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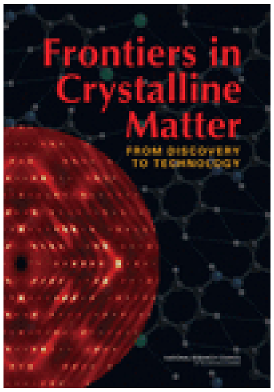

Frontiers in Crystalline Matter: From Discovery to Technology

Committee for an Assessment of and Outlook for New Materials Synthesis and Crystal Growth; National Research Council

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For much of the past 60 years, the U.S. research community dominated the discovery of new crystalline materials and the growth of large single crystals, placing the country at the forefront of fundamental advances in condensed-matter sciences and fueling the development of many of the new technologies at the core of U.S. economic growth. The opportunities offered by future developments in this field remain as promising as the achievements of the past. However, the past 20 years have seen a substantial deterioration in the United States' capability to pursue those opportunities at a time when several European and Asian countries have significantly increased investments in developing their own capacities in these areas. This book seeks both to set out the challenges and opportunities facing those who discover new crystalline materials and grow large crystals and to chart a way for the United States to reinvigorate its efforts and thereby return to a position of leadership in this field.

Summary

A CHANGED LANDSCAPE: CHALLENGES AND OPPORTUNITIES

For much of the past 60 years, the U.S. research community dominated the discovery of new crystalline materials and the growth of large single crystals, placing the country at the forefront of fundamental advances in condensed-matter sciences and fueling the development of many of the new technologies at the core of U.S. economic growth. The opportunities offered by future developments in this field remain as promising as the achievements of the past. However, the past 20 years have seen a substantial deterioration in the United States' capability to pursue those opportunities at a time when several European and Asian countries have significantly increased investments in developing their own capacities in these areas. This report seeks both to set out the challenges and opportunities facing those who discover new crystalline materials and grow large crystals and to chart a way for the United States to reinvigorate its efforts and thereby return to a position of leadership in this field.

The two activities in this field—discovering new crystalline materials and growing large crystals of these materials—have long been intertwined. Here, "crystalline material" refers to materials in which long-range periodicity of atomic positions is critical for the material's functionality. It is noted that such materials form a class distinct from nanomaterials, the functionality of which is defined by attributes governed by one or more nanometer-sized dimensions of the sample specimen, whether crystalline or amorphous. Once a new crystalline material is found to be either sufficiently interesting scientifically or relevant for an application—

or as often happens, both—large single crystals of that material are needed for detailed study. Because of common heritage, shared resources, and strong educational bonds, it is natural to combine these related activities—the discovery and growth of crystalline materials (DGCM)—in a single study. The growth of thin, two-dimensional crystalline films also is included in this study because it shares many common scientific and technological goals with the growth of bulk, three-dimensional materials.

The research activities falling under the DGCM umbrella are broad, spreading over traditional academic disciplines such as chemistry, materials science, and physics and undertaken in institutions such as university, government, and industrial research laboratories. Research in DGCM covers subject matter such as electronic, magnetic, optical, and structural phenomena. This diversity notwithstanding, there is a clear identity associated with researchers involved in DGCM. As can be seen from the attendance at scientific conferences in this area, it is a fairly small community, with exacting and specific technical needs and educational requirements.

While academia, the national laboratories, and private industry all have important roles in this field, industrial research laboratories historically have provided a particularly critical environment for the flourishing of DGCM activities. There, technological advancement in sectors such as the semiconductor industry, optical communications, and displays has required not only applied research to improve the performance of materials such as silicon, glass, and liquid crystals but also basic research into their fundamental properties. Advances made in DGCM in these laboratories were the consequence of a continual interplay between device development and basic research in physics and chemistry as well as close contact among the relevant technical communities—the material scientists, the crystal growers, and the developers of technical devices. This environment also served as a critical training ground, where the specialized techniques needed for success were passed on to new generations of crystal growers.

Almost a century after the discovery of Bragg's law, by which x-rays scattered from crystalline matter were used to establish its periodic structure, DGCM research not only has a strong legacy of foundational discovery but also retains great intellectual vitality, high technological relevance, and seemingly unending promise for discovery. The demand for crystals and new materials remains strong. The past 20 years have witnessed great advances in measurement capabilities in the United States across the whole range of facilities. At small and medium-size facilities, factors such as computer-assisted automation, new spectroscopies such as scanning probes, and the commercialization of diagnostic techniques have played a large role in driving demand for new materials. At the large national laboratories, several new U.S. synchrotron x-ray sources have been built, and new capabilities in neutron scattering have been installed at the National Institute of

Standards and Technology (NIST) and at the Oak Ridge National Laboratory. In addition, the National High Magnetic Field Laboratory, which opened in 1994, represents new capabilities in high magnetic field research, including a unique capability for studying the energy states of electrons in crystalline metals. These facilities represent some of the best characterization facilities in the world, creating opportunities to study, in great detail, novel magnetic, electrical, and structural properties of materials for which large single crystals are available. However, balance is needed between supporting the development of world-class characterization facilities and supporting the best materials growth; simply put, using the best neutron scattering facility in the world with suboptimal samples will engender suboptimal results.

The excitement and the promise of DGCM-based research already have been reflected in major initiatives abroad. For example, through projects such as Exploratory Research for Advanced Technology (ERATO), Japan now leads in the growth of strongly correlated oxides and organics both in bulk and thin-film form. China has significantly increased its commitment to develop expertise in crystal growth and basic materials research. And in certain areas such as ferroelectric crystals for information storage and actuator applications, China has developed the capability to produce large single crystals not currently available in the United States. The importance of international competition extends beyond national pride, however. Historically, those institutions that develop new materials are the ones with the best chance to exploit the resulting science and technology opportunities, the latter through intellectual ownership.

Despite the promises offered in this field, DGCM research in the United States today is substantially weaker than it was 20 years ago. The large industrial laboratories that historically led the nation in discovering new materials and in developing techniques for growing pure crystals no longer engage in these activities to a significant degree. DGCM research also has not found a "natural" home in the academic world in the United States. The nature of the work is inherently multidisciplinary and does not readily fit into the traditional, departmental structure of U.S. universities. Further, the start-up and operating costs of a DGCM researcher can be significantly higher than those of the typical university single investigator. Consequently, despite fundamental discoveries by DGCM researchers that have led to the establishment of entirely new subfields in condensed-matter physics, materials science, and chemistry, the presence of these researchers in U.S. universities is low. The net result of industrial laboratories' no longer engaging in DGCM research and the low level of research in the academic sector is that scientists and engineers in the United States face significant constraints because of inadequate access to crystals for scientific research and technology development, which frequently puts them, and the United States in general, at a competitive disadvantage.

RECOMMENDATIONS

This report was commissioned in the context of the deteriorating DGCM capacity in the United States. The National Research Council's Committee for an Assessment of and Outlook for New Materials Synthesis and Crystal Growth was charged with assessing this research area, identifying future opportunities, and recommending strategies to enhance opportunities in the United States (see Appendix A). In response to that charge, the committee concludes that DGCM remains a critically important area in condensed-matter research, and because of a change in the landscape in the United States, the continued competitiveness of the United States in this field requires that concrete and substantive steps be taken. The steps recommended by this committee are presented in the following paragraphs and are discussed more fully in Chapter 4 of the report.

Recommendation 1. Develop a focused, multiagency initiative to strengthen U.S. efforts to discover and grow new crystalline materials.

Crystalline materials research impacts a broad set of technologies encompassing energy, defense, information, communications, and industrial standards, and it straddles a number of traditional academic disciplines such as chemistry, materials science, and physics. Thus, an initiative for establishing and sustaining programs specifically directed toward driving the discovery and synthesis of new crystalline materials should be coordinated among agencies that fund research in these areas, including the National Science Foundation, the Department of Energy, the Department of Defense, and the Department of Commerce (NIST). The broad goals of such an initiative should be to establish crosscutting synthesis capabilities, educational thrusts, and openly available cyber resources that will enable broad research efforts. Programs funded through such an initiative would range from small-scale equipment run by single investigators to large-scale, centralized facilities for the discovery, growth, and characterization of crystalline materials, a range necessary to address the spectrum of research needs of this field.

Recommendation 2. Develop discovery and growth of crystalline materials "centers of expertise."

Funding should be provided for one or more "centers of expertise" that are capable of addressing the broadscale issues arising in the DGCM area. Centers have a role that cannot be filled by small programs. In contrast to small programs, centers can provide the infrastructure needed to house specialized facilities and the robust multidisciplinary environment needed for cutting-edge materials development. The purpose of these centers would be to address a range of problems, including those requiring large-scale facilities, facilities for using toxic chemicals, and facilities requiring significant technical support. In addition, the mission of one or more centers should be to address problems of crystal growth of immediate interest to U.S. industry. Working on a cost-recovery basis, these industry-oriented centers would be responsible for forming strong industrial partnerships, engaging in technology development with their industrial partners, and maintaining the expertise and infrastructure needed for industrial crystal growth. These centers also should support a small number of education and training programs that explicitly address the discovery and growth of crystalline materials and should complement the university-based education in DGCM addressed below in Recommendation 3.

Recommendation 3. Develop and sustain programs specifically designed to strengthen and sustain education and training in the field of the discovery and growth of crystalline materials.

In order for the United States to have a strong and sustainable effort in the discovery and growth of crystalline materials, federal agencies should develop programs and policies that focus on providing the specific and often unique education and training needed for those engaged in discovering new crystalline materials and synthesizing large crystals. Special attention should be given to developing federally funded programs that encourage academic organizations to prepare cross-disciplinary curricula and opportunities for educating the United States' next generation of DGCM scientists.

Recommendation 4. Promote cultural changes to develop and solidify academic programs in the field of the discovery and growth of crystalline materials.

The culture of U.S. science, as currently promulgated in the departmental or discipline-centric environment of universities, frequently does not reward DGCM synthesis research as much as it rewards measurement science. In order for the United States to have a strong and sustainable effort in the discovery and growth of crystalline materials, federal agencies should develop programs and policies that make it attractive for universities in the United States to hire crystal growers and promote robust research programs in this area by providing ample funding specifically for such work. The committee specifically urges that more crystal growers be hired into tenure-track positions at universities.

Recommendation 5. Develop a network approach for research-enhancing collaborative efforts in the discovery and growth of crystalline materials while preserving intellectual ownership.

New approaches to communication are needed to advance the field of discovery and growth of crystalline materials. The internal collaboration common in industrial laboratories formerly engaged in DGCM activities greatly aided the development of materials by providing rapid responses to synthesis needs as well as rapid feedback from measurement to synthesis. A similar approach to communication among researchers should be promoted through programmatic means by the federal agencies. The committee envisions a "DGCM network" as a novel approach to scientific collaboration that would both fulfill conventional needs for greater communication and enable the new modes of collaboration afforded by cyber infrastructure. The envisioned DGCM network would provide a virtual forum for organizing synthesis efforts, crystal growers would be able to announce the availability of new compounds, and a measurer would be able to request collaboration with a crystal grower to meet the measurer's need for a specific sample. The envisioned DGCM network would also provide access to information in the physical archive of already-synthesized samples stored in individual laboratories throughout the country, further enabling collaborations. At the same time, policies and procedures for participating in the network would be designed to enhance collaborative work while protecting the intellectual contributions of researchers who discover or develop novel crystalline materials.

Frontiers in Crystalline Matter

FROM DISCOVERY TO TECHNOLOGY

Committee for an Assessment of and Outlook for
New Materials Synthesis and Crystal Growth

Board on Physics and Astronomy

Division on Engineering and Physical Sciences

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NOTICE: The project that is the subject of this report was approved by the Governing Board of the National Research Council, whose members are drawn from the councils of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine. The members of the committee responsible for the report were chosen for their special competences and with regard for appropriate balance.

This project was supported by the Department of Energy under Award No. DE-FG02-06ER46271 and the National Science Foundation under Award No. 0551196. Any opinions, findings, conclusions, or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect the views of the organizations or agencies that provided support for the project.

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Cover: The technique of x-ray diffraction has long been one of the primary tools used to determine the atomic and molecular structures of crystalline materials and films. The diffraction pattern shown on the left is of the molecular compound N-(*p*-chlorobenzylidene)-*p*-chloroaniline, and the crystal structure associated with that pattern is shown in the background. Data for figures courtesy of Richard Welberry, Eric Chan, and Aidan Heerdegen (Australian National University) and Peter Chupas (Argonne National Laboratory); work performed at the Advanced Photon Source, Argonne National Laboratory.

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The **National Research Council** was organized by the National Academy of Sciences in 1916 to associate the broad community of science and technology with the Academy's purposes of furthering knowledge and advising the federal government. Functioning in accordance with general policies determined by the Academy, the Council has become the principal operating agency of both the National Academy of Sciences and the National Academy of Engineering in providing services to the government, the public, and the scientific and engineering communities. The Council is administered jointly by both Academies and the Institute of Medicine. Dr. Ralph J. Cicerone and Dr. Charles M. Vest are chair and vice chair, respectively, of the National Research Council.

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Preface

The National Research Council of the National Academies convened the Committee for an Assessment of and Outlook for New Materials Synthesis and Crystal Growth to assess current work and new opportunities in the United States in the field of the discovery and growth of crystalline materials. The Solid State Sciences Committee of the Board on Physics and Astronomy developed the charge for this study in consultation with the study's sponsors at the Department of Energy and the National Science Foundation. The committee was charged to define the research areas in this field, to determine the health of activities in the United States in those areas, to identify future opportunities, and then to suggest strategies to best meet those opportunities. The complete charge is reproduced in Appendix A.

The committee that prepared this report is composed of experts from the many academic disciplines falling within this field and includes members from the different types of institutions—academic, government, and industrial research laboratories—involved with this research (see Appendix B for biographical sketches of the committee members). The full committee met in person three times (see Appendix C) to address its charge. The committee formed subgroups to study specific areas in further detail and to develop the text of the final report. At its meetings, the committee heard from experts in the field and from the federal agencies that support research in this field. Conference calls and e-mail correspondence were used to coordinate the work of the committee between meetings. This final report reflects not only the committee's concerns regarding the current level of activity in the United States in this field but also its enthusiasm and excitement for research opportunities presented now and in the foreseeable future in these areas.

As committee chair, I am grateful to the committee members for their wisdom, cooperation, and commitment to ensuring the development of a comprehensive report.

Paul S. Peercy, *Chair*
Committee for an Assessment of and Outlook for
New Materials Synthesis and Crystal Growth

Acknowledgment of Reviewers

This report has been reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise, in accordance with procedures approved by the National Research Council's Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making its published report as sound as possible and to ensure that the report meets institutional standards for objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process. We wish to thank the following individuals for their review of this report:

Meigan Aronson, Stony Brook University/Brookhaven National Laboratory,
Gregory S. Boebinger, National High Magnetic Field Laboratory,
Ian Fisher, Stanford University,
Patrick A. Lee, Massachusetts Institute of Technology,
Allan MacDonald, University of Texas at Austin,
Cherry A. Murray, Lawrence Livermore National Laboratory,
Mark R. Pinto, Applied Materials, Inc.,
Nicola Spaldin, University of California at Santa Barbara, and
Yoshinori Tokura, University of Tokyo.

Although the reviewers listed above have provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations, nor did they see the final draft of the report before its release. The

review of this report was overseen by Paul Fleury, Yale University. Appointed by the National Research Council, he was responsible for making certain that an independent examination of this report was carried out in accordance with institutional procedures and that all review comments were carefully considered. Responsibility for the final content of this report rests entirely with the authoring committee and the institution.

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