Design, Discovery and Growth of Novel Materials

For Basic Research:

An Urgent U.S. Need

Report on the DOE/BES Workshop:

“Future Directions of Design, Discovery and Growth of Single Crystals for Basic Research”

Ames Laboratory, Iowa State University
(October, 10-12, 2003)

Organizing Committee:

Lynn Boatner, Oak Ridge National Laboratory
Mac Beasley, Stanford University
Paul Canfield, Chair, Iowa State University and Ames Laboratory
Robert Cava, Princeton University
Doon Gibbs, Brookhaven National Laboratory
Thomas Lograsso, Iowa State University and Ames Laboratory
David Mandrus, Oak Ridge National Laboratory
John Mitchell, Argonne National Laboratory

Executive Summary

The design, discovery and growth of novel materials, especially in single crystal form, represents a national core competency that is essential for scientific progress and long-term economic growth. Indeed, many of the major discoveries of condensed matter science during the last fifty years have been made possible by the discovery of new materials. Recently revealed phenomena such as high T_c superconductivity and the quantum Hall effect, for example, represent new states of matter that emerge from the collective behavior of large numbers of electronic, magnetic and lattice degrees of freedom. Such materials challenge our fundamental understanding of matter and provide novel materials functionality. New materials also lie at the core of many new and existing technologies, such as semiconductor electronics, solid state lasers, radiation detectors, compact disk storage, both cellular and optical communications, solar cells, fuel cells and catalysts. Such materials further hold the promise for new technologies ranging from efficient indoor and traffic lighting, to multi-component data storage, integrated bioelectronic sensors, and thermoelectric power generation. Single crystals are often required to achieve a materials' full functionality as well as to completely elucidate its properties.

A Department-of-Energy-sponsored workshop was held on Oct. 10-12, 2003 in Ames, Iowa with the purpose of assessing the state of novel materials and crystal growth in the U.S. Leaders of broad areas of synthesis and condensed matter science reviewed present U.S. strengths, levels of support, and competition from abroad. The principal finding of the workshop is that the current U.S. infrastructure and personnel levels are insufficient to meet the growing demand for high quality, specialized samples, and to maintain international competitiveness in an area vital to the nation's condensed matter science enterprise. We further risk being unable to fully exploit the nation's world-leading leading capabilities in neutron and x-ray science, even as powerful new facilities come on line. This situation is exacerbated by the several decade-long decline of traditionally strong industrial expertise in crystal synthesis, by the relatively small number of synthesis scientists being trained in U.S. universities and national laboratories, and by increasing support for single crystal materials synthesis in Europe and Japan.

The principal recommendation of the workshop is that the Department of Energy should act to close the gap in U.S. based design, discovery and growth of novel materials for basic research by growing and coordinating the nation's existing crystal growth efforts, by adding qualitatively new capabilities, and by significantly enhancing Ph.D. and postdoctoral training opportunities in universities, national laboratories and industry. Specifically, the workshop recommendations are: 1) to broadly increase the level of funding for individual research activities in new materials and single crystal growth, 2) to establish a novel, national materials design, discovery and growth network with unprecedented interconnectivity, and 3) to create multi-investigator materials preparation facilities that feature specialized capabilities, provide samples on - a priority basis, and offer training in advanced techniques. We believe these recommendations will strengthen the U.S. base in materials synthesis at all levels, optimize the use of national resources, and integrate the materials synthesis community more effectively into the larger U.S. condensed matter science enterprise for maximum impact.

Introduction

The discovery and development of novel, complex materials with interesting and potentially useful properties is crucial to scientific progress and economic growth. Indeed, science is increasingly charted by the discovery and development of new materials. Recent Nobel prizes (quantum hall effects, conducting polymers, buckeyballs, high temperature superconductors, heterostructures and the integrated circuit) were made possible by the synthesis and development of new materials with exciting properties. The discovery process is often driven by purely scientific interests (curiosity), with the technological benefit being realized at a later time.

The search for new or improved materials is also driven by the need to improve existing technologies as well as to realize new technologies based on novel functionality. Virtually every technology is materials-limited. It is evident that the properties of materials limit the switching speeds in computers, the optical transmission of digitized light signals, the magnetic memory density in computers, the heat generated in large scale computers, the means by which we produce artificial light, the conversion of sunlight into electric energy, the ability to catalyze chemical reactions efficiently, the working parts of fuel cells which convert chemical energy into electricity, the electrodes and electrolytes of modern batteries, and the temperature, current and magnetic field at which a superconductor can function in electric power generation and distribution.

The availability of advanced, often complex, materials with enhanced physical properties strongly affects the research agenda of the Condensed Matter, Materials Science and Chemistry communities. In particular, the ability to make single crystals of such advanced materials is often one of the critical steps on the path to understanding their electronic, magnetic, structural and optical properties. The design, discovery, and development of advanced materials with enhanced properties will take materials science and technology to the next level. We have entered an era in which the complexity of materials has suddenly come upon us – materials with much greater complexity in composition leading to potentially enhanced physical properties. Along with this, we have found materials with much greater complexity in their electronic structure, often reflecting a delicate balance among the competing spin, electronic charge, and excitations and crystal lattice interactions. Most importantly, along with this increased complexity has come new and/or enhanced functionality.

The past ten to twenty years have witnessed a continued flourishing in the discovery of new materials with remarkable properties. Colossal magnetoresistance, large thermoelectric power, and high temperature superconductivity are a few examples. Unfortunately, over this same period, support for researchers engaged in the design, discovery, growth and characterization of novel materials (historically a mixture of industrial as well as governmental funding) has not kept pace with construction of new, large-scale measurement facilities, nor with research efforts abroad. In order to place this in context it is useful to recall that one of the ways of parsing research efforts in condensed matter physics and chemistry is to draw the distinction between two complementary research methodologies: new science made possible by new measurements and that made possible by new materials. These two methodologies are complementary and intertwined. Often new measurement techniques will lead to the discovery of new phenomena in existing materials. Just as often, new materials will yield new phenomena that test the limits of existing measurement techniques. Unfortunately, over the past 10-20 years, these two symbiotic methods of research have become seriously imbalanced. To understand how the imbalance between these two methods of research occurred, we note that prior to 1990, much of the new materials discovery was performed at industrial laboratories, such as AT&T Bell Laboratories and IBM, and in an even earlier era at GE and Westinghouse. Recent trends have resulted in a dramatic decline in these industrially sponsored basic research efforts. Over the last decade, many of the important discoveries in new advanced materials, as well as an alarmingly large fraction of the supply of samples for research, have come from outside of the U.S.

During this same time frame the U.S. Department of Energy has made, and continues to make, major investments in x-ray, e-beam, and neutron facilities. These facilities make it possible to investigate the properties of new materials in unprecedented detail in order to learn the underlying physics and chemistry that give rise to the extraordinary properties found in advanced materials. In addition, the DOE supports a large number of researchers throughout the national laboratory system, as well as in universities, whose research efforts are focused on the characterization of novel materials. The productivity of these facilities and researchers is highly dependent on the ready availability of newly discovered materials as well as on high quality samples of those materials known to be of specific interest. Given the clear symbiotic link between groups that discover and grow crystals of novel bulk materials and the groups that perform specialized characterization measurements, the shrinking of the materials growth community, specifically during this time of rapid expansion of capability in the measurements community, has led at a minimum to a critical imbalance and some would argue to a crisis.

The most obvious manifestation of the synthesis/measurement crisis is the disparity between the demand for cutting edge compounds driven by enhanced measurement capability, and the aforementioned loss of leadership in new compound discovery and supply of single crystals of new compounds. This disparity is leading to a bottleneck in the U.S. materials-research enterprise and, as a result, the U.S. is in danger of ceding much of its historical leadership position in condensed matter science research to Japan and Europe. Advanced materials are recognized as vital to U. S. interests and are an area where we must maintain our leadership position. It is within this context that a two-day, BES workshop on the design, discovery, growth and characterization of novel research materials was held in Ames Iowa, October 10–12, 2003. This report is a summary of the conclusions and recommendations of that workshop.

Overview

The importance of the design, discovery and growth of new materials has been emphasized in the 1999 NRC report on Condensed Matter and Materials Physics *Basic Research for Tomorrow's Technology*. This report highlights several strategic themes for the next decade, including "materials with increasing complexity in composition, structure and function" and "materials synthesis, processing and nanofabrication." The report goes on to state that "Materials synthesis is an area of extreme importance to condensed matter and materials physics. In many areas of condensed matter and materials physics research, the availability of research samples of sufficient quality and size is the limiting step to continued progress."

The design, discovery, growth and characterization of novel materials, especially in single crystal form, needs to be a major emphasis in the US-DOE science portfolio. Historically, materials growth has played a crucial role in both the country's defense research activities as well as in its industrial research activities. During World War II, the central role of piezoelectric crystals for torpedo hydrophones and quartz crystals for microwave resonators justified continuous support for basic research in crystal growth. The discovery of the transistor at AT&T Bell Laboratories was made possible by the growth of high purity, germanium single crystals, leading to the birth of the multibillion-dollar electronics industry. Hard magnets such as $Nd_2Fe_{14}B$ provide the basis for applications ranging from actuators in cars to drives in computers. Similar examples can be found in transparent conductors such as indium-tin oxide for electronics applications, and gallium arsenide heterostructures for compact disc storage and cell phone amplifiers.

Underpinning these technologies is the U.S. complex of basic condensed matter science. The design, discovery and growth of novel materials is the engine of the “new science by new materials” methodology for basic research. Research programs in areas such as superconductivity, mixed valence and heavy fermion materials, magnetism, metal-to-insulator transitions, charge- and spin-density wave materials, high-T_c superconductivity, buckeyballs and carbon nano-tubes, colossal magneto-resistance, etc., have all relied on the design, discovery, and growth of novel compounds. These examples and others emphasize that groups engaging in materials discovery and growth play an enabling role for research directions in the condensed matter physics and chemistry community.

Indeed, materials growers provide an essential resource to DOE missions at large facilities, within individual research groups, and at the technology interface. Each of these "customers" has increasing needs for high quality specimens:

- Large single crystals are indispensable for neutron scattering, and their availability determines if fundamental questions about materials physics and chemistry can be addressed at all. DOE has invested heavily in neutron scattering by funding the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory while maintaining existing neutron scattering facilities. Upon completion, the SNS will enable the U.S. materials research and condensed matter physics community to probe structure and excitations at a level unprecedented worldwide. Ultimately, the success of the U.S. neutron scattering enterprise is tied to an increased availability of single crystals of novel materials.

- DOE investment in synchrotrons nationwide (APS, NSLS, ALS, SSRL) has enabled beamlines that can provide exquisite detail about the physical and chemical properties of novel materials. Experiments at these facilities impose stringent requirements on degree of crystalline perfection (mosaicity, homogeneity, surface purity), resulting in an increasing demand for high quality samples at these facilities.

- DOE-supported and other scientists in national laboratories and universities specialize in the measurement of detailed physical, chemical, and metallurgical properties of novel or interesting compounds. The demands on the sample purity, composition, size or homogeneity can be extreme for such measurements. Automation of routine data collection has greatly increased measurement throughput, highlighting a growing need for enhanced production of research grade samples of novel materials.

- Opportunities materializing from improved single crystal growth and new materials functionality will drive future technology breakthroughs. For instance, high quality SiC crystals can enormously benefit the semiconductor industry in high-power electronics and high-frequency applications; single crystal turbine blades can function at higher temperatures and have a superior corrosion resistance than polycrystalline units; large single crystals of luminescent materials such as $Cs_3Lu(PO_4)_2$:Ce will be the future basis of medical imaging; lattice- and thermal expansion matched materials will provide substrates for various high-T_c superconductors; advances in GaN-AlN-InN crystal growth and epitaxy will advance high-power, high-temperature electronics; spintronic materials will enable increased memory density and magnetic computers; large-scale fabrication processes of multilayer photovoltaic devices will improve efficiencies of the direct conversion of solar to electric energy.

The picture is clear. Existing and future facilities, individual researchers, and new technologies supported by DOE need an ever-increasing supply of well-designed, high quality research samples. An imbalance has developed between the supply and demand for such samples, a disparity exacerbated by the shrinkage or closure of major industrial crystal growth laboratories over the past decade.

The negative consequences of such an imbalance have been recognized by other countries. Japan, in particular, has major crystal growth facilities such as the Institute for Solid State Physics (ISSP) at the University of Tokyo housing about 15 optical floating-zone furnaces and the Universities of Tohoku, Kyoto, and Nagoya which each operate five such furnaces. Furthermore, in April of 2002, a "Center for Crystal Science and Technology" was established at Yamanashi University. In a similar manner, the European Bio-Crystallogenesis Initiative (EBCI) is a joint project of 13 laboratories from 5 countries to obtain suitable single crystals for basic structural research. The need for high quality research materials, and the scientists who can design and grow them, needs to be a mounting emphasis in the US research portfolio at a level that can compete on the international stage with such established and emerging materials growth centers.

The challenge to the U.S. scientific infrastructure is threefold: (1) to re-establish a balance between its "new materials" and "new measurements" efforts (2) to reverse the trend of reliance on foreign sources for high quality research specimens, and (3) to redirect the flow of skills back to the design, discovery, and growth of novel materials. The development and growth of novel materials requires a sustained commitment of time, money and human resources over substantial time scales, often much longer than the usual three-year grant period. It is thus extremely important that BES/DOE rise to this challenge of reinforcing and expanding the U. S. effort in new materials design and growth.

Outline of the new materials design, discovery, growth and characterization process.

A research material goes through several stages as it progresses from discovery, to new material, to a known material of specific scientific and/or commercial interests. At each stage an intellectual (and in some cases economic) winnowing process selects 'interesting' materials for further study. To contextualize the recommendations of this report, it is valuable to trace these steps and to indicate where bottlenecks can and do appear in the process.

A useful concept for understanding the different stages of a material is the “New Materials Pyramid” shown in the figure. At the pyramid base is the first stage, namely, the design, discovery, and growth of the full range of compounds by the full range of synthesis techniques. This vast array of synthesis possibilities is driven by the nation’s core of independent, usually small, research groups and combines many different approaches: from materials exploration to focused synthesis on specific compounds, to synthesis science and the development of new techniques. This network is diverse, including chemists, physicists, materials scientists, metallurgists, etc. and distributed across universities, national laboratories and industry. On average, the number of significant discoveries of new materials in a given group is small, requiring that these groups create and examine many materials using a range of criteria to judge them: the search for new materials and phenomena is a resource- and labor- intensive process. Effort is also expended to learn more about well-known materials, or about novel materials of more limited interest, thereby increasing general knowledge. In the case of a significant discovery, on the other hand, the discovery group (and in some cases much of the synthesis community) may be occupied for years. Over the past decade, with an increasingly limited national synthesis capability, this process has been significantly slowed, leading to bottlenecks in the supply of materials to researchers.

In the second stage, certain new materials will become selected by the community as especially important based on novel functionality, new insights into existing problems, or novel structures. Such selected materials have broad appeal that crosscuts the measurement community. For a truly exciting material this can be a time of rapid growth of knowledge. A recent example of such a phenomenon was the six-month period following the announcement of superconductivity in MgB_2, during which hundreds of papers were submitted and understanding of MgB_2 grew explosively. For such mid-life materials that have scaled the pyramid base, small crystals or polycrystalline samples often suffice for essential characterization. However, as understanding grows and the nature of the experiments become more detailed, the need for specialized samples also grows. At this point, it may be difficult to find a group, even the discovery group, that has the capacity to make such specialized samples in the size or numbers required. This also slows the pace of fruitful research.

In the third stage at the tip of the pyramid compelling, highly studied materials reach maturity, and large, high-purity crystals are often essential to comprehensive understanding. Neutron scattering experiments require centimeter-sized specimens; synchrotron experiments require samples with extremely low mosaic spreads or extreme homogeneity; NMR and Mossbauer experiments require samples with specific isotopes. Sample availability again becomes a research bottleneck—a rate-limiting step for progress—that becomes harder and harder for small, isolated synthesis groups to overcome.

An additional problem exists when specialized growth facilities are needed for materials that have uniquely dangerous properties such as radioactivity, high toxicity, or where growth requires extremely high (>2 GPa) pressures. For such cases, even the first stage of the materials pyramid is not accessible, since the facilities do not exist for such dangerous, expensive synthesis techniques.

In summary, new materials travel along a reasonably well-defined trajectory, throughout which the needs of experimentalists for size and quality of samples evolve in parallel. Bottlenecks to productivity exist along this trajectory associated with communication disconnects, sample availability, and infrastructure limitations. We believe it is vital to preserve the intellectual diversity of small design discovery and growth groups at the base of the new materials pyramid. However, it is possible to increase the productivity and efficiency of the base by developing and supporting more groups engaged in exploratory materials synthesis, and by developing and supporting the network that joins them. We also believe there is a clear need for facilities at the apex of the pyramid to address the bottlenecks associated with highly specialized materials, and training.

Workshop recommendations

The BES Workshop on *Future Directions of Design, Discovery and Growth of Single Crystals for Basic Research* was held in Ames, Iowa on Friday, October 10 through Sunday, October 12, 2003. It was convened to explore the issues outlined above and to express specific recommendations to BES for improving the state of materials synthesis and crystal growth in the U.S. science portfolio. The main finding of this workshop can be summarized briefly:

> *Current infrastructure and personnel levels are insufficient to discover novel materials and to grow high quality, specialized samples at a level commensurate with demand by facilities and experimental groups and to maintain international competitiveness in materials-driven research. The linkage among existing synthesis groups is not optimal, contributing to*

bottlenecks in the creation and dissemination of research specimens to the condensed matter community.

Three broad recommendations to DOE-BES were identified to address this finding:

> **1** Increase the level of funding for individual research activities in the design, discovery and growth of novel materials for basic research. This would include appropriate funding increases in existing programs as well as the creation of new programs at universities, national laboratories, and select industrial labs.
>
> **2** Establish a novel materials design, discovery, and growth network to enhance the links among the various existing and future BES research efforts through meetings, personnel exchange, and materials databases. A more tightly interacting research community will more effectively leverage DOE's investment and reduce duplication, dead-ends, etc., and better integrate the materials synthesis community with the condensed matter science community.
>
> **3** Create a set of multi-investigator materials preparation facilities. In addition to their existing research efforts, PIs at these centers would provide high quality materials for users, advance specialized techniques, and train new crystal growth scientists.

We believe the first two recommendations can be addressed in a straightforward manner by BES. The workshop group was particularly enthused by the concept of a materials network linking individual groups. It was strongly felt that such a network would yield a profound enhancement in the way materials growth is undertaken and in new materials output in the U.S. although the precise form of the network is still to be defined. Still, it must be emphasized that while efficiencies of effort are possible and desirable, given the scale of the problem, new resources will be necessary to achieve the needed balance as analyzed in this report. The third recommendation will require a substantial, visionary, and long term commitment from BES for additional staff and equipment. This recommendation represents a potential strategy for elevating US materials synthesis and crystal growth to levels commensurate with existing and future Asian and European initiatives.

In the text that follows each of these goals will be discussed in greater detail.

Recommendation 1: Increase the level of funding for individual research activities

Empowering existing synthesis groups to enhance their materials output as well as the creation of new programs will encourage more researchers to engage in this area of condensed matter science. Expected outcomes from such increased funding include:

- faster and more frequent discoveries in basic research of novel materials
- greater availability of high quality research samples throughout the U.S.
- reduced reliance on foreign research samples—enhanced control of the U.S. research agenda

The creative engine that drives new materials research should continue to rely on a broad roster of researchers based in universities, national laboratories, and a few industrial settings. The independence and competitive nature of such programs is valuable and should be preserved. A wide variety of ideas and techniques increases the chances of finding new, scientifically interesting, and potentially technologically useful materials. The goal should be to multiply the number of 'interesting' materials by expanding the pool of researchers skilled in the practice of designing, growing and characterizing novel compounds. This will lead to greater availability of novel materials for research at individual and facility-based programs nationwide.

Also arguing for an increased number of design, discovery, and growth programs would be a decreased reliance on samples grown by sample preparation groups in either Asia or Europe.

Substantially increasing support for existing BES programs and creating new materials preparation groups would be a major step toward realizing the outcomes identified above. One possible model is for the DOE to commit to a 10–20 % annual growth in the new materials design, discovery and growth budget for each of the next 5 - 10 years. Such a commitment to growth would address each of the above points by allowing for the training and employment of more researchers in this key area of new materials research.

Recommendation 2: Establish a novel materials design, discovery and growth network

Materials synthesis researchers, those supported by BES as well as other agencies, comprise a diverse cohort of physicists, chemists, metallurgists, and material scientists. Each of these scientists brings unique skills and perspectives to the design, discovery and growth of novel materials. Such individuality is essential to future vitality and productivity in the field. However, a new level of cooperation, data sharing, and interchange through a formal ‘materials network’ of these individual programs could yield a whole greater than the sum of its parts.

Enhancing communication and formalizing links among existing and future BES research programs will leverage DOE’s investment, paying dividends in new materials output and efficiency. Reducing duplication and minimizing dead-end trails will be the immediate outcomes of such a network. Robust collaborations, new ideas, and shared expertise and infrastructure are some of the long-term benefits. The detailed workings of the materials network have been left as a future planning activity for BES; however, a recommended outline of its desirable features was developed at the workshop. In particular, the network would:

- Organize annual and/or topical meetings of BES supported materials growth researchers
- Establish and maintain a materials growth, characterization and availability data bank
- Manage a personnel exchange among BES-supported materials preparation efforts.

Annual and/or topical meetings of BES-supported materials researchers-will foster stronger ties. The meetings would focus on current scientific discoveries as well as the status of joint research projects, status and needs of large BES user facilities, and the training of new scientists in the broad field of novel materials design, discovery growth and characterization.

Another objective of the materials network would be to establish and maintain a novel materials growth and availability data bank. This data bank would collect in one place information about the various materials that the different groups receiving BES funding have made: growth procedures, additional information about growth details, and comments about sample size, quality, stability, and even availability. The purpose of this data bank would be to provide BES sponsored researchers a directory of available and well-characterized samples and sample producing techniques.

This novel materials design, discovery growth and characterization network would also establish and coordinate a program that would encourage and facilitate the exchange of students, post-docs and researchers among BES supported efforts. These exchanges could be of arbitrary length, depending on the nature of the projects or training desired. Such a program would take advantage of the range of facilities and skills present in the different BES sponsored research efforts. Increased training of research scientists skilled in the art and science of novel materials design, discovery growth and characterization is an anticipated outcome. In addition, the exchange of personnel is an effective means to establish strong ties among various research efforts.

In many ways, this materials design, discovery and growth network embraces the model currently exercised by the DOE Center of Excellence in Synthesis and Processing. Here, an annual budget of "glue" funding is provided to bring together like, or complementary, programs at several national laboratories and universities. The premise is that the added money will allow programs to stretch beyond working in isolation and foster breakthrough results through these new collaborations. Typically some travel is supported, as is an annual workshop. The CSP has been and continues to be an extremely strong element of the BES portfolio. We anticipate that a network built upon the principles of this program would be a successful means to connect and energize the network participants, and that a similar level of funding ($300 K) would be a starting point for a successful network program. It is anticipated that the scope of the materials network may exceed that of a single CSP, however, because of the breadth of materials issues of current interest.

Recommendation 3: Create multi-investigator materials preparation facilities

Materials preparation facilities distributed over several BES labs would become centerpieces of a novel materials design, discovery, growth and characterization network. These facilities would directly respond to the growing need for highly specialized samples for BES researchers and neutron/x-ray sources. These materials growth facilities would be an integral part of the materials network, contributing their own existing new materials research efforts while satisfying needs of the upper part of the materials pyramid. As such, these centers would provide for the U.S. materials community:

- Growth of high quality research materials for users
- Specialized techniques of materials synthesis that require extraordinary infrastructure
- Advanced understanding of crystallization and phase diagrams
- New exploratory growth techniques and the science of synthesis
- Training for materials growth staff and scientists

As part of their mandate, BES-supported crystal growth facilities will apportion a fraction of their research scientist time to the production of research grade samples. Resource allocations would be based on proposals submitted from the larger BES research community and peer reviewed. These proposals could request samples of specific size, of specific composition and quality, or of specific isotopic composition. Alternatively, a proposal could request determination of temperature-composition phase diagrams necessary to facilitate crystal growth. Where relevant, a tech-transfer process could take place, with new or specialized techniques passing from an individual design and discovery group to the facilities.

The facilities would create and grow samples that require extraordinary infrastructure or techniques unlikely to be found in other settings. Examples of such samples would be highly radioactive or toxic materials or samples that require extraordinarily high temperature, pressure or other extreme environments for growth. Another class of such materials would be compounds that simply require extremely complex or expensive purification and/or growth techniques.

As centers for new materials design and growth education, these facilities would also lead the research community's understanding of crystallization and phase diagrams. This understanding is often vital for better control of crystal growth. In addition the facilities would be active in creating, refining, and disseminating new exploratory growth techniques.

Training for scientists in a wide range of materials synthesis skill-sets is not widely available in the U.S. BES-supported facilities could fill this training gap by holding "Crystal Growth Schools" akin to the neutron and synchrotron summer schools held most years in the US as well as Europe. By cooperating with smaller design and discovery efforts, skills and expertise would flow into the larger, materials growth facility. This training process would not only be desirable for the creation of staff for this center but also would provide a "finishing school" for researchers interested in a broad, new materials research background.

Siting the facilities at national laboratories will exploit the strengths of existing facilities and ancillary capabilities. DOE investments in advanced characterization (synchrotrons and neutron sources) as well as theory and computer modeling (Ultrascale Scientific Computing Facilities, Esnet and NERSC) present opportunities for cross-fertilization. For example, the complexity of crystal growth itself is a formidable challenge to computer modeling due to the length and time scales, as well as the frequent occurrence of non-laminar flow. The observation of in-situ growth processes (single crystal growth from melt, Molecular Beam Epitaxy and Pulsed Laser Deposition thin film growth) using modern synchrotron and neutron scattering facilities may be the only way to obtain vital information about growth mechanisms and how to influence them. Integrating synthesis/fabrication as an independent and complementary entity to existing DOE user facilities is a model recently embraced by the five NSRCs, and the present facility model can learn from this paradigm.

It should be noted that BES supported materials growth facilities such as these would require a substantial investment by DOE. In this sense the third workshop recommendation will not be accomplished incrementally or via augmentation of current support. It calls for a bold commitment on the part of DOE to a strong future in bulk materials synthesis in the US. The value of such a network of facilities was readily apparent to the participants of the workshop.

Summary

The design, discovery and growth of novel materials, especially in single crystal form, represent a national core competency that is crucial for scientific progress and long-term economic growth. High quality, specialized samples are key to the future of condensed matter science, leading toward a fundamental understanding of new states of matter and underlying the technologies that flow from them. Unfortunately, the principal finding of the present Workshop is that the current U.S. infrastructure and personnel levels are insufficient to meet the growing demand for high quality samples, and to maintain international competitiveness in synthesis science, particularly in the area of single crystal growth. Our principal recommendation is that the Department of Energy should act to close the gap in U.S. based design, discovery and growth of novel materials for basic research by growing and coordinating the nation's existing crystal growth efforts, by adding qualitatively new capabilities, and by enhancing the Ph.D. and postdoctoral training opportunities in universities, national laboratories, and industry. These recommendations will strengthen the U.S. base in materials synthesis, optimize the use of national resources, and integrate the materials synthesis community more effectively into the larger U.S. condensed matter science enterprise.

Appendices:

A: **BES Workshop Schedule**
Attached file

B: **Final Participant List**
Attached file

C: **Work shop organizing committee**

Lynn Boatner, Oak Ridge National Laboratory
Mac Beasley, Stanford University
Paul Canfield, Chair, Iowa State University and Ames Laboratory
Robert Cava, Princeton University
Doon Gibbs, Brookhaven National Laboratory
Thomas Lograsso, Iowa State University and Ames Laboratory
David Mandrus, Oak Ridge National Laboratory
John Mitchell, Argonne National Laboratory

Appendix A: Workshop Agenda

BES Workshop on Future Directions of Design, Discovery and Growth of Single Crystals for Basic Research

Friday, October 10, 2003

6 pm to 8 pm	Opening Reception: The Hotel at Gateway Center

Saturday, October 11, 2003

7:45 am	Shuttle Pick-up at Hotels
8:00 – 8:20	Workshop Check-in and Gathering
8:20 – 8:30	**Welcome** by Tom Barton, Ames Laboratory Rm. 275
8:30 – 8:45	**Introduction and Opening Remarks** Rm. 275 William Oosterhuis, Condensed Matter Physics and Materials Chemistry, Materials Sciences and Engineering Division, Office of Basic Energy Sciences
8:45 – 9:30	**State of the Art and Current Research Frontiers in Intermetallics** Rm. 275 Zachary Fisk, Florida State University
9:30 – 10:15	**State of the Art and Current Research Frontiers in Oxides** Rm. 275 Robert Cava, Princeton University
10:15 – 10:30	Break
10:30 – 11:30	**State of the Art and Current Research Frontiers in Organic/Inorganic Hybrid** Rm. 275 *a)* Christian Kloc, Bell Laboratories/Lucent Technologies, 10:30 – 11 am *b)* Paul Kögerler, Ames Laboratory, 11 – 11:30 am
11:45	Lunch at Scheman, 2nd Floor Lobby
1:00 – 1:30 pm	Charge to Breakout Sessions
1:30 – 3:30	Breakout Sessions
3:30 – 4:00	Break
4:00 – 5:15	Summary
5:30 – 7:00	Social at Reiman Gardens, Hors d’oeuvres and Cash Bar
7:00 pm	Dinner at Reiman Gardens

Sunday, October 12, 2003

7:45 am	Shuttle Pick-up at Hotels

8:00 – 9:30	**Neutron and Photon Scattering Open Discussion** Rm. 275 Facilitators: Doon Gibbs, Brookhaven National Laboratory and Robert McQueeney, Ames Laboratory
9:30 – 9:45	Break
9:45 – 11:45	Breakout Sessions
Noon	Picnic lunch at Scheman, 2nd Floor Lobby
1:00 – 2:00 pm	Workshop Summary; 2 pm Workshop Concludes
2:00 – 3:00 pm	Breakout Chairs Meet Rm. 275

Breakout Session Schedule

Concurrent Sessions, October 11, 1:30 to 3:30 pm

Training of the Next Generation: Educational Opportunities and Needs.
Rm. 275
Co-chairs: Paul Canfield, Ames Laboratory
Mercouri Kanatzidis, Michigan State University

Design and Discovery of Novel Materials and States: New (and current)
Rm. 250
Modes and Methods.
Co-chairs: Robert Cava, Princeton University
Brian Sales, Oak Ridge National Laboratory

Needs of BES Growth Facilities.
Rm. 252
Co-chairs: John Mitchell, Argonne National Laboratory
Peter Flynn, University of Illinois

Steady State Operation: Visitors, Staff, Organization.
Rm. 260
Co-chairs: Doon Gibbs, Brookhaven National Laboratory
Malcolm Beasley, Stanford University

Samples Growth Challenges.
Rm. 262
Co-chairs: Ian Fisher, Stanford University
Tom Lograsso, Ames Laboratory

Concurrent Sessions, October 12, 9:45 to 11:45 am

Training of the Next Generation: Educational Opportunities and Needs.
Rm. 275
Co-chairs: David Mandrus, Oak Ridge National Laboratory
Brian Maple, University of California-San Diego

Design and Discovery of Novel Materials and States: New (and current)
Rm. 250
Modes and Methods.
Co-chairs: Tom Lograsso, Ames Laboratory
Christian Kloc, Bell Laboratories/Lucent Technologies

Needs of BES Growth Facilities.
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Co-chairs: John Sarrao, Los Alamos National Laboratory
George Crabtree, Argonne National Laboratory

Steady State Operation: Visitors, Staff, Organization.
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Co-chairs: Paul Canfield, Ames Laboratory
Larry Jones, Ames Laboratory

Samples Growth Challenges.
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Co-chairs: Lynn Boatner, Oak Ridge National Laboratory
Cedomir Petrovic, Brookhaven National Laboratory

Appendix B: Participants

Participant Name	Affiliation	E-mail	Phone	FAX
Abernathy, Douglas	Oak Ridge National Laboratory	abernathydl@ornl.gov	865.576.5105	865.241.5177
Ager, Joel	Lawrence Berkeley National Lab	JWAger@lbl.gov	510.486.6715	510.486.4114
Beasley, Malcolm	Stanford University	beasley@stanford.edu	650.723.1196	650.725.2189
Boatner, Lynn	Oak Ridge National Laboratory	1b4@ornl.gov	865.574.5492	865.584.4814
Bozovic, Ivan	Bozovic Consulting	ibozovic@pacbell.net	650.324.4576	650.321.2320
Buttrey, Douglas	University Of Delaware	buttrey@che.udel.edu	302.831.2034	302.831.2085
Canfield, Paul	Ames Laboratory	canfield@ameslab.gov	515.294.6270	515.294.0689
Cava, Robert	Princeton University	rcava@princeton.edu	609.258.0016	609.258.6746
Chan, Julia	Louisiana State University	jchan@lsu.edu	225.578.2695	
Cheong, Sang-Wook	Rutgers University			
Crabtree, George	Argonne National Laboratory	crabtree@anl.gov	630.252.5509	630.252.7777
Derby, Jeffrey	University of Minnesota	derby@umn.edu	612.625.8881	612.626.7246
Feigelson, Robert	Stanford University	feigel @soe.stanford.edu	650.723.4007	650.723.3752
Fisher, Ian	Stanford University	irfisher@stanford.edu	650.723.5821	650.725.2189
Fisk, Zachary	Florida State University	fisk@magnet.fsu.edu	580.644.2922	850.644.5038
Flynn, Peter	University of Illinois		217.244.6217	217.244.2278
Fratello, Vincent	Integrated Photonics, Inc.	vjf@integratedphotonics.com	908.281.8000	908.281.0191
George, Easo	Oak Ridge National Laboratory	georgeep@ornl.gov	865.574.5085	865.576.3881
Gibbs, Doon	Brookhaven National Laboratory	gibbs@bnl.gov	631.344.4608	631.344.3075
Hackenberger, Wesley	TRS Technologies, Inc.	wes @trstechnologies.com	814.238.7485	814.404.3605

Participant Name	**Affiliation**	**E-mail**	**Phone**	**FAX**
Harmon, Bruce	Ames Laboratory	harmon@ameslab.gov	515.294.8902	515.294.4456
Ibers, James	Northwestern University	ibers @chem.northwestern .edu	847.491.5449	847.491.2976
Johnston, David	Ames Laboratory	johnston@ameslab.gov	515.294.5435	515.294.0689
Jones, Larry	Ames Laboratory	jonesll@ameslab.gov	515.294.5236	515.294.8727
Kanatzidis, Mercouri	Michigan State University			
Kloc, Christian	Lucent Technologies	ckloc@lucent.som	908.582.2747	
Kogerler, Paul	Ames Laboratory	kogerler@ameslab.gov	515.294.3481	515.294.0689
Lee, Peter	Argonne National Laboratory	pllee@aps.anl.gov	630.252.0162	630.252.5391
Lee, Young	MIT	younglee@mit.edu	617.253.7834	
Lograsso, Thomas	Ames Laboratory	lograsso@ameslab.gov	515.294.8425	515.294.8727
Mandrus, David	Oak Ridge National Laboratory	mandrusdg@ornal.gov	865.574.6282	865.574.4814
Maple, M. Brian	University of California - San Diego	mbmaple@ucsd.edu	858.534.3968	858.534.1241
Matthiesen, David	Case Western Reserve University	dhm5@po.cwru.edu	216.368.1366	216.368.8618
McCallum, R. William	Ames Laboratory	mccallum @ameslab.gov	515.294.4736	515.294.3902
McQueeney, Robert	Ames Laboratory	mcqueeney @ameslab.gov	515.294.3545	515.294.0689
Miller, Gordon		gmiller@iastate.edu	515.294.6063	515.294.7812
Misewich, James		misewich@bnl.gov	631.344.3501	631.344.4071
Mitchell, John	Argonne National Laboratory	mitchell@anl.gov	631.252.5852	630.252.7777
Nelson, Christie	Brookhaven National Lab	csnelson@bnl.gov	631.344.4916	631.344.3238
Nolas, George	University of South Florida	gnolas@cas.usf.edu	813.974.2233	813.974.5813

Participant Name	Affiliation	E-mail	Phone	FAX
Oosterhuis, William	U.S. Dept. of Energy	w.oosterhuis @science.doe.gov	301.903.4173	301.903.9513
Petrovic, Cedomir	Brookhaven National Laboratory	petrovic@bnl.gov	631.344.5065	631.344.2739
Plummer, Ward	University of Tennessee	eplummer@utk.edu	865.974.2288	865.974.3895
Ramirez, Arthur	Bell Laboratory	aramirez@lanl.gov	908.582.4742	
Randles, Mark	Northrop Grumman SYNOPTICS	mark.randles@ngc.com	704.588.2340	704.588.2516
Rosenkranz, Stephan	Argonne National Laboratory	srosenkranz@mac.com	630.252.5475	630.252.5475
Sales, Brian	Oak Ridge Nat. Lab	salesbc@ornal.gov	865.576.7646	865.574.4814
Sarrao, John	Los Alamos National Laboratory	sarro@lanl.gov	505.665.0481	505.665.7652
Sasaki, Darryl	Sandia National Labs	darrly.sasaki @science.doe.gov	301.903.4578	301.903.9513
Steigerwald, Michael	Columbia University	msteiger @chem.columbia.edu	212.854.0185	
Tranquada, John	Brookhaven National Laboratory	jtran@bnl.gov	631.344.7547	631.344.2918
Tritt, Terry	Clemson University	ttritt@clemson.edu	864.656.5319	864.656.0805
Vogt, Tom	Brookhaven National Lab	tvogt@bnl.gov	631.344.4916	631.344.2918
Zhu, Jane	DOE/Basic Energy Sciences	jane.zhu @science.doe.gov	301.903.3811	301.903.9513
zur Loye, Hans-Conrad		zurloye @mail.chem.sc.edu	803.777.6916	803.777.8508
Ciszek, Ted		ted_ciszek @siliconsultant.com	303.674.3424	