MINUTES OF THE

OCTOBER 10-11, 2000

BASIC ENERGY SCIENCES ADVISORY COMMITTEE

(BESAC) MEETING

Gaithersburg Marriott Washingtonian Center
Gaithersburg, MD

Geraldine Richmond
Chairperson

Minutes for the
Basic Energy Sciences Advisory Committee Meeting
October 10-11, 2000,
Washingtonian Central Marriott Hotel, Gaithersburg, Maryland

BESAC members present:

Boris W. Batterman
Jack E. Crow
James A. Dumesic
Laura H. Green
Walter Kohn
Anne M. Mayes
C. Bradley Moore
Zhi-Xun Shen, Vice Chair
Joachim Stohr
Kathleen C. Taylor
Collin L. Broholm
Patricia M. Dove
Mostafa A. El-Sayed
Anthony M. Johnson
Marsha I. Lester (Tuesday only)
C. William McCurdy, Jr.
Geraldine L. Richmond, Chair
Sunil Sinha
Samuel I. Stupp
Edel Wasserman (Tuesday morning only)

BESAC members absent:

David D. Awschalom
Robert B. Horsch
Richard E. Smalley
D. Wayne Goodman
Cherry Murray
David E. Tirrell

Also participating:

Philip Bucksbaum, University of Michigan
Patricia Dehmer, Director, Office of Basic Energy Sciences, DOE
Jonathan Dorfan, Director, Stanford Linear Accelerator Center, Stanford University
Mildred Dresselhaus, Director, Office of Science, DOE
Janos Hajdu, Uppsala University
Murray Gibson, Argonne National Laboratory
Keith Hodgson, Director, Stanford Synchrotron Radiation Laboratory, Stanford University
Linda Horton, Oak Ridge National Laboratory
Dan Imre, Brookhaven National Laboratory
Richard Lee, Lawrence Livermore National Laboratory
William Millman, Acting Director, Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, DOE
David Moncton, Executive Director, Spallation Neutron Source Project
Frederick O'Hara, BESAC Recording Secretary
Eric Rohlfing, Atomic, Molecular, and Optical Sciences Program, Office of Basic Energy Sciences, DOE
Brian Stephenson, Argonne National Laboratory
Iran L. Thomas, Associate Director, Office of Basic Energy Sciences; Director, Office of Basic Energy Sciences, Division of Materials Science
John Vetrano, Pacific Northwest National Laboratory

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

Tuesday, October 10, 2000

Chairwoman **Geraldine Richmond** called the meeting to order at 8:32 a.m. She welcomed the members, had them introduce themselves, and reviewed the agenda of the meeting. She introduced **Patricia Dehmer** to give an overview of the Office of Basic Energy Sciences (BES). Dehmer remarked that the budget saga began in February with the President's submission of the FY 2001 budget, which requested $244.2 million more than was appropriated the previous year. A good deal of this increase ($163 million) was construction funding for the Spallation Neutron Source (SNS). In this proposed budget, funding for the core programs was flat or decreased slightly (without accounting for inflation), putting the laboratory programs at risk. Although both the House and the Senate cut amounts and items from this request, the conference committee reported out and Congress passed a budget that was, essentially, the President's request. A major consideration in the funding for the SNS was the decision of the Tennessee legislature to exempt the project from sales tax, thus saving DOE millions of dollars over the life of the project. Major increases in the BES budget were for

Research	$ 40 million
Major Items of Equipment	12
Facility Operations	12
SNS	160
Waste Management	8
General Plant Projects and Equipment	0.5
Small Business Innovative Research and Technology Transfer	1

If it were not for the efforts of the scientific community [e.g., the American Physical Society, American Institute of Physics, American Chemical Society, Neutron Scattering Society of America, national laboratories, Defense Programs (DP) laboratories, university presidents, industries (such as Intel), user facilities, individuals, Office of Management and Budget, and Dear-Colleague letters from senators and congressmen] in July and August, this budget outcome would not have happened.

BES received the full $36.1 million it requested for the National Nanotechnology Initiative. The two reports issued by BES were used heavily to impress the need for this research on funders. During the past 20 years, tremendous advances have been made in visualizing and making things at the nanoscale. The major challenges for the BES nanoscience program are to:

- attain a fundamental understanding of nanoscale phenomena,
- design and synthesize materials atom by atom to produce materials with desired properties,
- understand how living organisms create materials and functional complexes, and
- create experimental tools and theory/modeling tools to accelerate nanoscale research.

With the nanoscience funds and as a part of a national program, BES will support (1) awards to investigators at DOE labs or at universities and (2) nanoscale-science research centers (NSRCs) at laboratories currently housing major BES user facilities. These NSRCs will

- advance the fundamental understanding and control of materials at the nanoscale,
- provide an environment to support investigators,
- optimize the use of BES national user facilities for materials characterization,

- provide state-of-the-art equipment,
- provide the foundation for the development of nanotechnologies,
- provide a formal mechanism for both short-term and long-term collaborations,
- provide a training ground for graduate students and postdoctoral associates in nanoscale research,
- build on the core competencies of the host laboratories,
- seriously advance the strategic vision of the host laboratories,
- partner with state government and local institutions, and
- complement one another.

She reviewed the Office of Science (SC) organization chart to orient members about where BES occurs in the organization, provided an extensive list of major research areas pursued by SC, and broke down the SC budget by major expenditure categories:

Base research at universities	$ 131	million
Base research at national laboratories	199	
BES user facilities	255	
Capital equipment	48	
General plant projects	11	
Accelerator Improvement Program	12	
Construction (SNS)	100	

She reviewed the new organization chart of BES. The Office now has two divisions: the Materials Sciences and Engineering Division and the Chemical Sciences, Geosciences, and Biosciences Division. The first of these two divisions has two teams: the Metal, Ceramic, and Engineering Sciences Team and the Condensed-Matter Physics and Materials Chemistry Team. The second division has three teams: the Molecular Processes and Geosciences Team, the Fundamental Interactions Team, and the Energy Biosciences Team). She noted that BES operates major user facilities for X-ray and neutron scattering and also a number of smaller facilities and collaborative-research centers that provide opportunities for linkages with local universities.

She broke down BES's funding to the national laboratories, showing that most of that funding is centered at Oak Ridge National Laboratory (ORNL), Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), and Lawrence Berkeley National Laboratory (LBNL). A series of graphs showed that, from 1988 to 2001,

- BES's budget authority has increased,
- base research has increased slightly with the office's commitment to university programs remaining constant with 163 universities being supported in FY 2000,
- facility operations has grown significantly (a trend that will continue and that does not portend well for the laboratories, whose mission is shifting from conducting in-house research to hosting outside users), and
- capital construction has varied widely and is at a peak with the construction of the SNS.

This overall lack of significant growth was paralleled by the data in an American Association for the Advancement of Science (AAAS) graph that showed that funding for the physical sciences has remained constant from 1970 to 2000 while funding for the life sciences has increased significantly (in constant dollars). What this means is that, after correcting for inflation, the physical sciences have actually experienced a decrease in support. It also implies that the Office of Management and Budget (OMB) deflators are too small. A more meaningful measure of inflations would be the American Association of University Professors' cost deflators, which show the "people-buying power" of research dollars. This measure is cross-disciplinary and may be more intense for scientific personnel. This premise was borne out when BES asked the national laboratories to provide staffing data for the past 10 years. Those data indicated a 20% decline in the level of staffing that the laboratories could afford. During this same period, national laboratories' staffing of user facilities increased 112%. These data mean:

- BES work at the DOE laboratories, which once was dominated by research performed by laboratory staff, is now dominated by world-class scientific facilities that serve the national scientific community, by collaborative research centers, by research associated with those centers, and by other research uniquely suited to the laboratories. This trend is supported by numerous blue-ribbon panels and will continue.
- Work at universities is a critical component of BES's research portfolio and will continue to be a significant portion of that portfolio.
- National laboratory activities are increasingly being linked to activities at other institutions.
- The "flat funding" for the physical sciences is not flat but actually represents a decrease in buying power for scientific research, and the OMB deflators give a disingenuous picture of funding for the physical sciences.

She concluded that (1) the BES research portfolio must maintain national leadership in special stewardship areas and must contribute to U.S. leadership in many more areas. (2) BES must continually establish appropriate new intramural and extramural programs. (3) BES must maintain state-of-the-art and next-generation facilities for the national scientific community. (4) The BES budget should be increased by 15% per year for the next 5 years with the same type of support from the scientific community that was witnessed during the past budget review.

She pointed out that BESAC is one of six committees advising SC. Its charter calls for it to review and make recommendations about the BES program; advise BES on long-range plans, priorities, and strategies; advise BES on funding levels; and advise BES staff on scientific issues of concern. BESAC operates under the auspices of the Federal Advisory Committee Act, which mandates that such advisory committees be the only mechanism by which federal officials obtain consensus advice. Within BESAC, subcommittees can be formed and operate to address technical or managerial issues; the findings of these subcommittees are reported to the full Committee, which can then consider those recommendations and accept or reject them in part or in whole. Findings and recommendations are made available to BES only through the whole Committee. Dehmer closed by reviewing the rights and responsibilities of BESAC members and by extending a warm welcome to the new members of the Committee.

Kohn asked what happened in the area of alternative energy sources (e.g., solar energy conversion). Dehmer said that DOE had large programs in that area that are centered at the National Renewable Energy Laboratory (NREL). Funding for many of the related research programs has been increased, including a major increase this year. It is an important area to this administration and is important to DOE regardless of the administration in power. Chemical energy changes, the introduction of biomass, and materials science (semiconductors and solar cells) are notable research programs. Kohn said that, because of the low cost of energy, the United States has not put enough emphasis on this research area. Dehmer noted that there were a lot of cofunded programs with international activities that have been very successful. BES tries to balance its core research program and its research portfolio. It is not a perfect balance; there is always a dynamic tension in what good is emphasized. The fulcrum changes over time.

Richmond called the Committee’s attention to the facts that the review of the Intense Pulsed Neutron Source (IPNS) would start immediately after the conclusion of this meeting and that the next BESAC meeting would be Feb. 26-27, 2001. She declared a break at 10:00 am.

The meeting was called back into session at 10:22 am. Richmond introduced the new director of the Office of Science, **Mildred Dresselhaus**, who reviewed the SC budget. She started with her ideas on taking over this job:

- The United States should be the world leaders in all major areas of science, demonstrating this leadership by
    1. supporting world-class research on national goals
    2. enabling rapid response to breakthroughs in other nations
    3. supporting excellence in university science education
    4. attracting bright, young students to science
- The United States should maintain clear leadership in some areas of science
    1. if required by national objectives
    2. if a field is a broad interest to society
    3. if a field significantly affects other science.
- The Department has to be a player with the National Institutes of Health (NIH), National Science Foundation (NSF), and other federal agencies.

SC is a main funder of science. It is in the top five in the physical sciences, environmental sciences, mathematics and computing, engineering, life sciences, and R&D facilities. She summarized the massive number of research facilities funded by SC.

The user community keeps growing; 17,000 researchers use SC facilities. For example, the number of users of synchrotron light sources went from 1600 to 5250 between 1990 and 2000. The facility-operation personnel increased from 1990 to 1994, but has remained the same since then; this while the number of national-laboratory-based researchers has decreased, which is a result of the constant budget of SC. She showed the AAAS graph showing the flat funding of physical-sciences research from 1976 to 2000.

The Department would like to get closer to the public support enjoyed by the life sciences. Another AAAS graph showed the funding for federal agencies for the past 10 years. NIH’s budget almost doubled during that period.

She then reviewed the legislative history of the FY-2001 SC budget, which increased from $2788 million to $3151 million, including an additional $161 million for the SNS, $70 million for high-performance computing, $6 million for user-facility upgrades, $36 million for nanoscience engineering and technology, and $25 million for the life sciences. This budget received broad-based support from the scientific, university, industrial, and legislative communities. She broke the SC budget into the categories of base research (universities), base research (national labs), BES user facilities, capital equipment, general plant project (GPP), accelerator improvement project (AIP), and construction.

Dresselhaus hopes to increase funding by 15% per year for the next five years. One question is where to put this money. She developed some benchmarking metrics to support this request:

- While the United States is among the leaders in some materials sciences, it is slipping behind in other fields.
- Interagency benchmarking: Where is work being done, and by whom is it funded?
- Among the best journals, who is being published, and who is funding that research?
- Return on investment

- Strategic planning: How can we improve our research portfolio overall?
- Benefits to the public
- Investment in the future
- Infrastructure improvement
- Letting people know what we do (collecting nuggets, compiling a list of the top 100 nuggets from 1977 to 2000, the top end of the scale to catch people's attention)

Items that she would like to see BESAC deal with include:

1. What is the Committee's assessment of research quality and how can it be further improved?
2. What is the Committee's assessment of the quality of facilities and their operation and how can they be improved? Are new types of facilities needed?
3. Is the balance of investments correct?

El-Sayed asked the purpose of collecting the nuggets. Dresselhaus replied that the nuggets give an emphasis on the upper end of research.

Kohn said that this would be a good time to increase research funding for nonpolluting and renewable energy sources. He asked if there was a recent report assessing this research field or should the Committee produce one. Dresselhaus was not aware of any such report but noted that BES research funded jointly with the Office of Renewable Energy just increased the efficiency of solar cells by 40%.

Mayes commented that the operation of user facilities is alive and well, but asked about basic research on environmentally friendly energy production. Dresselhaus said that energy security and defense security have gotten a lot of DOE attention. Energy efficiency and renewable sources have had a difficult time getting research dollars. She acknowledged that increased effort should be devoted along those lines. The politics have not been favorable in the past.

Richmond said that SC has been active in the training of scientists, but there are fewer students. More emphasis needs to be placed on precollege science training. Dresselhaus said that DOE will succeed in that in concert with the NSF.

Stupp said that it was not just a matter of numbers but also the quality of human capital in the research community. Dresselhaus voiced the opinion that the students today are excellent; we need to talk about what the careers are like and make those careers more attractive. BES may be having trouble getting personnel, but high-energy physics is in a real crisis. We cannot support many students.

Green commented that the number of personnel available to run the facilities is not increasing. We need to support the permanent personnel at these facilities.

Moore asked what process BES would like BESAC to use in assessing the budget. Dresselhaus said that the Committee's chairperson should be the one to answer that. Richmond said that the topic could be discussed the in the following morning's session. Dehmer said that the Committee could organize itself into subcommittees to look at specific topics. A lot of data is available that would be appropriate for BESAC to look at for several of these metrics. BESAC also has the Management Review Subcommittee, whose charge could be extended. There is an opportunity to reconstruct the research portfolio now. A year or two from now, such an opportunity may not exist.

Stohr said that improvements could be made in interagency cooperation, particularly among DOE, NIH, and NSF. He had run into problems in the past because of different philosophies and processes. Dresselhaus noted that they also have different funding sources in Congress. She said that this is her job and that she will look for ways to make such cooperation easier in the future.

Richmond introduced **Eric Rohlfing** to speak about the history and technology of fourth-generation light sources. He noted that a series of workshops had been held beginning in 1992. These workshops identified a linear-accelerator-driven (linac-driven) free-electron laser as the best technology for increased brightness. Scientific applications of such a machine were discussed, but a broad case was not made. Material damage (of the sample) was, however, identified as a critical issue. A concept paper was developed in 1997 that posited the use of the Stanford Linear Accelerator Center (SLAC) to drive an X-ray free-electron laser (FEL); it was dubbed the Linac Coherent Light Source (LCLS). Subsequently, the SC facilities roadmap has incorporated a marker for a next-generation light source, but it did not commit to a specific design or technology. Also on 1997, a BESAC panel investigated synchrotron radiation sources and science at four BES light sources. It placed its highest priority on funding exploratory research on fourth-generation light sources and recommended that another panel be convened to advise BES on the development and applications of such a facility. That follow-on panel, commonly referred to as the Leone panel, considered what new science could be done with new capabilities, such as coherence, ultrashort pulses, high intensities, and short wavelengths (in the X-ray region). It also asked what a reasonable R&D plan would be, what such sources would look like, and how they would serve the user community. The report of that panel stated that “the state-of-the-art light source facility of the future will include a complete marriage of accelerator principles and laser art, which has not been previously recognized widely.” It recommended that DOE

- emphasize the hard X-ray region,
- focus R&D on how to develop a linac-driven X-ray FEL,
- simultaneously support laboratory-scale laser sources,
- use third-generation synchrotron sources,
- improve X-ray detectors and optics, and
- improve the scientific case for coherent X-rays.

The proposed LCLS would be an R&D facility for coherent, intense X-rays. It would not be a next-generation user facility but a step toward such a facility. The project would be a collaboration among SLAC, ANL, BNL, Los Alamos National Laboratory (LANL), Lawrence Livermore National Laboratory (LLNL), and the University of California at Los Angeles (UCLA). DOE funding would be highly leveraged by lab contributions. The construction cost is currently estimated at $100 million. The facility’s 0.8- to 8.0-keV X-ray FEL would be designed to produce spatially coherent, subpicosecond X-ray pulses with a peak brightness about ten orders of magnitude greater than current synchrotrons. Specifically, its beam would have a wavelength between 1.5 and 15 Angstroms, the pulse width would be 300 fs, the repetition rate would be 100 Hz, each pulse would contain about 10^{12} photons, and the beam would be fully transversely coherent but not longitudinally coherent. An undulator would be used to produce a coherent beam by self-amplified, spontaneous emission (SASE). SASE FEL theory is well developed and is now used in simulations. The FEL starts from random noise in spontaneous radiation, and the electrons are bunched together by the electric fields of an undulator. Several experimental verifications of the SASE process have been published.

An R&D plan and a construction plan have been postulated. It is possible that the conceptual design could be completed in 2001 and critical R&D completed and construction started in FY 2003.

A 250-GeV linear collider with an integrated FEL facility that would produce a beam with a wavelength of 20- to 1-Angstroms has been proposed at the TeV-Energy Superconducting Linear Accelerator (TESLA) at Deutsches Elektronen-Synchrotron (DESY). A test facility is operational there, but no plans have been made to go to a wavelength shorter than 110 nm.

From another perspective, the next-generation light source would be a tabletop device that would produce 0.75 TW, 13-fs, 9.6-mJ pulses at 10 kHz. The Leone report recommended supporting the development of these tabletop X-ray sources and using them, along with third-generation sources, to explore the scientific applications of ultrafast X-ray pulses. A solicitation for proposals was issued by BES in FY 2000, and five new university grants and one new lab project were begun in FY 2000, joining two projects continuing from FY 1999. The new awards were for

- The Phonon Bragg Switch,
- Multiphoton Quantum Mechanics and Optimal Generation of Coherent X-Ray Harmonic Emission,
- Development and Utilization of Bright Tabletop Sources of Coherent Soft X-Rays,
- Ultrafast Coherent Soft X-Rays: A Novel Tool for Spectroscopy of Collective Behavior in Complex Materials,
- 100-fs X-Ray Detector, and
- Femtosecond X-Ray Beamline for Probing Ultrafast Dynamics in Condensed Matter.

The coherent control of high-order harmonic generation (HHG) for soft X-ray production with a deformable mirror, focusing mirror, and grating was recently demonstrated in a paper published in *Nature*. This experiment is a long way from the LCLS, but it is enough for doing tabletop experiments. The hope is that sophisticated X-ray science, combined with new experimental facilities and advanced laser science, will produce increased brightness, temporal resolution, and photon energy to make possible new scientific techniques and capabilities that will lead to next-generation user facilities in the next decade. But the Leone panel recommended that “a more compelling and rigorous set of experiments that can be achieved only if such a new coherent light source becomes available” be developed to justify the investment in such a facility. In response to this recommendation, BES sponsored a series of workshops to better define the broad scientific case and it requested from the LCLS Scientific Advisory Committee a document that (1) detailed the first experiments that would be carried out on the proposed LCLS, (2) formed the basis of the LCLS’s experimental requirements, and (3) provided BESAC and BES the rationale for a decision on whether or not to proceed with the conceptual design of such a facility.

Wasserman asked how one knew the costs at all these scales. Rohlfing said that the tabletop research is small scale and will remain so. The LCLS construction is projected $100 million. If you add the operation infrastructure, equipment, etc., it is $150 million. Dehmer commented that a construction project takes many steps; here, we are approaching the first step, the conceptual design. Such a design requires a scientific case, the development of which would cost a few million dollars. At the end of the conceptual-design phase, broader support would be expected from the scientific community. Then a more-detailed design would be carried out. Doing a conceptual design does not commit one to any further steps (or costs). The Leone panel recommended a stronger scientific case before going forward with the conceptual design. This Committee could make any of a number of choices. BES is willing to take any advice from

BESAC. Should a conceptual design be pursued? Should more scientific evidence be waited for? Should external reviewers' comments be waited for? Or what?

El-Sayed asked how short a pulse they get at Grenoble. Rohlfing answered, 50 ps. El-Sayed said that one can go much below that range. Kohn asked if anyone would make a brief presentation on the Leone report. Richmond said that during the afternoon session, six presentations would be made on various areas regarding that report. She suggested that the Committee listen to these presentations and then discuss what to recommend to BES.

Batterman said that, when synchrotron sources were being built, there was no question that they would work. Now, there is no guarantee that these new machines will deliver what they promise. In addition, if this machine works, it will not only probe the specimens but also produce the specimens, ranging from the matter of bombs to that of stellar environments.

McCurdy asked if this was a proposal for a user facility in the mold of the Advanced Light Source (ALS) or Advanced Photon Source (APS) national user facilities. Hodgson said that this facility would serve only 5 to 15 stations rather than the 50 of a full-blown user facility. A lunch break was declared at 12:08 p.m.

The Committee was reconvened at 1:12 pm. Richmond introduced **Keith Hodgson** to begin the discussion of what experiments might be the first ones conducted if the LCLS is built. The five presentations that he introduced were selected to describe the most promising scientific endeavors from the many possible areas of scientific inquiry that might be pursued with this research tool. During all the discussions of the LCLS, Stohr and Shen recused themselves from the deliberations and joined other members of the LCLS collaboration in the audience so they would be available to respond as members of the LCLS collaboration to any information needs of the Committee.

Hodgson began the discussion by describing the LCLS and comparing it with other past and current light sources. Six institutions are collaborating on the LCLS: the APS at ANL, the National Synchrotron Light Source (NSLS) at BNL, LANL, LLNL, the Stanford Synchrotron Radiation Laboratory (SSRL) at SLAC, and UCLA. During the past 10 years, there have been many advances in accelerators (particularly on beam dynamics and linear colliders), undulators (particularly on error control), and instrumentation and detector performance. Together, these advances make the LCLS possible. The development of the advice presented in the following five presentations was guided by the deliberations of the LCLS Scientific Advisory Committee. A website (www.ssrl.slac.stanford.edu/lcls) has been established to provide information about the facility to the scientific community.

The LCLS would be located in the SLAC Research Yard between End Station A and End Station B. One hall would contain the undulator and diagnostic instruments, a second hall close by would house experimental stations, and a further hall would house experimental stations for a longer beamline.

Currently, R&D continues to strengthen the baseline design for the LCLS. Experimental studies at NSLS have produced high-gain harmonic generation (HGHG). Work at DESY on the TESLA Test Facility (TTF) FEL is progressing well. The collaboration at BNL between the visable-infrared SASE amplifier (VISA) and the LCLS is advancing. And recently, the Low-Energy Undulator Test Line (LEUTL) at the APS has reported saturation at 390 and 530 nm, the shortest wavelength at which saturation has been observed.

The USDOE is not the only one that is thinking of constructing such a facility. BESSY II (Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung) in Berlin and Spring 8 in Japan are considering such a move, and the Daresbury Synchrotron Radiation Source has formed a study group to explore various FEL options. More to the point, the TESLA Test Facility at DESY in Hamburg is coupling a 300-MeV superconductivity linac with 80- to 180-nm lasers with a gain of 10^3 to 10^4. The second phase of this operation (in 2002 to 2003) will upgrade the facility to produce lasing down to 3 nm in the third harmonic. The ultimate objective of this work is to produce the TESLA 1-angstrom X-ray FEL (XFEL) in 2009 or 2010. A trilateral collaboration on R&D for XFELs has been signed by SLAC, DESY, and KEK (the High Energy Accelerator Research Organization in Ibaraki, Japan).

Jonathan Dorfan then presented the SLAC perspective and proposed involvement with the LCLS. The facility would be an intense, coherent, ~1-angstrom X-ray source that would allow an exciting and diverse research program and would open new vistas of inquiry and discovery. The United States is well positioned to establish the first source of this kind because the unique infrastructure of SLAC provides many of the key elements for a rapid, risk-averse implementation. SLAC has a long tradition of successfully developing novel accelerator-based facilities and would welcome the opportunity to join with its national partners to host this scientific adventure if it comes to pass. SLAC would give the LCLS its highest priority during the development of a conceptual design and construction. Its most recent construction project, the *B* Factory, was completed ahead of schedule and within budget; it is a $120 million device built in collaboration with 600 scientists from 9 nations. SLAC managed the conceptual design and the construction, and within one year, the *B* Factory was producing design-performance integrated luminosity and peak luminosity. In addition, the SPEAR3 at SLAC is proceeding very well, and the recent Lehman review was extremely complimentary of the progress of this upgrade.

If the LCLS comes to pass, SLAC will deploy its premier engineers and technical staff to ensure its success. The vacuum and radiofrequency (rf) engineering teams on SPEAR3 came directly from the *B* Factory team, and the lead engineer on LCLS R&D was the chief engineer of the *B* Factory. SLAC will dedicate the last one-third of the linac to inject into the undulator of the LCLS and will dedicate at least 75% of the annual operating time of that section of the linac to LCLS operation. If given the go-ahead late this fall, SLAC could complete the conceptual-design report and undergo a Lehman review in time for a FY-2003 construction start.

The LCLS project fits into the DOE Strategic Plan and would achieve a peak brightness exceeding existing X-ray sources by more than 10^9, a time resolution exceeding third-generation synchrotron sources by a factor of 10^3, and a coherence-degeneracy parameter that exceeds present sources by a factor of more than 10^9. The flux density could be varied by a factor of 10^6 by focusing, the X-ray absorption could be varied by a factor of 10 to 100 by tuning the energy, and the X-ray absorption would depend on the atomic number and vary by a factor of 10^5. The presentations that follow provide specific detailed examples that fall within a broader scientific-case document being prepared at the APS. They cover five topics (femtochemistry, nanoscale dynamics in condensed matter, atomic physics, plasma and warm dense matter studies, and structural studies on single particles and biomolecules), and they illustrate how the LCLS can probe or manipulate matter and create new states of matter. Additional accelerator and optics R&D is expected to extend the capabilities of the LCLS even beyond the conditions posited for these first experiments. Along these lines, ultrashort bunches could be obtained through a combination of stronger compression of the electron bunch (for which no new hardware is required) and/or for photon-bunch compression or slicing.

Richmond asked what the pulse length might be, and Dorfan responded that 10-fs pulses were indicated to be theoretically possible. El-Sayed asked about the feasibility of single-molecule imaging. Hodgson said that such imaging will probably be produced but will involve averaging.

Hodgson then introduced **Dan Imre** to talk about the first of the five topics, femtochemistry. Imre pointed out that the description of static molecular properties in terms of bond lengths and angles has served us well. But chemical transformations are about dynamics. What is desired is to have a motion picture of the nuclear motions as a function of time to show how chemical reactions occur. What is needed is a tool that looks quickly and gives a great amount of detail. One process that scientists would like to be able to look at is the dissociation of water. Very light systems like that require a time resolution of a few femtoseconds; heavier systems can be studied with pulses a few hundred femtoseconds long.

The LCLS would make it possible to map out the nuclear motions with a resolution of 0.1 angstroms, which is clearly sufficient. The wave function changes with time could be mapped out, and the chemistry could be watched as it happens. Femtosecond lasers are fast enough, but their wavelength (>200 nm) does not allow for any spatial information on the atomic scale. Spectroscopy of the transition state is an attempt to compensate for the inability of lasers to provide spatial resolution. No current experimental technique takes such a direct approach. Ultrafast electron diffraction (UED) is the only experimental system that attempts to break that limit. However, UED will never break the picosecond time limit because of the fundamental relationship between the number of electrons in the bunch and the pulse length. UED can, at best, produces a time resolution of 10 ps; LCLS would produce a time resolution of at least 200 fs, 50 times better.

Johnson asked how the desired mode is isolated. Imre replied that an electronic excitation is used so the cleanest wavefunction would have the broadest excitation. Lester asked what time resolution he was talking about, and Imre said that the resolution is the measurement of the difference in time. Lester said that the dream experiment would need a resolution of less than 50 fs. Imre replied that many systems would produce plenty of data at 50 fs, although that would not include the dissociation of water.

Imre went on to describe pump-probe experiments, in which the reaction is started with the laser and the subsequent reaction is watched with the LCLS. The gas-phase photodissociation of an isolated diatomic molecule would be the simplest of reactions to study with this technique because $t = 0$ is easily defined, the initial wave function is well defined, and the wave function remains localized throughout the reaction. Condensed-phase photochemistry could also be performed this way and, indeed, has been performed on CH_2Cl_2 with third-generation sources. However, those sources have only a limited time resolution. Richmond asked if he could think of any nonhalogenated species that this process would work on, and Imre replied that, if you understand one system, you can understand how other systems work. Sinha asked what would be measured, and Imre responded a distribution of bond length that moves quite a lot. Sinha noted that the diffraction spectrum is going to be over millions of molecules, preventing the researcher from getting the needed resolution. Hajdu responded that a post mortem could be done in each experiment, and the potential information available is tremendous.

The femtosecond resolution of the LCLS will also allow the investigation of dynamics in nanoparticles. Under most experimental conditions, size-dependent properties tend to be masked by the presence of a wide size distribution. The high intensity of the LCLS will make it possible to conduct experiments on *single* particles.

Finally, nanoparticles melt at a temperature that is very different from the melting point of the bulk material. The LCLS's high resolution will allow study of the melting of a single nanoparticle. Melting will be able to be done with a laser, and the melting dynamics will be able to be watched with the LCLS. The time resolution of the Mie scattering spectrum at 1.5 angstroms will make it possible to map out internal particle vibrational modes as well as the surface capillary modes of a single nanoparticle because the LCLS will be very sensitive to the shape of the specimen and Mie spectra are extremely sensitive to changes in particle size and shape. With a large detector, a spectrum will be obtained that is a function of the angle of observation, giving the researcher another dimension of information.

Stupp asked how much damage would be produced. Imre said that the question of damage is a major problem that will be dealt with at length in a later presentation. Stupp asked how relevant the technique was as the molecules get larger and larger. Imre responded that two types of experiments were reported on: dissociation and large systems (like photosynthetic molecules). In the latter, the changes in the active site are looked at, not all the responses of the whole molecule. Stupp noted that larger-scale motions can dominate the response, and Imre responded that the specimen had to be chosen to match the capabilities of the tool. Kohn asked if the technique would be able to image the photodissociation of a large molecule into two large segments, and Imre responded that one would get so many different bond lengths that it would be very difficult. Kohn asked if the work that had been performed had been done in close association with molecular dynamics calculations, and Imre responded that the results shown had been derived from calculations based on quantum mechanics and that they produce real-time images.

Imre concluded by stating that the LCLS is the only tool that will, in the foreseeable future, make it possible to observe nuclear motion during a chemical reaction in real time, and the LCLS can be applied to a wide range of problems in the field of chemistry.

Brian Stephenson then discussed the second of the first set of proposed experiments, nanoscale dynamics in condensed matter. He pointed out that the nanoscale is important in dynamics because it often determines the mechanism of dynamics during materials processing, such as annealing and other processes in which the overall behavior of a material is determined by defects. However, producing nice pictures is not always easy, particularly in situ. The LCLS should allow the observation of basic dynamic processes that occur at the atomic scale and overall dynamics that are mediated by defects and collective mechanisms at the nanoscale. Observing equilibrium dynamics is desirable. Moreover, a technique that will measure both the time and length scales simultaneously will tell a lot about what is going on.

Existing scattering techniques for studying dynamics can probe thermal fluctuations to lengths down to 10^{-1} nm at high frequencies (10^{7} to 10^{15} Hz) and to lengths down to 10^{3} nm at lower frequencies (10^{-3} to 10^{7} Hz). They can also excite and probe fluctuations to lengths down to 10^{3} nm at frequencies from 10^{-3} to 10^{15} Hz. With the LCLS, X-ray photon correlation spectroscopy (XPCS, which has already been used on third-generation light sources) and X-ray transient grating spectroscopy (XTGS) should be able to extend these capabilities into frequency-length regimes as yet untouched.

The LCLS should also allow the testing of the reptation model of the diffusion of long-chain polymers because it would allow observing the diffusion of one polymer in another. Three techniques could be used on the LCLS to observe this diffusion: XPCS, which would produce a "movie" of the speckle moving through the bulk polymer; XPCS with a split pulse (one of which travels along a variable path length before being reintroduced into the original beamline, producing two identical pulses offset by a variable time difference), allowing the determination of a correlation time when noticeable motion is detected; and XTGS, which would split the X-ray pulse from the LCLS into three beams, drive the system with a chosen charge, and observe the response as a delay time. Mayes said that it seems that this capability should already be within our grasp. Stephenson replied that polymers with as high as possible a density difference must be used, and it has not gotten done because of the higher intensity that is needed.

An issue that needs to be resolved or controlled is the avoidance of heating the sample by more than 1 degree. Three variables need to be considered: How many photons are available per pulse? How many photons are needed per pulse to give a sufficient signal? And how many photons per pulse does it take to produce a temperature rise of 1 degree? Plots of available experimental data gathered with unfocused pulses at various energies indicate that windows of opportunity exist if the energy is set to just below an absorption edge; there, the LCLS beam could impinge on a sample without overheating it. The expectation is that the LCLS could be used in a number of applications of XPCS and XTGS that people have tried with third-generation sources and failed at. Kohn questioned whether some of those attempts were on the borderline of what can be done now. Stephenson replied that they were beyond the borderline; research has been conducted with the third-generation sources for 5 years now, and the limits of the technologies are being pushed. Mayes asked about biological samples. Hodgson replied that a damage limit has been mapped out for biological samples; with soft samples, the sample would have to be moved around, or it would accumulate a high local dose very rapidly.

A break was declared at 2:58 p.m. The session was reconvened at 3:17 p.m. to hear **Philip Bucksbaum** describe the atomic physics that could be done with the LCLS. He started by saying that the LCLS, as a high-intensity, high-energy photon source, would provide a unique opportunity to study fundamental aspects of X-rays' interacting with atoms, ions, molecules, and clusters and that the understanding of X-ray–atomic interactions is central to all next-generation X-ray sources.

In current laser–atom experiments, the field modulates the atomic potential at visible-laser frequency, the outer electron has time to tunnel free, and the strong interaction between the free electron and the ion core can be observed. With an unfocused LCLS beam, the field would modulate the atomic potential at X-ray-laser frequency, the electrons would not have time to tunnel free, and the processes involving deeply bound core electrons could be studied. Thus, three new fundamental processes should be observable:

- multiple ionization sufficiently rapid to form hollow atoms,
- multiphoton ionization (two photons acting together) to yield absorption below the edge, and
- giant Coulomb explosions of clusters of atoms that are close together.

These processes would be observed with several types of detectors: charged-state spectrometers, electron-energy spectrometers, ion-recoil detectors, and X-ray fluorescence detectors (to observe relaxation).

An example experiment would be the multiple photoionization of neon to form hollow atoms. Neon will display this effect well, the k-shell photoionizations will be relatively high, it produces a simple and well-understood spectrum, the Auger decay rate is relatively long (2.5 fs), almost all the relaxation is Auger, and that Auger relaxation is more than 100 times the radiative fluorescence. Possible ionization processes that the LCLS might produce with neon include photoionization, Auger decay (making another electron or two come off), sequential multiphoton photoionization, and direct multiphoton ionization. The intensity of the LCLS would make several of these processes possible or probable, such as *k-l* double vacancies (simultaneous ejection of an electron in the *k* and *l* shells).

Focusing the beam would permit observation of coherent two-photon photoabsorption to the point of saturation (i.e., when the photoionization rate equals the Auger decay rate). A lot of single absorptions will occur, also; but a 1.5-keV-electron per pulse detector should be able to be built that would be specific for the two-photon signal.

With clusters as the sample, the physics is very different. What can be looked at are the charge state, electron energy, and ion recoil. With an LCLS beam focused to 0.01 µm, each atom in the cluster would be classically ionized nearly 1,000 times. The atoms would continue to ionize because the Auger rates are about 1000 times faster than the ionization rate. Each atom should be able to be stripped down to a high charge state. Understanding these processes in detail is central to the imaging of biomolecular samples.

McCurdy asked what can be learned about atomic structure, what systems might you be able to use, and what experiments might you be able to do with two-photon absorption in the X-ray region. Bucksbaum replied that you will be able to learn more about correlation, which is a subject where almost all the information currently comes from valence-shell experiments. What we would like to do is to look at these multiphoton processes and to study how correlation affects photoabsorption. McCurdy asked about relativistic effects in the heavier systems. Bucksbaum said that he did not know the answer to that, but anything that changes the inner shells will be able to be investigated. Kohn noted that electron correlations are very small. Bucksbaum said that the enhancement of the inner shell is many orders of magnitude. Mayes asked what the possibility was that another country might do some of these experiments first. Bucksbaum responded that no one else is building an LCLS; if they did, they would attack these basic problems first; the detectors are already available. Sinha asked how the beryllium windows would hold up. Bucksbaum replied that, generally, there would be no problem; however, there are some aspects where the high intensity of the beam would cause damage.

Richard Lee then discussed the fourth of the first set of experiments, plasma and warm dense matter studies. He pointed out that dense states of matter are important because of their wide occurrence. Hot dense matter (HDM) occurs in supernovae, stellar interiors, accretion disks, plasma devices, and directly driven inertial-fusion plasmas (e.g., imploded cores). Warm dense matter (WDM) occurs in the cores of large planets (e.g., Jupiter), systems that start solid and end as a plasma (e.g., exploding wires), and X-ray-driven inertial-fusion implosions.

The LCLS could be used in (1) just creating WDM, measuring the fundamental nature of the matter via its equation of state and watching the surface expand; (2) probing resonances in HDM, measuring kinetic processes, studying redistribution rates, and developing kinetic models by tuning the LCLS to a resonance and watching the fluorescence; (3) probing dense matter, measuring n_e, T_e, $\langle Z \rangle$, $f(v)$, and damping rates by looking at the scattered signal.

The LCLS is unique in that it could both create and probe high-density, finite-temperature matter. Creating WDM requires rapid, uniform bulk heating, which, in turn, requires high photon numbers, a high photon energy, a short pulse length, and a high peak brightness. Conducting pump/probe studies of HDM requires an impulsive source of high-energy photons. And measuring plasma-like properties requires short pulses with a signal that is greater than the plasma emission. No existing source can probe HDM or create WDM to probe. Thus, the LCLS's 10^{10} increase in peak brightness would allow access to novel regimes.

Johnson asked if, when the beam is being focused on the sample, the analog of interference rings is introduced. Lee replied no and that the reason why is that the wavelength of light does not interact with the medium in the same way. The critical density is so high that the X-rays do not interact to make waves. Shen asked where nuclear matter would fit in this array of dense materials, and Lee responded that it would be in the cold matter.

Lee went on to point out that WDM is the regime where neither condensed-matter methods nor plasma theoretical methods are valid. Indeed, materials' equations of state are generally patchwork quilts pieced together from various theories. Only in 1998 was a single approximation of the equation of state for copper devised by employing corrections and adjustments to the patchwork of theoretical results for that element. However, experimental data on deuterium (D_2) ice along the Hugoniot has shown that the theories are deficient, and equations of state for aluminum disagree even though they all match the Hugoniot for that element, which is well known. The LCLS is expected to overcome these difficulties by heating matter rapidly to produce isochores from which the state of material on release could be measured with a short-pulse laser (the surface movement would actually be measured, allowing the calculation of the isentrope).

Another application of the LCLS would be to excite a line transition in HDM and provide excitation levels that would produce a signal that would easily be observable in the emission. The LCLS would be able to do this because its pump rate is larger than the decay rate. No other method is available to probe a hot plasma.

The final application cited was the use of the LCLS to conduct scattering studies that would provide data on free, tightly bound, and weakly bound electrons. These data would allow the measurement of T_e, n_e, $f(v)$, and plasma damping of solid-density, finite-temperature matter.

In summary, he noted that equation-of-state measurements illuminate the microscopic understanding of matter, and other properties of the system (e.g., conductivity and opacity) depend on the same theoretical formulations. However, measuring the properties of high-T_e and -n_e matter requires a short-duration, high-intensity, and high-energy probe. As such, the LCLS is expected to provide measurements of kinetics behavior, plasma coupling, line-transition formation, and high-energy-density (HED) plasma formation.

Sinha asked what the Compton shift would be, and Lee answered, 50 eV. Kohn asked if the laser source under construction at LLNL (the National Ignition Facility or NIF) is going to compete with the LCLS in any way. Lee replied that the NIF is not practical. A source with a pulse of greater than 10 ns cannot be used for this purpose, and the NIF will only produce one shot a day, only some small fraction of which could be used to study WDM. Green asked why this technique was interesting and whether this research could not be done in pressurized ovens. Lee answered that the high temperature and pressure cannot be produced simultaneously with traditional laboratory approaches; other than with a device like the LCLS, these conditions could exist only in planetary cores. Mayes asked why everyone on the team was from Europe or Canada. Lee replied that laser plasma physicists are located at large laboratories, of which there are only three in the world. Mayes went on to ask if he was confident that, if you build it, they will come. He responded, yes.

Janos Hajdu then discussed the last of the examples of first experiments that would likely be conducted on the LCLS, structural studies on single particles and biomolecules. He said that the bottleneck in characterizing biomaterials is that only crystallized materials can currently be investigated because of the radiation damage imposed by the technology. The LCLS beam would interact with the matter through scattering and absorption. How the beam is focused determines whether that beam is appropriate for biomaterials or other types of specimens. The beam would interact with the matter by (1) the photoelectric effect followed by Auger emission, shakeup excitations, and interactions among decay channels; (2) elastic scattering; and (3) inelastic scattering.

The problem is framed by five considerations:

- Biological samples are highly radiation sensitive.
- Conventional methods cannot achieve atomic resolution on nonrepetitive (or nonreproducible) structures.
- The maximum resolution is a function of sample quality in scattering by a crystal, but not in scattering by a single molecule.
- The limit to damage tolerance is about 200 X-ray photons per square angstrom in conventional crystal experiments.
- But the conventional damage barrier can be stretched by very fast imaging.

In the Coulomb explosion of a macromolecule from intense X-ray pulses, the light atoms boil off first, and all the atoms have different X-ray cross-sections. The sample dynamics of such an explosion were modeled with XMD interfaced with GROMACS. The model considered heating, bond breaking, ionization, and ionization dynamics and kept an inventory on all electrons in the sample. He showed movies of such simulations that varied the pulse intensity and pulse length with drastic variation in the molecular response, ranging from no damage to explosive dissociation. The conclusion drawn from these simulations is that ionization and subsequent sample explosion cause diffraction intensities to change. The results from these simulations were used to calculate limits of resolution (in terms of pulse duration and photons per pulse) for several biomaterials, ranging from lysozymes to single virus particles.

The first experiments that likely would be attempted would be on the structure of the viral genome, nanoclusters, the structural kinetics of nanometer-sized samples, nanocrystals, two-dimensional crystal arrays, X-ray diffraction tomography of whole cells, and X-ray scattering from insect cells.

Several questions arise; for example, how to hold a single virus in the beam. One way is to spray it in as nanodroplets, in a hydrated state, at cryogenic temperatures, in a high vacuum, and with a residency time of a few microseconds. Another way is to embed the sample in vitreous ice, with a goniostat, at cryogenic temperatures, and at a high vacuum. A prototype high-mass quadrupole/time-of-flight mass spectrometer has been constructed and used to analyze an MS2 bacteriophage virus, which has a mass of 2,484,700 daltons. The phase problem can be approached by using (1) continuous molecular transforms of single particles, (2) the tools of classical crystallography (for samples with reproducible structures), or (3) holography.

Most biochemical processes involve the diffusion of reactants. As a result, kinetic studies suffer from the mixing problem. Decorated nanoclusters (sample particles that have had other species attached to their surfaces) may help to overcome this limitation. The technique also has implications for structural kinetics.

Eventually, it would be desirable to investigate living systems, the smallest of which are mycoplasmas. They have a 300-nm diameter, a cell membrane 8 nm thick, a solvent content of 60 to 70%, 1 DNA, 400 ribosomes, 10,000 RNA molecules, 50,000 protein molecules, and 400,000,000 water and solute molecules.

Stupp asked what this technology would provide to biology. Hajdu responded that, if this machine works, the number of known structures will expand tremendously. He noted that 80% of all drugs target unknown structures and have mechanisms that are not well understood. This device would also allow the visualization of the human genome and explicate proteins' interactions with each other.

Moore asked if focusing the beam is straightforward. Hajdu said that the stream of molecules would be hydrated and injected into the beam. With each beam pulse, you would be able to tell if you had hit a molecule or not. At 120 pulses a second, it would be all right if you did not hit a molecule with every pulse.

Sinha asked if the simulations were gotten from crystals. Hajdu replied that they had simulated crystals, but not this time. Sinha then asked Hajdu if he could calculate what happened to solid-state material. Hajdu replied that that was definitely the case and that the situation was simpler with small samples. With small samples, early in an exposure, one in five ejected electrons would deposit its energy; late in an exposure, the total energy may be absorbed. Trapped electrons will produce a slower Coulomb explosion.

Richmond asked how quickly you have to make your measurement. Hajdu said, the quicker, the better; the size of the window of opportunity depends on the molecule and the beam energy and ranges from 10 to 230 fs, according to the simulations. Richmond asked if the simulations could be extrapolated to other samples like heavy atoms, and Hajdu pointed out that the simulations that have been performed are of biomaterials, their damage mechanisms, and their cross sections. El-Sayed asked if one would be able to see what happened in such a short time, and Hajdu said that many of the processes would be captured by techniques already developed for biology.

Batterman asked if the mirrors will reject the higher harmonics, and Hodgson responded that higher harmonics will not be an issue. Kohn asked what could be done about the structure and dynamics of proteins, and Hajdu responded that a lot of calculations and simulations have been done in this field, and the proteins of choice are those on the surface of viruses that govern the dynamic interactions with other molecules and proteins. We will only be able to look at averages of a relatively small number (a few hundred) of protein molecules, but we would be able to look at something 5 to 10 times larger than lysozyme. Stupp asked how these proteins of choice would be attached. Hajdu said that one can design specific binding sites on the surface of the virus that will bind specific peptides; the gaps can then be filled with lipids, and the surface of the virus can be mapped.

Johnson asked if this device can be used as a pair of optical tweezers, and Hajdu responded affirmatively, that ion traps can be used.

Broholm noted that several presenters had spoken about tuning the wavelength of the laser and asked how difficult that would be. Hajdu noted that the LCLS would have only one undulator, and it would take from a minute to an hour to tune; in addition, there would be other ways to tune the system. Broholm asked if the electron beam could be swept over to another target, and Hajdu said that it could be done. Batterman asked how rapidly the linac energy could be tuned, and Dorfan said that it depends on the stability of the beam desired; currently, the beam is tuned with feedback loops, taking on the order of minutes.

Johnson asked what the commercial driver of this research is, and Hajdu said that has not been considered yet; it might take 2 or 3 years of operation to determine the commercial applications. The presentations given have constituted an in-depth look at *some* of the science that could be done. They by no means reflect the full breadth of the research that could be done.

Mayes asked what the construction and operating costs would be. Hodgson said that the project had been costed at $90 million in 1998; inflation would bring that to $100 million. Adding beamlines, equipment, etc. would bring it to about $150 million. It would take about 3 years to build; then getting all the components to work together would take a year or two. Five teams of 15 users would cost $10 to $15 million a year to support.

Crow asked if there were any significant issues in instrumentation or detectors. Hajdu responded that the detectors already exist, and the data streams that would be produced would be much slower than those handled today.

Richmond noted that the Leone panel had asked for a rigorous list of experiments that would be performed and that a scientific case be made for the LCLS. She proposed that, during the coming evening, each member formulate (1) his or her advice on where to go from here and (2) an assessment of whether the science presented here was compelling enough to justify continuing to pursue the LCLS or (alternatively) whether additional scientific review was necessary. El-Sayed asked when BESAC might receive the results of the independent reviews. Richmond said that those reviews will not be addressed to BESAC.

The chair called for public comment; there being none, the session was adjourned at 5:27 p.m.

Wednesday, October 11, 2000

Richmond called the meeting to order at 8:40 a.m. She announced that Pat Dehmer had received the Presidential Rank Award, which is given to the top 1% of federal executives.

Richmond noted that the concerns about the scientific case for the LCLS raised in the Leone report, including the possibility of sample degradation, had been discussed at length during the previous day's session. The question before BESAC was whether those discussions were sufficient to make a recommendation to BES on whether or not to proceed with planning for the construction of the LCLS. She polled each member individually to determine if the concerns about the scientific case had been adequately addressed.

Sinha said that the previous day's discussions had allayed much of his skepticism about whether the things people dreamed about could be done with this facility. He believed that a scientific case could be made for its construction. It would be a bargain initiative that would take us into a new regime of science with very exciting possibilities. He asked if the Committee was to decide now about going beyond the five experiments described and also consider other possible research. Dehmer said that the issue was narrowly defined to the five experiments described and whether, on the basis of this information, the Department should go forward with planning or not.

Richmond asked Sinha what he had in mind. He replied that there are natural applications of this type of source, like atomic physics, nonlinear processes, and this matter of warm dense matter. In solid-state and condensed-matter applications, there is always the lingering issue about damage to the sample, but, if one can control the flux at the sample, it appears that one can use mirrors, monochromators, or repetitive pulses to avoid vaporizing the sample. Other types of experiments (e.g., femtosecond chemistry) may also have problems that need further analysis. The machine would have three unique properties: coherence of the beam, variable pulse lengths, and high peak brilliance. Not all of these capabilities are needed in all experiments, but the availability of all of them would certainly make the machine very flexible. Moreover, the facility would have a number of, as yet undefined, technical/industrial applications.

Stupp noted that, the way the case was presented to the Committee made it clear that the problem of sample damage could be dealt with. He suggested hearing more peer reviews before committing construction funding, but DOE should proceed with the conceptual design.

Crow was impressed with the biological applications of this technique. He said that NIH's participation should be encouraged.

Moore expressed an interest in seeing the expert reviews. This project is still early in the planning stages.

Dumesic would defer to more expert opinion; he would like to see experimental and theoretical tests and analyses.

Johnson said that a lot of science could be done with this source that could not be done without it. It took a decade to compress the pulse from 6 fs to 5 fs in the visible spectrum. How more difficult will it be with X-rays? More knowledge is needed about the dispersion mirrors. Stohr explained that there are two parameters that can be varied to influence the pulse: compressing the photon bunch and compressing the electron bunch. It is unlikely that the pulse cannot be reduced much more below 50 fs, but the expert opinion is that, with the variety of techniques available, the 50-fs pulse is achievable. Johnson asked if there were any space-charge effects in the electron beam, and Stohr said that those effects were minimized because the beam would operate in the relativistic regime. Johnson also asked about heating in the case of a single particle in a bulk commodity: is enough known about the heat capacity of the particle? In addition, he believed that the possibility of an X-ray-driven, inertial fusion implosion was not discussed very much, and that was the most interesting and compelling part of the plasma-physics presentation. Despite the political ramifications of the National Ignition Facility, if the best science on inertial-confinement fusion can be done with the LCLS, then that fact should be emphasized. In response to the question about the heat capacity of a single particle, John Vetrano said that the question of heat buildup in particles has not been a problem in electron microscopy, and Kohn commented that, if it were a nanoparticle, it would have an average heat capacity.

Green noted that these experiments will touch the regime of one to a hundred molecules. She wanted to hear more about the mechanics of pulse production. She found the femtochemistry all interesting and the structural investigation of biomaterials most exciting, although these theoretical studies must have quantum-mechanical corrections. Most important was the use of this light source to get protein and molecular structure without diffraction techniques. Such studies are what was hoped transmission electron microscopy would do but has not done in very many cases. She concluded that the information presented clearly meets the Leone criteria, that the LCLS pushes the envelope in every direction, and that there is a chance of failure because every direction is being pushed. However, it is an effort that she would like to see supported.

El-Sayed noted that these experiments are extensions of what has been being done. The displacements produced are very, very small at this time scale, so better and better resolution is needed. Any effects of damage will wash out because very short pulses and lower intensities can be used. Achieving these brief pulses at high intensity will be difficult but is worth trying.

Dove commented that important applications will come out of this technology, and more are being thought up as more is being learned about it.

Batterman commented that he had been around when synchrotrons were being sold to the scientific community. Some of the promises of the synchrotron were a bust; the field that was revolutionized was crystallography, which had not been considered in the scientific justification of synchrotrons. The five experiments are each unique. The atomic physics that could be done is exciting, to say nothing of the plasma physics; that is a regime that can be studied only with this technique. If these experiments do not work, something will still be learned. He strongly supported the project.

Broholm was impressed by the presentations. The leap in brilliance alone is a good reason to pursue the technology. The presentations demonstrated that many of these techniques will be possible.

Mayes was also enthusiastic about the what had been presented the previous day. This machine is likely to be a “nugget generator.” It would cover a lot of new ground over a wide area of science. The Leone report asked if a large body of users would come forward. The presentations of the previous day included many non-United States investigators, which shows the wide interest, but the U.S. scientific community needs to be enlisted.

Taylor said that, in the beginning, researchers will be developing a technique as well as investigating materials. That period is when breakthroughs are made. She encouraged pursuing work that would support the work that would be done at this facility. The science being done four years from now will not be what is envisioned today.

Kohn concluded that not going forward would be unthinkable. He took a conservative view of this project. He had great confidence in the group working on the design, but there are possible showstoppers. If the engineering can be accomplished, it is certain that exciting science will be done with this device. But even the most rigorous peer-reviewed, published justification was done with simulations based on (reasonable) assumptions. It is a good case but not a totally convincing case. He suggested that the demonstration of scientific importance not be considered complete but that further, more thorough consideration of the scientific promise of this 50-fs window on imaging be supported. He would have liked to have seen the other examples pushed to the same level of review and completeness as the biomaterials experiment. He was glad to hear that a panel of reviewers more competent than BESAC will be reviewing this scientific case. He asked what BESAC’s decision commits it to. Dehmer said that it commits DOE to proceed with the conceptual design; after that, a decision would have to be made on whether to proceed with a detailed design; then a decision would have to be made whether to proceed with construction. Kohn said that that procedure would be appropriate.

McCurdy said that he did not want to dampen creativity with detailed criticism of the experiments. Still, a few questions should be raised in the spirit of improving the plans for the initial LCLS experiments. In his opinion, the first two proposed experiments (those on femtosecond chemistry and nanoscale dynamics) were the least persuasive because the facility’s 240-fs pulses and 50-fs correlation with probe pulses are about a factor of 10 from what would be required to perform most experiments on the dynamics of systems containing first-row atoms. Thus, the prospects for time-resolved experiments had not been well established, especially with respect to elucidating the dynamics of photodissociation on multiple potential surfaces. Analysis is needed that compares the kinds of dynamics that might be probed with this facility with the dynamics that can be addressed with current femtosecond laser technology.

The atomic physics proposal does not make use of the time resolution of the facility, but instead makes use of the prospects for tunable sources with wavelengths in the vicinity of 1

Angstrom. Those experiments are clearly of the "first-experiment" category and will almost certainly work and provide new information on fundamental processes while providing diagnostics of the performance of the facility. In any case, because of their role as diagnostics, atomic physics experiments will almost certainly be the first ones to be done at the LCLS.

In the proposed experiments in atomic physics (and also in the biomaterials experiment), he was struck by the absence of any discussion of the computer-driven detection schemes that have already begun to revolutionize experiments in atomic and molecular physics. An example is the COLTRIMS experiment (in cold-target, recoil-ion-momentum spectroscopy), where large amounts of data are taken by imaging detectors and mined for coincidences. This approach performs a large ensemble of possible experiments simultaneously and then selects the ones of interest after the fact. Other examples include (1) the experiment that Eric Rohlfing described involving the use of genetic algorithms to optimize the conditions to produce a particular harmonic and (2) modern adaptive optics in astronomy and elsewhere. Because the proposed experiments are the basis of the scientific justification of the facility, it is critical that they extract the maximum scientific impact from the beam time that is dedicated to them. By the time the LCLS would be coming on line, the power of real-time and lab-scale computing will have increased by another factor of 5 to 10. For that reason, it was somewhat disappointing not to see experiments in the atomic physics proposal that would use the most advanced detection technology to address at least the angular dependence and correlation in the photoejection of more than one electron.

The proposal on warm dense matter was one of the most persuasive presentations because it clearly pointed out a unique opportunity provided by the LCLS.

The best studied of the possibilities was clearly the "Single Particles and Biomolecules" proposal. He noted that Kohn had described the thoroughness and care of the analysis published in *Nature*. McCurdy, however, was unsure that, given the possibilities provided by computing technology, the use of Coulomb explosions to provide structural and dynamical information about small clusters should be given up on so easily.

Finally, he asked about the context of the conceptual-design decision for this facility:

- What other possibilities are on the table for fourth-generation light sources?
- What is the opportunity cost, if any, of making that decision for LCLS?
- What other potential facilities will be competing for BES attention and funding?

Dehmer responded that, in terms of light sources, the LCLS is the next frontier in terms of brilliance. If you restrict yourself to very short wavelengths and brief pulses and high intensity, that rules out all the other light sources. At this point in time, vast decisions are not being made. What is being considered is whether to take the next step. In terms of the overall budget of BES, it is a small step, but it is an important one given BES's unique responsibility in the area of advanced light sources.

Thomas said that the cost basis of this decision is not really known. A preliminary cost estimate would likely come out of a conceptual design.

Richmond announced that Marsha Lester had to leave the meeting early but had left some notes about her assessment. Lester had some concerns about the time resolution of pump-probe experiments, the synchronization of those experiments, and whether the proposed time scale is fast enough to obtain the desired information. She was also concerned about the spatial resolution and backdrop diffraction of molecules that are excited in the pumped laser and whether the remaining ground-state molecules are subject to X-ray scattering.

Richmond said that her perspective, as one who had been on the Leone panel, was that this was a refreshing change in the breadth of science presented and the excitement of the scientific community. It would be great to have guarantees, but then science would not be so much fun. Overall, she saw no show-stoppers and would be very disappointed if these experimental opportunities were not attempted. She suggested that it would be appropriate for BESAC in future meetings to (1) talk more about the engineering of pulse generation and detection, (2) hear outside reviewers' comments, (3) involve potential users early in the design and planning, and (4) confer with NIH about shared funding.

Dehmer noted that NIH and BES are jointly upgrading several facilities, but she considered the LCLS as different. It is an accelerator project. It is not known if it will succeed. BES has taken a lead role in next-generation accelerator engineering; if you are looking at a next-generation accelerator, you should put the budget authority with BES with, perhaps, a much smaller role for NSF. To put such budget authority in an agency whose responsibility is the health of the nation may not be the best way to go. If this country is going to correct a perceived imbalance between life-science funding and physical-science funding, this is the best type of activity that the Office of Science and the NSF can put forward.

Shen said that the Birgeneau panel considered why other agencies were not asked to share in the funding of the operations of research facilities.

Continuing her list of appropriate future actions for BESAC, Richmond added to (5) explore the issue of commercial applications, which had been brought up by Johnson, and (6) have a peer-reviewed publication on the femtosecond-chemistry application of the LCLS. El-Sayed noted that such justifications were rarely published by journals. Richmond said that, if simulations could be done to back up the assertions, that would be helpful and publishable. Hajdu commented that this is not the type of thing that top journals would publish. Green suggested that publishing the proceedings of the workshops might be a good way to put forward the scientific case.

Sinha moved to support going forward with the conceptual design of the LCLS pending positive technical reviews. Johnson seconded. Moore commented that advisory decisions should be made with the maximum information. Shen and Stohr abstained from the vote for reasons of conflict of interest. The remaining members of the Committee voted unanimously in favor of the motion.

Richmond stated that the Committee would revisit this issue in February to get an update. Also, the issues brought by Mildred Dresselhaus need to be considered, especially what would be the priorities if the funding for BES was increased 15% per year for the next five years. Other topics that will be addressed in the next meeting will include the results from the LANSCE/IPNS review and the management team review of the Chemical Sciences, Geosciences, and Biosciences Division. Crow suggested that the Committee get an update on the HFIR upgrade and the evolving needs of that community. Kohn asked if the staff could prepare a review of BESAC's activities regarding nonpolluting energy sources. Mayes noted that the Committee should address how to do a portfolio analysis. A break was declared at 10:22 a.m.

The meeting was reconvened at 10:43 with the introduction of **Iran Thomas** to report on the Materials Sciences and Engineering Division. He reviewed the new organization chart for the division and noted that the merging of two prior divisions into the present one was interesting because funding for engineering was now included with that for basic science. A major objective of the division is to achieve the same level of control over chemical potential as nature does with biological processes, an area of research that BES has pursued since the early eighties. The imaging of proteins is just the beginning; next will be more complicated structures, such as poly saccharides.

He reviewed the current staffing situation in the division. Offers are out to candidates for two positions, and one more position has been approved and will be posted soon.

A review of the awards funded gave a good insight into what the division did during the past year. New research grants outweighed renewal grants by $4.5 million to $2.5 million. Funding of the Experimental Program to Stimulate Competitive Research (EPSCoR) was the largest category of awards at about $6.4 million. Close behind was the Phase II funding for the Small Business Innovative Research program. At about $6.3 million, this is becoming a sizable piece of the research budget; it is focused on areas important to BES, such as instrumentation. Major research initiatives and their approximate funding within the division include Complex and Collective Phenomena ($2.9 million), Carbon Management (an interagency and interoffice initiative to reduce carbon emissions; $3.1 million), and Computational Materials Sciences Network ($1 million).

A number of activities within the division received increases in funding this year:

Nanoscience	$13.5 million additional
Nanoscience Computation	3.4
Nanoscience Facilities Utilization	2.7
Facilities Utilization	12.6
LANSCE Upgrade	1
ALS Upgrade	0.9
HFIR Instrumentation Upgrade	2
SPEAR3 (done jointly with NIH)	8
EPSCoR	0.9
Core Research	1
SNS Other Project Costs	1.2
Waste Management	8
Small Business Innovative Research and Technology Transfer	0.5

Some activities received decreased funding:

HFIR HB-2 Extension (completed)	$4 million less

SC and DP are jointly funding a nanoscience network to advance the discovery and understanding of nanoscale phenomena. SC was assigned the lead, and all funding for the joint projects was put into the SC budget under a memorandum of understanding. The strategy being employed is to use “glue” funding to stimulate and facilitate synergistic, multilaboratory collaborations among the existing nanoscience programs. The selection criteria include excellence in science, mission relevance to DP, demonstrable new potential, and distribution of funding to at least two DP and two other national labs. An April workshop identified five scientifically challenging research themes that met these criteria: nanoscale tribology, nanostructured energy storage, tailored nanostructures, nanoscale features of deformation, and nanostructural photonics.

In other news:

- The division also started a pilot effort in the Computational Materials Science Network to advance frontiers by assembling diverse sets of researchers working together to solve problems that require cooperation across organizational and disciplinary boundaries.
- The first concrete has been poured for the SNS. The site is being graded, and the ion source and targets are being constructed and tested. Experiments are expected to start in 2005 or 2006, depending on the availability of funding.
- A website on the HFIR upgrades has been constructed. It provides descriptions of what is being done each day and what has been accomplished so far. This is the first time that the replacement of the beryllium reflector has been fully documented.

Moore asked how the division was planning to address the $200 million decrease in SC's core-research funding. Thomas said that individual program managers will have to cope with the cutbacks, possibly not funding some research proposals. Moore asked what BESAC can do. Thomas replied, the BESAC members can fight for increased funding for the physical sciences. A compelling case has to be made to Congress about our society's need for chemistry, physics, etc.

Dehmer said that, typically, the planning process starts at the previous year's funding and then adds increments to that, including a small cost-of-living increase. However, research does not get such cost-of-living increases. As a result, the core research base essentially goes down; 3 to 4% increases in agency discretionary funding should be written into the funding plans and requests.

Richmond introduced **William Millman** to speak about the Chemical Sciences, Geosciences, and Biosciences Division. He noted that they are completing the staffing of the division, with one new staff member, one offer outstanding, and one last vacant position to be filled. He reviewed the organization and staffing of the division. He reviewed the major new initiatives of the division. In the Carbon Management Program, 68 new grants were issued to universities and 41 new field work proposals (FWPs) were agreed to with national laboratories; in addition, 26 university grants and 7 laboratory FWPs were continued. In the Complex and Collective Phenomena Program, 6 university grants and interagency agreements and 2 laboratory FWPs were initiated; in addition, 5 university grants and 2 laboratory FWPs were continued from FY 1999. In the Fourth-Generation Tabletop Light Source Development Program, 5 university grants and 1 laboratory FWP were started; in addition, 1 new grant started in FY 1999 was continued, and 1 existing grant was redirected.

He pointed out that a number of activities within the division received increases in funding this year:

Nanoscience	$9 million additional
Nanoscience Computation	2
Microbial Cell	2
Plant Genome	0.5
Computational Chemistry	2
Nanoscience Facilities Utilization	0.4
ALS Upgrade	0.2
Core Research (Chemical Sciences)	3
General Plant Projects and Equipment	0.6
Small Business Innovative Research and Technology Transfer	0.4

Some activities received decreased funding:

Facilities Utilization	$4 million less
Core Research (Geosciences)	0.2
Core Research (Biosciences)	0.5

The majority of these decreases resulted because of the completion of the replacement of the beryllium reflector of the HFIR. The overall change in funding for the division was an increase of $16 million.

The division supports the activities of three councils for assessing and guiding research in chemical sciences, Earth sciences, and biosciences by conducting workshops, the proceedings of which are published in the peer-reviewed literature. This fiscal year, the three councils have proceeded to select their nominees for membership and have identified topics for four workshops.

The floor was opened to public comment. **Murray Gibson** of ANL said that BESAC can help the core program by articulating the case for science, telling what is done, such as the synthesis of materials and instrumentation development. The scientific community needs to tell the story of how core-research science has contributed to the national science endeavor. BESAC might play a very useful role in making such an effort effective.

Richmond thanked the BESAC members for their input and expressed the Committee's appreciation to the presenters for their efforts. The meeting was adjourned at 11:47 a.m.