Review of BES Division of Materials Sciences Programs at Brookhaven National Laboratory

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Overview of Basic Energy Sciences Programs at Brookhaven National Laboratory

The DOE Basic Energy Sciences (BES) program at Brookhaven National Laboratory (BNL) supports research in materials sciences, chemical sciences, the National Synchrotron Light Source (NSLS), and biosciences with a FY2001 budget of $75.5M. Combined with BES funding of construction projects for the Spallation Neutron Source, the BES program is one of the cornerstone programmatic areas of BNL and, thus, is of crucial interest to laboratory management.

During this last year, BNL has made a particular effort to increase internal support of BES science at the Laboratory through two concrete steps. First, it has supported, into the second year, a large ($1.5M) LDRD program in Nanoscience. The use of these internal laboratory resources for this program is indicative of BNL's commitment to BES science. Second, it has continued to expand its Postdoctoral Research Associate program through special financial support and through the inception of the Goldhaber Fellowship program.[1]

The NSLS continues to be one of the most heavily used DOE synchrotron sources and is essential to the DOE goal of providing extraordinary tools for extraordinary science. The NSLS user community continues to expand in numbers (~2800) and disciplines, and the facility is committed to enhancing its role as a national resource for materials, chemical and biological research. In this last year BNL appointed a new Chairman, Steven Dierker, and began exploring methods of supporting users by providing improved access to the *full* range of synchrotron-based experimental techniques for specific programs in materials and chemical science. The first example of this approach is that of a pilot program in catalytic chemistry, to be followed by others, possibly including soft matter, high pressure studies and high magnetic fields. The NSLS is also contributing to the national R&D program leading to the next generation of advanced light sources. For example, the BNL concept of high-gain harmonic generation and laser seeding of FELs has advanced and been the subject of a series of important publications. In addition, the NSLS has shared in the success of the near-UV VISA program this year. A white paper on the feasibility of constructing an upgraded, high brightness light source, specifically, the Photon Energy Recovery Linac (PERL) at BNL is currently in preparation for submission in the spring.

With the permanent shutdown of the High Flux Beam Reactor, BNL is working with other neutron facilities in the U.S. to provide expertise in neutron scattering and

[1] One of this years recipients is Dr. Y.J. Kim, a research associate under the supervision of J.P. Hill in the Physics Department.

instrument development. This includes a collaboration between BNL and Oak Ridge National Laboratory to relocate the U.S.-Japan spectrometer to a cold guide beam port at Oak Ridge's HFIR. Arrangements have been made to form a BNL-NIST Scientific Alliance, which will locate a BNL scientist at the NIST neutron facility. BNL is leading the effort to propose a novel inelastic scattering instrument to be built at the Spallation Neutron Source (SNS). These efforts are coordinated by the Center for Neutron Science, headed by Stephen Shapiro.

There has been a major effort to tie together the various BES programs at the Laboratory. Most recently, a new Materials Science Department has been formed within the BES directorate, joining together BES programs in the former Materials and Chemical Sciences Division of the Energy Sciences and Technology Department. David Welch is the Interim Department Chair, while a permanent chair is sought. In addition, the programs in Materials Science have been united with those in Condensed Matter Physics through the formation of a Materials Center. The Center is headed by Doon Gibbs and is intended to coordinate internal programs in materials science at the NSLS, the new Materials Science Department, the Condensed Matter Physics section of the Physics Department, and the Chemistry Department. Thus far, this program has arranged for better access by Center members to all the experimental resources on the site and begun to coordinate seminars and research initiatives.

Especially during the last year, BNL has been very active in establishing a major nanoscience program. The theme for this program is controlling the physical and chemical response of nanoscale functional materials. Two chemistry Nanoscale Science Engineering & Technology (NSET) proposals were awarded nanoscience grants: Catalytic Nanomaterials and Charge Transfer at the Nanoscale. In addition, the growing program in transmission electron microscopy (TEM) at BNL received a major boost in support, as did a Materials Synthesis Program in the Physics Department. Our initial proposal for a Nanocenter was declined; however, a new proposal has been submitted, again with a focus on functional materials, but with the research program aligned more with the nanoscience theme.

The present review is concerned with all BES programs at BNL funded by the Condensed Matter Physics and Materials Chemistry Team of DOE's Division of Materials Science (DMS), including all programs in BNL's Condensed Matter Physics and selected programs in the newly formed Materials Science Department. The remaining programs in the Materials Science Department are funded by the Metal, Ceramic, and Engineering Sciences Team of DMS, the Division of Chemical Sciences, or elsewhere in DOE. More detailed summaries of individual programs, including personnel, budgets and scientific highlights are presented below and will be discussed during the review. Brief introductory descriptions of the Condensed Matter Physics and Materials Science Programs follow. Although the NSLS is not presently being reviewed, we have also included an introductory description of its scientific programs as well.

Condensed Matter Physics

The Condensed Matter Physics program at BNL is managed by Doon Gibbs, and consists of about 30 scientists and 40 staff people in all. They are arranged into research groups, which are mainly focused on DOE facilities, including the:

- Neutron Scattering Group (headed by John Tranquada)
- X-ray Scattering Group (John Hill)
- Powder Diffraction Group (Tom Vogt)
- Electron Spectroscopy Group (Peter Johnson)
- Theory Group (Alexei Tsvelik)

In addition, there are two Centers: the Center for Neutron Science, headed by Stephen Shapiro and the newly formed Materials Center, headed by Doon Gibbs. This year, the annual operating budget for Condensed Matter Physics was approximately $6.5 M, supplemented by about $500 K in LDRD funds. Additional, smaller amounts of funding come from outside the Division of Materials Science of the DOE, as described in detail below.

The scientific program in Condensed Matter Physics is focused on basic science, and is driven by the interests of the principal investigators and their collaborators, consistent with the DOE mission. The main themes of the research include:

- Strongly correlated and complex systems
- Magnetism
- Surfaces and interfaces
- Nanoscience
- Neutron Science

Most of the experimental work is technique oriented in that it tends to be centered on DOE facilities, principally including the NSLS, Advanced Photon Source (ANL), High Flux Isotope Reactor (ORNL), Center for Data Intensive Computers (BNL/SUNY-SB) and the LBL Super Computer Facility (NERSC). Some research is also carried out at non-DOE facilities, such as at the reactors NIST (Washington, D.C.), ILL (Grenoble), PSI (Zurich), ISIS (Oxfordshire), ANTSO (Sydney) and at the ESRF (Grenoble), to name several. Most of the research is highly collaborative both within Condensed Matter Physics, as well as with other BNL Departments, especially Materials Science, the National Synchrotron Light Source and Chemistry. There are also extensive collaborations external to BNL including universities, other national labs and industry.

Much has changed in Condensed Matter Physics since the last review three years ago. In the first place, there is a new Associate Laboratory Director for BES (Rick Osgood) and a new Coordinator for Condensed Matter Physics (Doon Gibbs). In

addition, Alexei Tsvelik, formerly of Oxford University, joined the Theory Group in April to lead the effort on strongly correlated systems. Following the departure of Michael Weinert to the University of Wisconsin—Milwaukee, Tsvelik has now become Theory Group Leader and is leading a search for a junior level scientist in electronic structure. The Theory Group has also recently hired Fabian Essler, formerly of Warwick University, as an Associate Physicist starting in January, and a number of postdocs and students. In an effort to revive BNL's traditionally strong Summer Visitor Program, Tsvelik and Sergei Maslov have recently submitted a proposal to the DOE to start a BNL Theory Institute for Strongly Correlated and Complex Systems. The Institute plans to host a series of long and short term visitors throughout the year, including several workshops dedicated to problems in strongly correlated and complex systems. In other groups, Tom Vogt has become the Group Leader of Powder Diffraction following the retirement of Dave Cox, and John Hill, the Group Leader of X-ray Scattering, replacing Doon Gibbs.

Responding to the general need for a larger materials synthesis effort in the U.S. and at BNL, Condensed Matter Physics has redirected efforts in three groups: (1) There is a significant Pulsed Laser Deposition (PLD) program in epitaxial growth of complex metal oxides in the Electron Spectroscopy Group spearheaded by Peter Johnson and driven by a postdoc (Weidong Si, who arrived last year). This program began as a collaboration with the University of Connecticut and was originally supported by an LDRD, (2) The Neutron Scattering Group has hired an expert in single crystal oxide growth (Genda Gu, who started in February), (3) The X-ray Scattering Group has hired an Assistant Physicist in soft matter with expertise in synthesis and characterization (Tianbo Liu, who started in April). These efforts are aligned with the larger synthesis effort at BNL, in particular, within the Materials Science Department and will form important synthesis components of two thrust areas within the proposed BNL Nanocenter. Using new funds acquired through the DOE Nanoscience Initiative (500K), we are currently searching to make a new hire in synthesis, who will be stationed within the Powder Diffraction Group.

It is also recognized that Condensed Matter Physics would benefit from a stronger program in a soft matter science than currently exists. With the hiring of Tianbo Liu in April and with awarding of an LDRD in biomineralization to Elaine DiMasi in October, the kernel of such an effort now exists within the X-ray Scattering Group. This effort will be coordinated by Ben Ocko and interact with soft matter programs at the NSLS initiated by Steven Dierker and Ron Pindak, formerly of Lucent Technologies, who joined BNL in November. It is anticipated that this larger group will respond to the DOE call for proposals in Nanoscience, with a BNL proposal in soft matter. Depending on the extent of funding in Condensed Matter Physics, we anticipate the possibility of forming a new Soft Matter Group in Condensed Matter Physics headed by Ben Ocko.

Future of Condensed Matter Physics

In the near term, we anticipate continuing efforts to rebuild and strengthen our Theory Group emphasizing strongly correlated and complex systems, and electronic

structure. Similarly, we will continue to seek opportunities to stabilize and expand BNL's neutron scattering capabilities at other U.S. facilities, and especially at the SNS. In this regard, we have recently established the BNL-NIST Science Alliance, which will permanently locate a BNL scientist at NIST. Moreover, we are currently engaged in negotiations with Meigan Aronson of the University of Michigan for a joint BNL/SUNY-SB faculty appointment which would be centered in the Neutron Scattering Group. A new Collaborative Access Team, headed by John Hill, has been formed and funded at the Advanced Photon Source to initiate a new program in inelastic x-ray scattering. In addition, we anticipate upgrading our powder diffraction beamlines at the NSLS, and are considering initiating a larger powder diffraction effort at BNL, possibly including new hires in the Materials Science or Chemistry Departments.

The BNL-wide effort to expand the program in materials synthesis will be a central theme of the next five years, including the ongoing efforts in advanced PLD, soft matter and single-crystal oxide growth. As already noted, a search is underway for a new hire to be stationed in the Powder Diffraction Group. A broader set of growth and synthesis techniques will be included within the proposed Nanocenter's program in functional materials. In this regard, it is worth noting that Condensed Matter Physics will play a leading role in two of the six thrust areas in the proposed BNL Nanocenter, specifically concerned with functional oxide materials and thin organic films. It is also important to note that we are participating in a series of NSLS Workshops concerned with developing a scientific case for PERL, and will form a study group to examine and propose avenues by which Condensed Matter Physics can participate in a long-term scientific program connected with such a short pulse, bright light source. Finally, it is our intention to strengthen our ties to local universities, both through increased scientific collaboration, and more especially through joint BNL/University appointments, as a means of leveraging our collective resources. Already, one of our staff, Alexei Tsvelik, has joined the SUNY-SB Physics Department as an Adjunct Professor.

The Materials Science Department

The new Materials Science Department (MSD) is headed by David Welch, as Interim Chair, and Jack Fajer, as Interim Deputy Chair. It has approximately 40 staff members and an annual operating budget of approximately $8M, including about $615K in LDRD funds. The department is organized into four groups:

- Superconducting and Magnetic Materials (Masaki Suenaga, Group Leader)
- Nanoscale Structure of Advanced Materials (Yimei Zhu, Group Leader)
- Molecular Materials (Jack Fajer, Group Leader)
- Electrochemical Sciences (James McBreen, Group Leader)

An overarching aspect of the research of all four groups is a strong focus on the structure of real or defective materials on many length scales, how such structure arises from various methods of synthesis and processing, and how it determines the functional behavior of materials. Thus, methods of transmission electron microscopy, both imaging

and analytical in nature, and methods of x-ray diffraction and spectroscopy, primarily at the NSLS, play critical roles in much of the research conducted in the MSD. [Two programs under review, "Structure-Sensitive Properties of Advanced Permanent Magnet Materials: Experiment and Theory" and "Synthesis and Structure of Conducting Polymers," are located in the Superconducting and Magnetic Materials and the Electrochemical Sciences groups, respectively.]

The Department performs interdisciplinary research in basic materials science (including chemistry) with some work in related application to the conversion, transmission, storage, and efficient use of energy. It is increasingly involved in the science of nanoscale materials. While newly formed at the department level (October 1, 2001), the MSD has long roots going back to the Metallurgy Division of the Nuclear Engineering Department in BNL's earliest beginnings. The present MSD receives the majority of its funding from the Office of Basic Energy Sciences, from both the Division of Materials and the Division of Chemical Sciences. However, there has always been a strong component of support from the various technology offices of DOE, in recent years primarily the Office of Energy Efficiency and Renewable Energy, and a strong connection to applications of superconductivity such as accelerator magnets and detectors, supported by the Office of High Energy Physics. The MSD also has a long tradition of interactions with industry by means of CRADAs and other types of collaborations.

The importance of materials synthesis and processing in the research of the MSD is illustrated by the active participation of several staff members and their research programs in the DOE Center of Excellence for the Synthesis and Processing of Advanced Materials (CSP), a distributed center for promoting coordinated, collaborative research partnerships related to the synthesis and processing of advanced materials. Members of the MSD are active participants, including one as project leader, in four of the eight projects of the CSP: "Defect Structures and Properties in Rare-Earth Cuprate Superconductors," "The Science of Localized Corrosion," "Nanocomposite Magnets," and "Smart Structures Based on Electroactive Polymers." The two programs from the MSD mentioned above under review this week, are important parts of the latter two CSP projects above.

Much of the research of the MSD is done in a strongly collaborative mode with researchers at other materials laboratories and universities, as the discussion of the CSP projects above suggests and as will be clearly illustrated by the two MSD programs now being reviewed. Furthermore, several staff members of MSD are adjunct professors at the State University of New York at Stony Brook and elsewhere, and graduate student research and training is becoming an increasingly important component of the research programs.

There are now strong collaborations within BNL between Condensed Matter Physics and MSD, i.e., work on high T_c superconductivity and the new superconductor MgB_2 and various areas of nanoscience, such as nanoscale magnets, correlated electron systems, and transition metal oxides. An increase in these intra-laboratory collaborations,

especially in areas involving synthesis and processing, as well as the characterization of nanoscale structure by TEM in a wider range of functional materials, and in materials theory, is a very high priority and will be facilitated by the new management structures at BNL such as the Materials Center and the formation of the MSD within the BES Directorate.

Future directions and strategic plans for the MSD involve not only the programs supported by the Condensed Matter Physics and Materials Chemistry Team of BES/DMS, i.e., those being reviewed today, but also several related programs supported by the Metal, Ceramic, and Engineering Sciences Team of BES/DMS which are closely connected to the programs under review, both those in Condensed Matter Physics and in the MSD. These new directions include:

1. A central focus on understanding defects and the "real structure" of nanomaterials, with particular emphasis on the properties of metal oxides;
2. A greatly expanded TEM program, with an emphasis on nanophenomena and structures and the roles of defects in them;
3. An expanded effort in the synthesis and processing of metal-oxide nanoparticles and nanocomposites, to be carried out both at BNL and with our collaborating universities;
4. Incorporation of a strong program in ab initio calculations in conjunction with other methods of modeling;
5. An increasing emphasis on non-superconducting functional materials, i.e., ferroelectrics, piezoelectrics; magnetoresistives, etc.

The strategy for implementing and strengthening these new directions include a number of features. They include stronger interactions among the MSD, Condensed Matter Physics, and the Center of Data Intensive Computing, and the integrating role of the Materials Center is critical here. Other aspects of the strategy include key senior appointments and an increased number of joint appointments with Stony Brook.