not occur without an active program." IPNS asserted that it has put forth a cost-effective program to meet these goals that should be started immediately to maximize its impact.

Crow asked what are the priorities were in the budget. Brown said that it depends on how the money comes in. IPNS has made a commitment to devoting 25% on immediate maintenance and upgrade. Its next priority is increasing availability.

McCurdy noted that the measures cited are the quality and amount of science produced and that the Subpanel is asking if you are being a sufficient steward of science. He asked how that operates in a year. Brown said that the Subpanel stated it well. You look at source strength, reliability, etc. IPNS's organization has been running for 20 years. It had a strong user group. But over time they lost interest. IPNS asked NIST how they operated. Now the IPNS has two committees: The Program Advisory Committee makes recommendations on each instrument and its users. Also, the University of Chicago has a committee that reviews our program each two years. They were the driving force on coming up with the upgrade plan.

Shen noted that IPNS and Lujan Center are very different in user support and asked what impact this group has had on the production of important science. Brown said that there is no question that they have had a significant impact. Shen asked if similar things can be done at LANL. Hurd said that the tie between visiting scientists and those that operate the facilities is very critical. Parkin said that LANSCE is doing exactly what was described for IPNS.

Sinha stated that the summer school that IPNS has run has been important in expanding the interest in and practice of neutron science. DOE should continue support for that.

Kohn said that he was nervous. We have this responsibility in 6 to 8 years to have a well-functioning user base for the SNS that is four times larger than what we have now. Unless in one way or another you double or triple the user base in those years, you are going to be in trouble. The facility must be worth the expenditure of money. Thomas said that BES expects to have an increasing number of users at startup of the SNS. It will take several years of operation until the user base is ramped up. Mason called the Committee's attention to the fact that the end of construction in 2006 is the arrival of the first neutron, not full operation. What is needed is to get the DOE user base to the current level of NIST's.

A break was declared at 1:05 p.m. The session was called back to order at 1:37 p.m. with the introduction of **Eric Rohlfing** to review the progress in the Linac Coherent Light Source (LCLS). The scientific case for the LCLS is directly tied to the decision on proceeding with LCLS construction (Critical Decision, Level 0: conceptual design). The "first experiments" are aimed at defining (in some detail) the first classes of experiments that would be mounted on the LCLS and form the basis for the experimental requirements for the LCLS conceptual design report (CDR). The papers on the first experiments were assembled through the LCLS Scientific Advisory Committee and simultaneously presented to BESAC and an external peer-review panel. On the basis of those presentations, BESAC unanimously voted to recommend that BES approve CD-0, contingent upon a positive external peer review. The external peer review was completed in November, and the reviewers comments were very similar to the BESAC comments and generally positive. Several reviewers noted a significant improvement over earlier efforts, and there was a tendency for reviewers to favor science outside their areas of expertise.

In atomic physics, the reviewers agreed that these studies are a basis for understanding intense X-ray–matter interactions, criticized the proponents for not being innovative, expressed concern about a lack of impact on the field, and expressed concern about the need to interpret nonlinear processes with a spiked temporal structure in LCLS pulses.

In plasma and warm dense matter (WDM), the reviewers saw a clear niche role for the LCLS, particularly as a pump source to create WDM. They expressed concern over the broader impact and relevancy of plasma and WDM to BES, but noted a clear relevancy to DOE DP.

In structural studies on single particles and biomolecules, the reviewers issued their most positive set of comments. This application is clearly at the forefront of the field with a huge potential impact, but there was some skepticism about whether there would be sufficient signal to overcome background noise to extract molecular-structure information.

In femtochemistry, the reviewers issued the weakest set of reviews, especially from those most directly associated with ultrafast dynamics. They expressed concerns with synchronization between the laser pump and the LCLS probe and said that there was a clear need for shorter pulses to have a real impact in dynamics, particularly in the gas phase.

In studies of nanoscale dynamics in condensed-matter physics, there were few review comments. The overall impression was that it was not clear that the LCLS parameters are ideally suited to experiments, and concern was expressed that the damage calculations for X-ray photon correlation spectroscopy (XPCS) look marginal.

In X-ray laser physics, there were few comments. Most of those comments strongly endorsed attempts to shorten the LCLS pulse based on scientific needs, particularly for femtochemistry.

BES has delayed approval of the conceptual design. There is strong support for the LCLS project, but the scientific case and the level of "community" support is not yet sufficient. BES will hold another BES Workshop on Scientific Applications of Ultrafast, Intense, Coherent X-Rays in May. It will not repeat what has already been done, but rather will focus on scientific applications of a source with LCLS specifications with an emphasis on ultrafast dynamics, nonlinear optics, and X-ray imaging. It will mix LCLS veterans with newcomers. The output from the workshop will be a report that complements and broadens the LCLS scientific case and makes recommendations for the FY 2003 budget.

The BES vision for the LCLS is that the LCLS is partly an accelerator/free-electron laser (FEL) R&D project, but it must also be a stand-alone scientific user facility. The LCLS is not a step along a predetermined path toward a larger X-ray FEL (XFEL) facility. Previously, it was viewed as a testbed for the next-generation XFEL machine, but at this point, BES does not know if that is the case.

Batterman commented that the converse of the statement that people get more excited about things outside their expertise is that looking at "old stuff" is perceived to be unexciting and is played down.

Lester said that it gave her a sense of relief that the expert review supports the BESAC assessment and that the staff has chosen a more conservative path in pursuing this program.

Johnson asked why BES is limiting the workshop attendance to 20 to 25 people. Rohlfing said that we are not going to reinvent the wheel. A smaller workshop will be more focused.

McCurdy noted that the presentations in October did not have much on new methods of detection and asked if that came up in the expert review. He also asked about the cost of the experiment. Rohlfing replied that the same reservations about the atomic-physics experiments were raised. BES expects that there will be an increased cost in going to a stand-alone device: $100 million to $175 million.

Johnson noted that the horizon of the atomic physics experiments was Day 1 and that that horizon would expand as experience was gained. Rohlfing agreed, but said that he had been asked to focus on Day 1.

McCurdy called attention to the fact that BESAC had expressed a concern about the length of the pulse for femtochemistry and asked if the expert reviewers specified a pulse length. Rohlfing said that they had recommended a pulse shorter than 250 femtoseconds, perhaps as short as 50 femtoseconds.

Richmond introduce **Keith Hodgson** to speak about the LCLS. He announced that John Galayda will be the first director of the LCLS program at the Stanford Linear Accelerator Center (SLAC) and introduced **Max Cornacchia** to give a project overview. Cornacchia began by pointing out that the LCLS design is for a single-pass free-electron laser that uses the existing SLAC Linac with a wavelength of 1.5 to 15 angstroms (0.5 to 5 angstroms in the third harmonic) and a peak brightness 10 orders of magnitude above the APS. The time-averaged brightness will be 2 to 4 orders of magnitude above that of the APS. It will produce subpicosecond pulses of fully transversely coherent radiation. The design and R&D studies have been started at ANL, BNL, LANL, LLNL, SLAC, and the University of California at Los Angeles (UCLA) as a collaboration.

In comparison, third-generation light sources have a high flux and brightness, short pulses (tens of picoseconds), and partially transversely coherent beams with a bandwidth equal to the inverse of the number of undulator periods. X-ray FELs have a flux and brightness that is many orders of magnitude higher than in third-generation light sources, pulses that are 1 to 2 orders of magnitude shorter than those of third-generation light sources, and fully transversely coherent beams (having a degeneracy factor of 10^9) with a bandwidth equal to the inverse of the number of undulator periods.

To build such a machine takes a bright electron source (photoinjector) and a bunch-compression system. Then the beam is accelerated in a linear accelerator and an undulator (120 meters long) with photon beamlines to transport it. SLAC would need an injector into the accelerator; there, the pulses would be accelerated and compressed before going into the undulator.

Self-amplified, spontaneous-emission (SASE) FEL theory has been well developed and verified by simulations and experiments. FEL radiation starts from noise in spontaneous radiation. A transverse radiation electric field modulates the energy and bunches the electrons within an optical wavelength, producing an exponential buildup of radiation along the undulator length. The main parameters are a wavelength of 1.5 angstroms, an electron energy of 14.35 GeV, a saturation peak power of 9 GW, a bunch length of 230 femtoseconds, 10^{12} coherent photons/pulse, an undulator length of ~120 m, an undulator gap of 6 mm, a peak brightness of 1.2×10^{33}, and an average brightness of 4.2×10^{22}. The standard operation will be in the first harmonic.

Other FEL-based light sources are being tested, built, or planned. The TESLA (TeV-Energy Superconducting Linear Accelerator) Test Facility (TTF) at DESY (Deutsches Elektronen-Synchrotron) is currently lasing with a gain of about 3000 observed at 80 to 180 nm. The same facility would become an X-ray TESLA. The Source Development Laboratory (SDL) at BNL-NSLS (National Synchrotron Light Source) is performing electron-beam testing. The High-Gain Harmonic Generation (HGHG) experiment at the BNL Accelerator Test Facility (ATF) was successful. The VISA experiment at BNL-ATF; projects in Japan, Italy, England, and Germany; and the Low-Energy Undulator Test Line (LEUTL) at ANL-APS (where saturation was observed for the first time in the world) are all looking at some aspect or other of this scientific problem. A crucial milestone in FEL physics was reached when the LEUTL experiment measured large amplification and evidence of saturation last summer at 530 and 385 nm.

The question remains how to achieve a short bunch in an FEL. What was needed was a simulation tool to optimize the electron beam in 6-dimensional phase space. What has been learned so far is that (1) preservation of transverse electron brightness leads to a shorter undulator and more relaxed tolerances, (2) the mechanism for achieving short electron bunches (230 femtoseconds) was confirmed by simulations, (3) shorter bunches can compromise transverse electron brightness because of collective phenomena that occur, and the 230-femtosecond bunch length is the result of optimization dimensions.

Batterman asked what the weakest link in the system was. Cornacchia answered that it was the gun; all of the simulation effort is in place.

The conceptual design report is on schedule, and first-draft contributions are being reviewed. The goal is to have it ready, in draft form, by early summer 2001.

In summary, substantial progress has been made in most areas; experimental confirmation of the photo-injector brightness is the most important short-term goal; integration of the photo-injector, FEL physics, and X-ray optics is continuing; the X-ray optics are to address the detailed requirements of the "first experiments"; and the focus for the next six to eight months will be on the CDR and preparation for the Lehman review.

J. B. Hastings was introduced to talk about "the sixth experiment," another of the experiments that might be run on the LCLS. This experiment would lead to the focusing of X-ray pulses, the generation of shorter X-ray pulses, and the increase of the longitudinal coherence.

The landscape of damage tolerance for proteins can be mapped by graphing intensity versus pulse length (in femtoseconds). At the LCLS baseline design of about 250 femtoseconds, sample explosion causes diffraction intensities to change to unusable levels even at low intensities (10^{11} photons per 100-nm-spot pulse). Calculated resolutions for various types of samples {e.g., $2 \times 2 \times 2$ clusters of lysozymes, a single RUBISCO molecule, and a single viral capsid [the tomato bushy stunt virus (TBSV)]} were large (often greater than 30 angstroms). The resolution could be improved dramatically if the pulse time could be reduced. For probing chemical processes, the situation gets interesting at 100 femtoseconds.

The LCLS baseline design parameters are: shortest fundamental FEL radiation wavelength = 1.5 angstroms; electron beam energy = 14.3 GeV; normalized root mean square (rms) slice emittance = 1.2 mm-mrad; peak current = 3.4 kA; FEL mode source size [FWHM (full width at half maximum)] = 78 micrometers; FEL mode source divergence (FWHM) = 1 microrad; peak brightness = 12×10^{12}; X-ray pulse length (FWHM) = 230 femtoseconds.

The focusing of LCLS pulses is a singularly important phase-space transformation of the LCLS pulse; this will take field strengths of about 10^{10} V/m to about 10^{16} V/m.

A schematic diagram was shown for a method for making short pulses with the LCLS accelerator and compressor. When one takes into consideration the 3rd to 6th dimensions, significant improvement is obtained in magnetic electron-bunch compression. A relatively conservative approach is to produce a chirp, producing a pulse with a 2% energy spread. One can then take advantage of the X-ray optics and do pulse compression or pulse slicing to give a short pulse length.

Optical pulse compression by energy chirping can produce a minimum pulse length of about 10 femtoseconds with a wavelength spread of 2% with grating-line separations of 5.5 micrometers, a grating vertical separation of 75 cm, a grating horizontal separation of 107 m, an incident angle at the grating of 0.2 mrad, and a grating length of 1 m (which is impractical). But no practical solution has yet been worked out.

One scheme to compress the pulse might be to line up crystals as monochromators. The sacrifice is 20% of the intensity. These optics are readily available, but the technique is not practicable.

Johnson asked how one got a linear chirp with an electron beam. Hastings said one did that by adding a third-harmonic section.

SASE FEL starts up from noise with no longitudinal coherence. If one can impose microbunching of the electron beam, the output is the amplified input; this would preserve the longitudinal coherence of the seed. A scheme to do this was shown. It involved splitting and reuniting the beam to produce a fully coherent beam. Hastings said that it is intriguing to contemplate such an experiment. Greene asked what the scale of the parallel paths was. Hastings said that it was on the order of a few centimeters. These are not experiments that would be carried out on Day 1, but this schema is to show how the technique may develop.

In summary, the LCLS design opens the possibility for adjusting X-ray beam parameters according to the needs of the experiments. Among these parameters are increased electrical field strength (focusing), shorter bunch lengths (electron bunch/X-ray pulse compression; slicing), and increased longitudinal coherence. All areas need extensive R&D efforts.

Stupp asked how the sample would be presented to the beam. Hastings said that the sample particles might be frozen and dropped one by one into the beam. Hodgson suggested the use of microdroplets or the use of the sample in the gas phase.

Johnson asked if, in addition to producing short pulses, they had any plans for increasing the contrast. Hastings replied that the pulses are produced by focusing in the transverse direction. If one looks at the temporal side, the signal is very clear.

A break was declared at 3:00 p.m. and the meeting was restarted at 3:15 p.m., when **Iran Thomas** reviewed the activities of the Materials Sciences and Engineering Division. He discussed the organization chart and identified the new staff members in the organization. He noted that the division got 745 proposals for the nanoscience initiative, and he introduced the staff that processed the proposals, which numbered more than all the other proposals received by BES in a year.

Pan American Advanced Studies Institutes (PASI) are short courses of two to four weeks duration, involving lecturers of international standing at the advanced graduate and postgraduate level from the Americas. PASIs may involve up to 8 to 12 lecturers and approximately 40 to 50 students from the different countries in the Americas. PASI proposals are due by April 15, 2001.

The decommissioning and demolition (D&D) of the High Flux Beam Reactor (HFBR) has been put in the charge of the Environmental Management (EM) Division, including the dismantling and shipping of instruments to other sites. The task has been done quickly and professionally.

The upgrades of the HFIR were going along well until tritium was discovered in a drain line. That discovery has slowed things down considerably. The neutron-scattering upgrades at the HFIR include new and upgraded instruments, a cold source, and new beamlines. The HFIR cooling-tower replacement has progressed. The tower has been demolished and removed from the site. Sludge has been removed from the basin, the new tower is under construction, and the project is currently under budget and ahead of schedule. For the beryllium-reflector replacement, the reactor has been disassembled to the reflector.

Tritium was unexpectedly discovered in a HFIR foundation drain in early October. It was traced to an underground process waste line. The source of tritium contamination was eliminated, and less than 10% of the tritium was released. The defective underground process line will be replaced during the current outage. This event delayed removal of the old reflector by four months. Crow asked what the impact of this event would be. Thomas said that an operational readiness review will have to be performed. Some positive things have come out of this event. The manager realizes now the effect of surprises on forecasting. An SAR (safety analysis report) has to be completed, too. Roberto said that the delay will be six months or less.

The SNS has undergone a significant staffing change, and a new organization is to go into effect March 1. David Moncton, SNS Executive Director, will return to ANL on or about March 1 after completing a successful two-year tenure with the SNS. A new director has been designated, Thom Mason. The project now will report to DOE through ORNL rather than directly. Mason will be an associate laboratory director at ORNL. LBNL successfully completed a major portion of the R&D on the SNS front end. They fabricated and tested the first production ion source and procured a large number of hardware components. LANL and Thomas Jefferson National Accelerator Facility (TJNAF) are working well together on the hybrid (normal/superconducting) linac. Mason noted that, since December, $30 to 40 million per month have been committed in procurements. Thomas continued that BNL has made good progress in the accelerator physics design and that the prototype dipole and quadrupole magnets have been fabricated to specifications and successfully tested. ORNL's R&D on the mercury-target concept supports the design. ANL and ORNL have selected the first three instruments and incorporated them into the project cost baseline. LANL has completed the preliminary design reviews for global safety, network, timing, and machine-protection systems. The SNS site is about the same size as ORNL with the excavation nearly complete (1.3 million cubic yards of earth moved).

Issues at the end of FY 2000 include the fact that the initial estimate of pre-operation costs was significantly higher than the original estimate. The architect/engineer's Title I cost estimate for conventional facilities was about $80 million over baseline because of increases in scope. Moncton had pulled back some of the cost cushions that had been built into the program and used those savings to upgrade the specifications of the Oak Ridge site. The bottom line is that, at the end of FY 2000, it was time to pause and rethink the DOE "stretch goals."

A pre-operations cost estimate was developed during 1997 and 1998. During the summer of 2000, Moncton's team developed their own preliminary pre-operations staffing plan, which had not been discussed with DOE. That plan was informally proposed to DOE in September 2000. It would have exceeded the February 2000 baseline ($105.5 million) by about $377 million if the project was completed on schedule (June 2006). The Moncton proposal was judged unacceptable by BES when it was presented because it assumed a rapid operations staff buildup to the facility's ultimate steady-state level, it double-counted costs included in the total estimated cost, and it did not take advantage of ORNL's infrastructure.

In November, SNS management scrubbed the pre-operations estimate. This estimate was reviewed by a panel of experts with experience in commissioning similar facilities. Additional cost-saving measures were recommended and were subsequently implemented. A DOE (Lehman) review in December 2000 was presented with a pre-operations cost estimate that was only $21.3 million above the February 2000 baseline and that retained the June 2006 completion date. The review committee concluded that this estimate was reasonable and appropriate to reach

CD-4 (Conceptual Design, Level 4). The pre-operations cost estimate is now at the February 2000 value of $105.5 million, and no change in that value is expected.

The root cause of this cost excursion is that the SNS stretch goals were too ambitious and accepted by DOE too readily. The issues are being resolved by addressing the scope required to meet Level 0 baseline requirements (at least 1 MW; June 2006 completion; $1,411.7 million total project cost) while maintaining the best features of the stretch goals and designing for later incorporation of most of the stretch goals. The main lesson here is that projects have to be very open, and DOE has to understand what project management is thinking. Overall, the SNS is in very good shape.

Mayes asked what happened to the instrument budget. Mason replied that the original budget was $45 million; it now stands at $60 million. Thomas said that the average cost of a state-of-the-art (SOA) instrument is $7 to 8 million, but they are much better than what was originally costed out. We hope to find even more funds for the instruments. Mayes asked what the upgraded power might be. Thomas said that it would go from 1 to 2 MW; he did not think that anyone sees any problem with that.

Wasserman noted that the six national laboratories were supposed to work together and asked how that has worked out. Thomas replied that it has worked out extremely well; the reviewers singled out the very good cooperation between LANL and TJNAF.

Mayes asked if the change in reporting path had any consequences for the SNS. Thomas said that if the path had not been changed, it would have induced great hardships on trying to go through the laboratory's organization for, say, procurement. Some scientific integration will result that will help the SNS, and some management burdens will be shifted to the laboratory director.

Crow asked if, at the August meeting, the Committee could see a schedule for the instruments' procurement, development, testing, installation, etc., including the activities at the IPNS and LANSCE. Thomas said that this community has not been broadened as much as possible. Bob Gottschall will set up some workshops on the new instruments (e.g., HIPPO at LANL). That action should produce an amplification of interest. Crow stated that some of the possibilities are known; what is not known is how many people will be supported on what instrument when and where.

Richmond thanked Thomas for promising to follow up on Crow's suggestion and presenting it at the next meeting. She introduce **William Millman** to discuss activities in the Chemical Sciences, Geosciences, and Biosciences Division. He discussed the division's staffing changes: two new permanent professional staffers, two new temporary professional staffers, two continuing temporary staffers, and three departing professional staffers.

New activities included the reception of 745 nanoscience preproposals for BES, competing for up to $18 million. Of these, 313 were encouraged to submit full applications. In addition, 46 laboratory field work proposals (FWPs) were received from 13 laboratories for up to $18 million. In computational chemistry, 37 proposals were received, competing for $1.9 million; 21 discouragement letters were sent, and 16 full applications were encouraged.

The Council for Chemical Sciences held a workshop on Emergent Properties and Functions in Nanoscale Chemistry, and five vacancies on the Council were filled. The Council for Earth Sciences has identified a topic for a workshop in geophysics and will hold a topical contractors meeting in December; its next meeting will be in March. The Council for Biosciences has a tentative date for its first meeting in May.

A workshop on catalysis futures was being held the same week as this BESAC meeting. The U.S. position in catalysis research was recently evaluated by COSEPUP (Committee on Science, Engineering, and Public Policy) as part of the study reported in *International Benchmarking of U.S. Materials Science and Engineering Research*. The United States is among the world leaders in catalysis research, but there has been a decline of long-term research in corporate laboratories, and there has been no concomitant increase in the efforts at universities. (There has been in other countries.)

The Catalysis Futures Workshop will look at understanding and controlling chemical reactivity, considering (1) enzymatic vs traditional catalysis, (2) new ways to approach catalyst synthesis and in situ characterization, and (3) global catalytic processes (geoscience efforts regarding catalysis and building molecules with biological, chemical, and biochemical methods).

The other workshop is 21st Century Chemistry & Materials: Exploiting Biology's First Billion Years, recognizing that biology gives us molecules (DNA, proteins, carbohydrates, etc.), structures (in the form of membranes, channels, fibers, machines, etc.), processes (such as molecular recognition, self-assembly, pathways, etc.), and concepts (such as combinatorial chemistry, adaptation, and evolution). Some of the things to be looked at are (1) designed templates for mineralization (e.g., proteins and carbohydrates); (2) designed structures and scaffolds [e.g., DNA, RNA, proteins (gene-based or synthesized in vitro or in vivo), and carbohydrates]; (3) motors, rotors, tractors, and other devices (e.g., tubilin; kinesin; ATP synthase; sensors, reporters, imagers, and detectors; and enzyme catalysts); (4) the roles of pores and channels in selective transport, separations, and concentration; and (5) interfaces (e.g., engineered cells or materials surfaces) for selective adhesion, designed membrane-like surfaces for molecular recognition, self-assembly (i.e., surfaces that encode molecular-recognition gradients or tracks), and adaptive surfaces (i.e., multipotential surfaces that respond to the molecular environment). The meeting will focus on the use of frontier physical sciences to understand biology and the exploitation of biology to create physically interesting systems. The meeting will cover biomachining, single-macromolecular science, material in intracellular and extracellular spaces, chemical modification of cells and nanomaterial implantation, cell-based devices, cells for chemical factories, genomic modification of cells, and physical science in proteomics. It will be held in the summer or fall of 2001.

Wasserman commented that corporate labs are reducing R&D in catalysis because universities are producing more relevant products and there are small companies that focus on catalysis. It is not just a simple cutback.

Kohn said that, in Berlin, the catalysis researchers are supported by theoretical groups and asked if the United States has anything like that. Millman said, no, nothing that comes close. It is partly because of the cultural differences between our countries. We have people in this country that are equally capable.

Stupp observed that this workshop would be a good opportunity for BESAC and DOE to give input into what should be pursued in this area.

Richmond then reintroduced **Patricia Dehmer** to give an overview of BES nanoscale science, engineering, and technology activities. Preapplications from universities were due January 12, 2001; formal applications are due March 14, 2001.

The visions for the Nanoscale Science Research Centers are to

- Advance science through in-house efforts to advance the fundamental understanding and control of materials at the nanoscale and through supporting investigators and groups working together on problems of a scope, complexity, and disciplinary breadth not possible working separately

- Furnish service to the scientific community by providing (1) state-of-the-art nanofabrication and characterization facilities to in-house and visiting researchers at no cost for nonproprietary work; (2) a mechanism for short- and long-term collaborations and partnerships among DOE laboratory, academic, and industrial researchers; and (3) training for students in interdisciplinary nanoscale research in cooperation with regional or national academic institutions
- Enhance laboratory core competencies by (1) advancing the strategic vision and building on the core competencies of the host laboratory, particularly the BES user facilities and research programs already in place; (2) optimizing the use of BES national user facilities for materials characterization; and (3) providing the foundation for the development of nanotechnologies important to DOE
- Provide local and national coordination, requiring proponents to (1) partner with state government and local institutions and (2) complement one another and other-agency centers (e.g., existing components of the NSF National Nanofabrication Users Network and the larger national laboratories with materials-sciences programs and user programs)

Several laboratories have expressed interest in hosting nanoscience research centers (NSRCs); ANL, BNL, LBNL, ORNL, and Sandia/LANL have submitted proposals. According to DOE project-management and budgeting conventions, funding for conceptual designs could be provided in FY 2001 from available funding; funding for Title I (preliminary design) and Title II (final design) could begin in FY 2002; and Title III (physical construction) could begin in FY 2003.

The proposals that have been put forward are the Center for Nanoscale Materials (ANL), Molecular Foundry (LBNL), Center for Functional Materials (BNL), Center for Nanophase Materials Science (ORNL), and Center for Integrated Nanotechnologies (LANL, Sandia, and University of New Mexico).

These facilities are research-oriented. BES would like to hear how BESAC responds to these proposals, which will be presented to BESAC later in this meeting.

Johnson asked if the diversity of students involved in this activity can be tracked. Dehmer responded that some of the proposals have already thought about this and will mention it in their presentations.

Shen asked if there will be coordination between or among the centers. Dehmer replied, yes.

Stupp asked how long they will be funded. Dehmer said that there was no sunset position. Stupp asked if this will extend their current activities. Dehmer said, no, we expect new ideas that build on core competencies.

Kohn asked if there are other states that are doing things similar to what California is doing. Dehmer pointed out that there are strong interactions with the State of Illinois.

Richmond asked if BES wanted general impressions or comparisons when the Committee commented on the proposals. Dehmer responded that full discussions are desired. Stohr asked if there will be a review of the proposals. Dehmer said, yes, but it has not been discussed what type.

McCurdy asked what the size of the proposed budgets and activities of the centers was. Dehmer said that the design money is a few million dollars. Conventional construction, beamlines, instruments, etc. would total $50 to 100 million. The operating lines put out by NSF are $1 to 4 million, which makes it difficult for universities.

Richmond opened the floor to public comment. There being none, she adjourned the meeting for the day at 4:55 p.m.

Tuesday, February 27, 2001

The meeting was called to order at 7:58 a.m. Richmond said that the morning would be devoted to the subject of nanoscience. She introduced **Daniel Chemla** to present an overview of the issues involved, synthesis and design at the nanoscale level, and the proposal for a nanoscience center (the "Molecular Foundry") being put forward by LBNL.

Chemla pointed out that two classes of issues exist in nanoscience:

- In going from the nano to the macro scale, the functional systems are likely to operate differently because of the specificity of nano building units; variations in multicomponent functional assemblies; changes brought about by function, nonlinearity, and collective behavior; and the interplay of function, dynamics, and space-time duality.
- Synergies are likely to be encountered between soft and hard matter; between the top-down and bottom-up approaches; and among experiment, theory, and computation.

At the nanoscale, three elements are important: (1) quantum size because of electron structure, optical effects, and magic sizes; (2) altered thermodynamics because of solubility and melting point; and (3) modified chemical reactivity because of surface area and specific sites.

In the past ten years, massive advances have been made in nanoscale science. Nanostructure studies at the ALS have produced 2-D Co/Cu magnetic quantum wells, the scanning tunneling microscope (STM), and angle-resolved photoemission spectroscopy (ARPES). In addition, tremendous progress has been made in nanoconstruction. The Molecular Foundry is intended to extend these efforts to the physical, chemical, and biomimetic synthesis and fabrication of nano building blocks, producing n-crystals, n-tubes, n-tube bundles, q-dots, q-rods, dendrimers, organic n-structures, patterned surfaces, cell membranes, etc.

One can use DNA to start to organize matter. Generic protocols can be developed for self-organization and self-assembly, allowing one to plan and control matter at all length scales to construct functional superstructures out of the nano-building units. These are the systems we need to build.

To perform a function, a system and its components must exhibit some degree of nonlinearity. Systems consisting of a very large number of individual components, each strongly interacting with a multitude of other components in highly interconnected assemblies, display novel collective behaviors that are fundamentally different from what would be expected from the sum of their parts. These are "complex systems."

The intrinsic nonlinearities of nano-objects are fundamentally different from the properties of the bulk parent compounds of individual atoms. A "function" implies changes in time (i.e., dynamics). The nano-object provides new opportunities for integration and interconnectivity on an unprecedented scale. The nonlinearities of highly interconnected nano-objects produce qualitatively new behavior. The nanometer-length scale is the meeting place of the two great fields of the natural sciences, involving hard matter and soft matter. Examples of nonlinearity include the time-energy picture of the quantum interaction between two particles.

The nanoscale brings up a number of interesting questions of dynamics. A "function" implies changes in time. The time scales of nanometer objects span many orders of magnitude, from milliseconds to attoseconds. Not only will it be necessary to investigate a wide variety of properties of matter at the level of a few molecules or nanostructures, but it will also be very important to follow the evolution of these properties at multiple time scales.

Hard and soft matter are going to be used in combination. The nanometer-length scale is the meeting place of these two fields of science. Cells are factories of reactants and reagents. A major question is how to harvest soft matter.

Working with nanomaterials presents some computational challenges in going from the atomic or molecular level (1 to 100 atoms) to nanostructures (10^3 to 10^6 atoms) to bulk (an infinite number of cells with 1 to 10 atoms in a unit cell). Such atomistic calculations will need to reflect the correct symmetry, surface, whole Brillouin zone, quantitative predictions, and connection to ab initio calculations.

The research cycle starts with design and proceeds through synthesis, measurement, and analysis back to (re)design. LBNL wants to shorten the time of this cycle by putting all these elements together. The Molecular Foundry would have four elements:

1. A collaborative research facility for nanoscale materials, providing design, modeling, synthesis/fabrication, state-of-the-art characterization tools, and expertise for the whole community.
2. An internal research program to investigate the conjunction of soft and hard materials and building units; multicomponent, complex, functional assemblies; and multidisciplinary capabilities in materials science, physics, the various forms of chemistry, biochemistry, molecular biology, and engineering.
3. Training and education for undergraduates, graduate students, postdoctoral fellows, and guests.
4. A portal to major national facilities, such as the ALS, National Center for Electron Microscopy (NCEM), and National Energy Research Scientific Computing Center (NERSC) with their nationally unique facilities, such as the e-beam nanowriter and the nanofabrication laboratory.

In terms of bricks and mortar, the Molecular Foundry at LBNL would be a terraced, two- to four-story structure with a bridge to the ALS, a gross area of about 90,000 sq ft, a net usable area of about 53,000 sq ft, laboratories, and offices. It would have facilities for synthesis and fabrication:

- inorganic synthesis (precursors, processes, automation);
- nanofabrication (lithography, thin-film processing, clean rooms);
- organic synthesis (small molecules and synthetic polymers);
- biopolymer synthesis (peptides, oligonuleotides, combinatorial synthesis); and
- cell culture (mammalian, microbial, plants)

and for imaging and characterization:

- ultrahigh vacuum scanning tunneling microscope–atomic-force microscope (UHV STM-AFM), field-emission scanning electron microscope (FESEM), transmission electron microscope (TEM), and focused ion beam (FIB);
- confocal and single molecule, fluorescence, optical tweezers; and
- ultrahigh-resolution spectroscopy beamline.

LBNL has a long history of nanoscience, having first proposed it in 1991 and having very successfully developed the NCEM and the Center for X-Ray Optics (CXRO). It has assembled a nano-crew that focuses its work at the nanoscale and has attracted talented young people. All of this is embedded in the existing laboratory facilities that include the NCEM, ALS, NERSC, and CXRO/MSD Nano-Writer.

LBNL's research programs currently include about 550 graduate students, 300 undergraduate students, 250 postdoctoral fellows, and more than 400 participating guests (not counting facility users). It participates in several academic collaborations, both regional (with the University of California at Berkeley, Davis, Los Angeles, Santa Barbara, San Diego, and San Francisco; Stanford University; and Scripps Institution of Oceanography) and national (with many other U.S. universities). In 2000, the ALS hosted more than 1000 users, and the NCEM hosted more than 200 users. The Laboratory's industrial collaborators include Intel, IBM, Dupont, Seagate, Advanced Materials, Glycomed, Novartis, and others. In addition to direct scientific interaction, trained scientists are what industry sees as LBNL's most important product. LBNL also works closely with the other national laboratories.

Shen asked how many postdocs were among the number of educational participants shown. Chemla replied that about 250 are supported. Kohn asked how many were related to this program. Chemla replied 50 to 100.

Mayes asked what LBNL's vision was for the facility in terms of assembling materials. Chemla said that he had shown a photograph for one: the use of DNA to organize gold on a surface. When the DNA is burned away, the organization is left.

Dehmer asked why LBNL would need the building. Chemla replied, to be efficient, the students (e.g., in chemical and ion physics) need to talk to each other and to do all the work in the same location. Moreover, LBNL wants to pull together interdisciplinary teams from the national laboratories.

Richmond introduced **Murray Gibson** to present ANL's vision of a nanoscale materials center. At ANL, a strong collaboration exists among different disciplines. The Center for Nanoscale Materials at ANL would focus on hard materials and look specifically at three themes in nanoscience: confinement (looking at magnetic structure), proximity (producing effects by putting two materials next to each other), and organization (the imposition of structure).

ANL currently has a program in nanomagnetism, which is funded by BES. It focuses on the control of exchange in patterned arrays, lithography, self-assembly, and the use of organic chemistry to make molecular magnets. ANL is also strong in nanoscale superconductivity, developing expertise in vortices in $NbSe_2$ that lead to interesting physical properties, including magnetism.

Characterization tools are very important. Electron microscopy of nanostructured materials is needed to perform lithography, spectroscopy, etc., and near-field scanning optical microscopy is needed to take chemical communication down to nanodomains. ANL would also like to integrate microelectromechanical systems (MEMS) as a nanolab to measure very small objects' properties [e.g., magnetic fields, electric fields, and nanomechanics (such as a vibrating magnetometer)].

ANL has already developed complex oxides for use in ferroelectric films and dots for high-density storage, and it plans to probe these effects at the nanoscale. It would also like to use diffraction contrast X-ray in nanoprobe experiments. For example, X-ray microprobes can study states and dynamics of ferroelectric fibers. ANL would plan to apply nanoprobe diffraction studies of nanopatterning (using subtractive etching). In such studies, a microfocused beam would allow illumination of individual nanostructures, a fuller understanding would be gained of subtractive processes as well as additive (growth), and novel materials would be investigated (e.g., multicomponent oxides).

ANL has strong collaborations with a number of institutions in the area, such as Northwestern University, the University of Chicago, Northern Illinois University, the University of Illinois-Chicago Campus, and the University of Illinois. More than $36 million spread over two years has been received from the State of Illinois to support this center.

Partnering with universities produces faculty and Argonne staff fellows, leverages program funds, and provides accreditation for educational outreach. ANL plans to establish satellite laboratories at its partners' sites. The Institute for Nanotechnology at Northwestern University is being constructed now, and is complementary to what is being proposed.

The proposed Center for Nanoscale Materials would integrate fabrication, characterization, and simulation to perform nanofabrication, advanced electron microscopy, scanning-probe microscopy, molecular and self-assembly, dynamic nanoscale spectroscopies, and advanced data analysis and simulation. To accomplish all this, ANL plans to add a building to the APS with a clean room, offices, laboratories, etc.

Stohr asked if there were also other capabilities. Gibson replied, yes, they are scattered around ANL and in cooperating institutions.

McCurdy asked what infrastructure the State of Illinois was going to underwrite. Gibson replied, the building that would house the institute at a cost of $36 million.

Johnson asked how they would make nanoscale diamonds, given the difficulty in making macroscale diamonds. Gibson said that their approach makes new small-grain diamonds with which you get a very smooth structure.

Richmond introduced **Don Parkin** and **Terry Michalske** to present New Mexico's vision of a nanoscale materials center. Parkin started by pointing out that SNL, LANL, and the University of New Mexico (UNM) have tremendous scientific capabilities and educational resources, including the National Magnetic Field Laboratory, the Lujan Center, and significant fabrication facilities. They are proposing the establishment of a Center for Integrated Technologies, the objective of which would be to develop the scientific principles that govern the performance and integration of nanoscale materials and educate a new generation of scientists, thereby building the foundations for future nanotechnologies. The center would synthesize theory and characterization (LANL), nanomaterials design and integration (SNL), and nanoscience education (UNM). These lead roles serve to focus the shared capabilities and responsibilities. The center's scientific thrusts would be nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and the nano/bio/micro interface.

The New Mexico vision is an integration from exploration to discovery to design; this is not a linear process, but a connected one.

Michalske continued that these thrusts focus interdisciplinary efforts: Nanophotonics and electronics will usher in a new frontier for integrated photonics and optoelectronics. In the near term, quantum-dot lasers and photonic lattices are allowing us to tailor, couple, and manipulate light in innovative ways. The vision here is to allow a broad integration of self-assembled nanostructures with lithographically defined features that will lead to new sciences and functionality. The applications are broad, from telecommunications to new light sources.

In regard to complex functional materials, quantum confinement in semiconductor nanoclusters was used to tune oxidation/reduction potentials for the breakdown of organic pollutants with only visible light. In addition, self-assembled nanocomposites enable the control of phase stability and structure, mixing hard and soft materials, which allows the production of nanocomposites that mimic natural materials.

In nanomechanics, conventional design rules do not apply. At the nanoscale, mass disappears. Nanostructuring by layering and 3-D particulate dispersions produces superior strength. Studies of quantized dislocation interactions are providing a new understanding of deformation at the nanoscale. Integrating the micro- and nano-length scales will provide new ways to measure nanomechanical properties, explore energy coupling, and evaluate performance. The result will be new materials with superior performance

Nano/bio/micro interfaces are a bridge to living systems. Work already completed in New Mexico laboratories includes

- the integration of semiconductor nanoscale discoveries [i.e., the vertical cavity surface emitting laser (VCSEL)] with biofluids to develop the Bio-Cavity Laser for single-cell diagnostics and
- the use of synthetic nanostructures to mimic the molecular-recognition machinery of living cells.

The integration of nanomaterials with biological structures is the key that will lead to new concepts for molecular recognition, transport, and energy/signal transduction.

The Center would provide cross-cutting capabilities to advance its scientific thrusts. In New Mexico, many of the unique capabilities needed to do this are already present. About 30 SNL personnel are on the UNM campus now. What is proposed is to provide the infrastructure and environment for successful collaborations with other NSRCs, universities, and industry. Two major facilities are in Albuquerque [e.g., the NanoFabrication and Integration Laboratory (NFIL)] and one in Los Alamos [the Integrated Theory, Synthesis, and Characterization Laboratory (ITSCL)]. In addition, there are dedicated resources and leveraged capabilities in each institution. The NFIL has a core of shared capabilities: a theory laboratory, characterization laboratory, interaction area, and leveraged institutional capabilities.

The region is home to LANL, SNL, Air Force Research Laboratory (AFRL), UNM, New Mexico State University, New Mexico Tech, Intel’s major U.S. microelectronics manufacturing facilities, and many prospering high-tech industries. The Southwest is home to many outstanding universities and high-tech industries. It is a great source of students, faculty, and collaborators for the center.

From a national standpoint, the center is distinguished by its focus on performance and its integration of nanoscale materials; at the same time, it complements the other four NSRCs. The center is forming strong connections with university nanocenters, including California’s NanoSystem Institute, Cornell’s Nano BioTechnology Center, and Harvard’s Center for Mesoscale Imaging.

Stohr said that he heard a lot of buzz words but wanted to know who the people are that would be driving this. Michalske said that they had approximately 50 people attend an organizational meeting two weeks ago. Their strength is in the scientists at the national laboratories and universities. Stohr asked what their strengths were. Michalske replied, nanophotonics, nanolithography, photonic crystals, quantum data, nanocell materials, and nanomechanics practiced by people that have worked in these fields for a long time.

Wasserman asked how work would be coordinated. Parkin said that they would set up communication links and have people reside at the other sites. This would not be new to them; they share BES programs across the three institutions now and have been dealing with the problem of coordination.

Kohn asked what capabilities are in place. Brueck responded, extensive capabilities in crystal growth for semiconductors, microengineered materials, and nanochemistry. Kohn asked what the student enrollment was. Brueck responded, approximately 100 graduate students in nanoscience.

Stupp asked how the center would connect to those outside the institution. Parkin replied, through joint workshops. Michalske said that the center would have an exchange of personnel and would use the unique equipment at the different centers.

Richmond introduced **Richard Osgood** to talk about BNL's proposed center. He said that BNL's scientific thrust is in functional nanomaterials (e.g., ferroelectrics, piezoelectrics, catalysts, and magnetics). BNL focuses on fundamental materials chemistry and physics. Major themes that it addresses are collective phenomena and chemical reactivity at the nanoscale. One of the most important results is that it enables an integrated materials program at BNL and leverages and expands work in other divisions.

The BNL Center for Functional Nanomaterials building would be contiguous to the National Synchrotron Light Source, Instrumentation Division, and Materials Science Division. Major university partners are State University of New York at Stony Brook, Columbia University, and Princeton University. The structure would be a two-story building including five major laboratory clusters: nanofabrication of unconventional materials, high-resolution microscopy, proximal probe microscopy, synthesis and in situ probing, and ultrafast optical science and probes to look at dynamics

Within BNL, the center would provide a first common "home" for materials science, expand interactions with nearby universities, expand student and joint appointments/fellowships, build on the long NSLS leadership in new material probes, and institute a cross-cutting thrust among five scientific departments plus the Instrumentation Division.

In the region, the center would provide a major Northeast materials center in key materials systems that have major industrial and fundamental scientific importance. It would be strongly collaborative with major regional university and industry research centers (e.g., the University of Delaware and Exxon). It would also have major new user or collaborative instruments.

Currently, BNL has an important graduate school population (not users); Stony Brook is a principal partner in running BNL; and BNL has an advisory board on which Columbia, Princeton, Yale, MIT, Cornell, and Harvard are represented. The center would expand the university role, focusing on the three nearby focus universities (Princeton, Columbia, and Stony Brook); major new user instruments with user support; an emphasis on student/faculty support/joint positions; and expanded collaborations with the University of Massachusetts, Rutgers, University of Connecticut, etc.

Planning meetings have been held, science proposals have been submitted, universities have been involved, and four joint appointments in nanoscience have been made.

The center would address four integrated thrust areas: (1) the physics of functional nanostructured materials, (2) nanocatalyst materials, (3) nanoscale and molecular materials chemistry, and (4) instrumentation for the preparation and characterization of nanomaterials in which there are many areas of interaction.

The center would build on strong existing programs at BNL and its partner universities (e.g., at BNL, correlated electron systems and oxide materials with a long history of work in piezoelectric soft modes; striped phases; neutron, photoemission, and X-ray scattering; and materials, fabrication, and applications).

BNL has a long history in studying piezoelectrics, which are crucial functional materials. They involve a collective electron response. And there has been nanoscience work with neutron scattering and with X-ray diffraction. BNL's program has a large chemical content (e.g., nanoscale catalysts) in which they are developing new catalysts and nanofabricating platinum. Issues being dealt with include size distribution, cluster density, and structure and reactivity. BNL is also working on the atomic-scale self-assembly of monodisperse tailored catalysts. It is directing its gas-phase people to look at theoretical experimental studies of small clusters. And BNL is going in a new direction to investigate functional molecular materials (soft matter).

Advanced instrumentation will play a crucial role in nanomaterials research, and BNL has a long history in instrument development, with a strong user-support network for work in very-large-scale instrumentation. For example, BNL developed a method for using electron beam lithography to produce Fresnel zone plates for X-ray focusing. These plates are fabricated at Lucent Technologies.

The center would take BNL in new scientific directions, provide new user instruments, establish a needed regional materials center, produce more university involvement, and make the DOE laboratories a stronger base for industrial collaboration.

Shen asked who the four joint appointments in nanoscience were. Osgood replied, Stan Wong, Arthur Suits, Richard Osgood, and Mike White.

Stohr asked if the proposal includes money for an SOA X-ray beam. Osgood replied that there is a small-angle X-ray scattering component that would be important in polymer chemistry.

Kohn asked if nanoscience offers promise in alternative energy. Osgood said, yes; for example, the Graetzel Cell is a low-cost solar concept.

Sinha commented that, even if there is duplication in what is proposed, these centers will serve regional needs, and there are important industries in the Northeast, Southwest, and West Coast that would benefit greatly. Also, industries are moving away from these research activities.

Johnson asked if there was a specific plan to hire staff as industrial collaborations disappeared. Osgood replied that there was. Additional students would be brought onsite, and additional faculty joint appointments would be made. In addition, there would be SOA instruments here, so skilled technicians would be needed to operate them.

Richmond introduced **James Roberto** to make the ORNL presentation for a nanoscience center. He said that the purposes of the proposed center at ORNL would be to

- advance nanoscale-materials research through the integration of the unique neutron-scattering capabilities of the SNS and the upgraded HFIR with nanomaterials synthesis, theory, modeling, and simulation;
- provide the research infrastructure to ensure full utilization of the SNS and the upgraded HFIR for nanoscale materials research;
- advance the fundamental understanding of soft materials, complex nanophase materials, and collective phenomena that emerge on the nanoscale; and
- provide a national and regional resource for nanoscale research in partnership with participating universities.

The philosophy is to be flexible, responsive, and highly leveraged and coordinated. These attributes would be attained by employing a minimal permanent staff, investigating only 10 to 12 research areas that continually evolve and change, engaging a significant university presence in staffing and governance, using an advisory committee to guide equipment acquisition and scientific direction, making infrastructure investments that reflect national and regional needs, and developing a facility that complements and extends the existing laboratory and university research.

The intense neutron beams at the SNS and HFIR will make broad classes of nanoscale phenomena accessible to structural and dynamical study. ORNL has identified three areas of particular importance: soft materials (including molecular interactions and nanostructures in polymers and folded proteins), interface science (including nanomagnetism, thin molecular films and membranes, and organic/inorganic interfaces), and nanophase materials (including nanostructured composites, ceramics, alloys, and materials with nanoscale spatial, charge, and magnetic ordering).

ORNL is in the process of upgrading the HFIR with new and upgraded instruments and a thermal-neutron intensity that is increased 2 to 3 times. In addition, ORNL will have the SNS, the world's most advanced accelerator-based pulsed-neutron source, producing neutron beams with more than 10 times the intensity of any existing pulsed-neutron source.

These capabilities open up the possibility of studying a rich array of physical properties, such as the self-organizing or -assembling behavior of polymers, micelles, and proteins and the characteristics of perovskite-structure complex metal oxides (CMOs).

Neutron-scattering opportunities include small-angle neutron scattering (SANS) for large-scale structures, reflectometry for molecular-scale interfaces, and hydrogen/deuterium (H/D) contrasts for atomic-level details. The science that would be enabled would include (1) polymers and block copolymers in nanotechnology and (2) novel nanostructures from block copolymers and biomolecule/nanotube assemblies.

The study of self-assembled molecules requires an understanding of the 3-D microphase-separated states of block copolymers, the comprehension of the dynamics of polymer-polymer diffusion, and the conduct of time-resolved studies of morphological changes. The possible morphologies of triblock copolymers include wires, planar structures, and 3-D structures.

Another application would be the study of molecular orientation at membranes (e.g., the penetration of membranes by the bee-sting protein, meliltin).

Complex nanophase material systems present many challenges, including synthesis (choosing the right path in a bewildering array of materials) and greatly expanded energy, length, and time scales. Neutron-scattering opportunities include studies in elastic and inelastic scattering and high-resolution powder diffraction. The science enabled includes highly correlated complex materials (stripes), reduced dimensionality (materials with no bulk analogs), magnetism and spin-dependent transport in magnetic nanostructures, and functional nanophase materials.

For energy, nanoscience can be applied to clathrate systems on the ocean floor, fuel-cell electrolytes and membranes, carbon foams, nanophase composites, thermal-barrier coatings, and battery materials.

A lot of dynamics in alloys and other systems can be studied with the new neutron sources: nonequilibrium phase-transformation kinetics, amorphous-to-crystalline transitions, grain-growth kinetics, porous materials, and reaction kinetics. A major difficulty is finding a way through the maze. That can be done through science-driven synthesis and simulation that combines terascale computing, unique crystals for neutron scattering studies, and the synthesis of complex nanoscale materials to produce more intelligent searching. Theory, modeling, and simulation (TMS) methods applicable to nanoscale systems are made possible by ever-more-powerful computers and corresponding advances in software and algorithms and by the merging of several computational techniques (e.g., quantum chemical and molecular dynamics) to provide highfidelity simulations of nanoscale systems based on first principles. TMS is a key enabler for narrowing the search for new materials, reducing the time needed to design and synthesize new materials, and designing and optimizing new nanoscale technologies. ORNL has leading expertise in terascale computing and applications to nanoscale materials design and synthesis modeling.

The center would be collocated with the SNS and ORNL's nanoscale materials programs, and it would be jointly operated with university partners with substantial support for student and faculty participation. At any given time, 50% of the staff would be from other institutions (faculty, students, and industrial and government laboratory researchers). It would include an interdisciplinary Nanomaterials Theory Institute, facilities for the synthesis of research materials, clean facilities for nanofabrication, and specialized equipment for characterization.

ORNL has strong partnerships with The University of Tennessee (UT), Vanderbilt University, and the State of Tennessee through the new UT-Battelle management and a group of "core universities" (Duke University, Florida State University, Georgia Institute of Technology, North Carolina State University, University of Virginia, and Virginia Polytechnic Institute). Other collaborators in the nanosciences include Harvard University, University of Minnesota, University of Massachusetts, University of Pennsylvania, and Princeton University. At the center, ORNL would like to form interdisciplinary research teams with university scientists and offer a unique research experience to a new generation of graduate students and postdoctoral researchers.

A 100,000-sq-ft building would be constructed with laboratories, clean-room facilities, computers, and office space located next to the SNS and its visitor housing. Researchers would have access to ORNL's material-characterization facilities and terascale computing center. An equipment list, prepared with input from 15 universities, includes equipment for chemical and physical characterization, materials synthesis and nanofabrication, special sample environments for neutron experiments, and computational infrastructure.

The center would incorporate a significant synthesis effort in nanoscale materials related to soft matter, interfaces, and nanophase systems, including polymers, macromolecular systems, exotic crystals, complex oxides, and other nanostructured materials and phases. Nanofabrication facilities would provide a national resource for research materials related to the center's focus areas. And the SNS and HFIR would benefit from access to the most interesting research samples.

Stupp asked what would allow the study of protein. Roberto said that after the instrumentation was improved by a third, one would get orientation information. At a few tens of angstroms, one would be seeing where a molecule is.

Kohn noted that theory plays a large role and asked what theoretical capabilities related to nanoscience existed at ORNL. Roberto replied that he could mention a few names known worldwide in this field, such as Malcomb Stocks and Peter Cummings. In addition to the work performed on polymers by the Laboratory's Chemical Technology Division, the laboratory also performs extensive research and development on nanoscale materials processing.

Johnson asked what the samples would be that would come from overseas. Roberto responded that we cannot do it all alone but would use this center to address that issue.

Sinha asked if ORNL is going to hire experts. Roberto said that the laboratory had already hired one and that it is easy to attract such talent with The University of Tennessee nearby.

Richmond thanked all the presenters and asked Dehmer to outline what input BESAC could make.

Dehmer asked what BESAC would like to see that has not as yet been presented and what the members' general reactions were to these center concepts.

Goodman asked Dehmer what DOE's vision was on the number of these centers. Dehmer said that she expected more than one would be funded in order to serve regional needs and that it is possible that all of these centers could be funded.

Shen said that he was impressed with all the presentations. Because of market forces, industry cannot afford this type of research anymore. What he would like to see emphasized is the effect that these centers and the research that they would support would have on the nation's industrial competitiveness. He said that he could see industries paying $100,000 for memberships in these centers.

Wasserman said that he also was impressed but that there are a lot of chemistry and nonbiological systems that could be of great interest. In addition, the contrast between NIST's support personnel and DOE's was mentioned as an important factor in using the centers effectively. The entire range of capabilities to carry out an experiment needs to be reflected in the staff support and would be a great help to researchers in related areas who end up using these centers.

Kohn raised the question of BES's involvement in alternative energy sources. He noted that the large surface areas and highly organized structure of nanomaterials could pay off in highly efficient solar reflectors. He offered the opinion that, if BESAC took the lead in dealing with the energy requirements and nanoscience, it could make a great contribution.

Greene stated that some of the ideas are very far reaching and that and having multiple centers would improve the chance of success. However, it would have been helpful to have had the full proposals in hand in order to comment on them intelligently.

McCurdy noted that the visions of what the proposals have to offer in terms of science (new accomplishments) will be essential to sell the budget and to obtain funding. Dehmer said that it is hard to predict the future; many of these presentations tried to give a hint of the benefits of this advanced science and technology.

Sinha said that one has to be careful that the funding from this nanoscience is not just used to advance more work that is already being done but, rather, breaks new ground in science.

Stupp said that his overall assessment was positive, but that he would like to see a concrete statement of how these institutions would be *user* facilities and how students and postdocs would benefit.

Mayes said that she wanted to see how these facilities would serve the broader needs of the country, to see nanofabrication facilities that users from across the country would be attracted to.

Kohn asked what the role of organizations other than BESAC would be in implementing this initiative. Thomas said that there is an interagency working group in nanoscience that was set up by the previous administration; it oversees the national nanoscience initiative and recommends directions for work by DOE, NSF, DOD, etc. DOE recognizes that what is lacking is the capability to make the things you want to study. It makes sense to collocate the nanoscience facilities with the sites where the samples are produced. It was recognized that DOE has the responsibility to establish these centers in conjunction with the extant world-class facilities, such as the light sources and neutron sources. Kohn noted that the Oak Ridge proposal referred repeatedly to the SNS but that the SNS is years away. He asked what would happen in the intervening time. Roberto commented that the upgrade to the HFIR would result in the operation of the highest-flux neutron source in the world. When that upgrade was completed and the facility was available to the scientific community, it would be able to provide samples for the proposed nanoscience center.

Richmond commented that the proposals for nanoscience centers could have included additional items on individual ties, energy efficiency, regional-economy effects, and other relevant aspects.

Crow asked if BESAC could have NSF come in and tell us about their nanoscience projects. Dehmer offered that BES could prepare a summary of NSF's activities.

Richmond thanked all the presenters and noted that the next meeting of BESAC will have a progress report and overview of neutron sources, an expanded discussion of LCLS scientific issues, and additional examination of the different nanoscience initiatives. The tentative date for the next BESAC meeting is August 2-3. New appointments to the Committee will take effect in October. She asked for public comment. Osgood noted that the proposed NSF nanoscience centers are smaller than those envisioned for DOE and that the proposed DOD centers do not emphasize instruments and sources.

There being no further public comment, the meeting was adjourned at 10:44 a.m.

Respectfully submitted by
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Recording Secretary
Mar. 21, 2001