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Frontiers of Materials Research: A Decadal Survey*

**This is the fourth materials research decadal since 1989.*
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Frontiers of Materials Research: A Decadal Survey

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Charge to:
COMMITTEE ON FRONTIERS OF MATERIALS RESEARCH: A DECADAL SURVEY

- Assess the progress and achievements in MR over the past decade;
- Identify the principal changes in the research and development landscape for MR in the United States and internationally over the past decade, and how those changes have impacted MR;
- Identify MR areas that offer promising investment opportunities and new directions for the period 2020-2030 or have major scientific gaps;
- Identify fields in MR that may be good candidates for transition to support by other disciplines, applied R&D sponsors, or industry;
- Identify the impacts that MR has had and is expected to have on emerging technologies, national needs, and science, broadly;
- Identify challenges that MR may face over the next decade and offer guidance to the materials research community for addressing those challenges; and
- Evaluate recent trends in investments in MR in the United States relative to similar research that is taking place internationally by using a limited number of case studies of representative areas of MR that have either experienced significant recent growth or are anticipated to see significant near-term growth. Based on those trends, recommend steps the United States might take to either secure leadership or to enhance collaboration and coordination of such research support, where appropriate, for identified subfields of MR.

Frontiers of Materials Research: A Decadal Survey

- The Committee met five times as a whole, with many additional teleconferences, among the leadership, the entire committee, and subsets of the committee.
- The Committee received input from more than 40 guest speakers and panelists at its meetings, who added to the members' understanding of the frontiers of materials research.
- This was a two year intense effort by 24 Committee Members.

General Observations

- Materials Science and Materials Engineering are both vast enterprises encompassing many diverse intellectual communities with different priorities
- Together they are really colossal, stretching from frontiers of fundamental science (topological matter, non-equilibrium processes) to industrial-scale manufacturing (additive manufacturing, Gorilla glass)
- It was a challenge to provide a full description of accomplishments and future prospects with an excitement in dealing with the diversity of opinions, backgrounds, and priorities.
- This 2019 Decadal Survey in Materials Research is truly a Consensus Report.

From Executive Summary:

"The statement of task was extremely broad, and the committee could not cover every aspect of MR, from the most fundamental to the most disruptive manufacturing, without leaving important and even crucial areas of MR out of the report, or providing only brief mention. This does not indicate that the committee felt these areas were less important or crucial."

FRONTIERS OF MATERIALS RESEARCH: A DECADAL SURVEY
Chapters of the Report

- CHAPTER 1. LANDSCAPE AND IMPACT OVER THE PAST 10 YEARS: SETTING THE SCENE
- CHAPTER 2: PROGRESS AND ACHIEVEMENTS IN MATERIALS RESEARCH OVER THE PAST DECADE
- CHAPTER 3. MATERIALS RESEARCH OPPORTUNITIES
- CHAPTER 4. RESEARCH TOOLS, METHODS, INFRASTRUCTURE, AND FACILITIES
- CHAPTER 5. NATIONAL COMPETITIVENESS

Text from Chapter 1 concerning the past decade

"By studying earlier decades and reading the reports that were produced, researchers know to expect the unexpected, which is precisely the allure of science. There have been surprises, to be sure, in the last decade. It is useful to examine a few examples of important developments that were not foreseen."

Graphene and topological insulators

“For example, … graphene … was given scant mention in the previous decadal survey in 2010. Since then, graphene has spawned an exciting field of other two-dimensional (2D) materials, and perhaps more importantly, it has instigated work on new physical phenomena, with potential utility in many electronics applications such as solar cells, transistors, transistors, camera sensors, digital screens, and semiconductors.”

Vitrimers and polymers with dynamic covalent bonds

“Self-healing of polymers realized a new paradigm with the development of polymers with dynamically reconfigurable covalent bonds. One example, a remarkable new class of plastics now known as vitrimers (a term for glass-like polymers), was unanticipated 10 years ago. Vitrimers exhibit properties similar to silica glasses but in which the covalent bond network topology can be rearranged by exchange reactions without depolymerization. They remain insoluble and yet processable as bulk materials.”

Gorilla Glass

“Smartphone touch screen technology, which made its appearance at the beginning of the last decade, created entirely new roles for glass. This glass serves three functions: it enables user input, protects the display beneath it, and transmits the information on the display to the user even after years of use, in addition to resisting breakage owing to accidental drops. The material has to be mechanically durable, scratch resistant, thin, stiff, dimensionally stable, flat, smooth, impermeable to water, and transparent to both visible light and radio waves. Corning was able to surmount all of these challenges in a very short time through application of deep understanding of glass composition and manufacturing technology.”

Text from Chapter 1 concerning the past decade

" … some important developments were the product of pure discovery-driven science (topological insulators), while others were concerted technological efforts (Gorilla Glass), and still others some combination of the two (vitrimers). This is a strong argument for supporting materials research across a span of technology readiness levels, and for creating environments in which basic and applied research, as well as academic and industrial research, interact intimately."

Key Findings and Recommendations

- **Key Finding:** Basic research in fundamental science directions meaning work that neither anticipates nor seeks a specific outcome, is the deep well that both satisfies our need to understand our universe and feeds the technological advances that drive the modern world. It lays the groundwork for future advances in materials science as in other fields of science and technology. Discoveries without immediate obvious application often represent great technical challenges for further development (e.g., high-Tc superconductivity, carbon nanotubes) but can also lead to very important advances, often years in the future.
- **Key Recommendation:** It is critically important that fundamental research remains a central component of the funding portfolio of government agencies that support materials research. Paradigm-changing advances often come from unexpected lines of work.

Chapter 1
Key Findings and Recommendations

- **Key Finding:** The integrated computational materials science and materials engineering methodology has had a significant impact on product development in specific industries, as the committee has learned through industrial input. There is potential for further impact through the inclusion of integrated data sciences into the materials research for all length scales and material types.
- **Key Recommendation:** All government agencies funding materials research should encourage the use, when appropriate, of computational methods, data analytics, machine learning, and deep learning in the research they fund. They should also encourage universities to provide students of science and engineering exposure to these new methods by 2022.

ILLUSTRATIVE RESEARCH OPPORTUNITIES

- **Key Finding:** Quantum materials science and engineering, which can include superconductors, semiconductors, magnets, and two-dimensional and topological materials, represents a vibrant area of fundamental research. New understanding and advances in materials science hold the promise of enabling transformational future applications, in computing, data storage, communications, sensing, and other emerging areas of technology. This includes new computing directions outside Moore's law, such as quantum computing and neuromorphic computing, critical for low-energy alternatives to traditional processors. Two of the National Science Foundation (NSF)'s "10 big ideas" specifically identify support of quantum materials (see *The Quantum Leap: Leading the Next Quantum Revolution* and *Midscale Research Infrastructure*).
- **Key Recommendation:** Significant investments by, and partnerships among, NSF, DOE, NIST, DOD, and IARPA will accelerate progress in quantum materials science and engineering, so crucial to the future economy and homeland security. U.S. agencies with a stake in advanced computing, under the possible leadership of DOE's Office of Science and NNSA laboratories and the DOD research laboratories (ARL, ONR, AFRL), should undertake to support new initiatives to study the basic materials science of new computing paradigms during the next decade. To remain internationally competitive, the U.S. materials research community must continue to grow and expand in these areas.

DEMAND FROM THE ULTIMATE APPLICATIONS

- **Key Finding:** Materials science and technology has an enormous impact on the quality and sustainability of Earth's environment across the entire spectrum of materials types. This is another important opportunity for university, national laboratory, and industry cooperation.
- **Key Recommendation:** Research in numerous directions that improve sustainable manufacturing of materials, including choices of feedstocks, energy efficiency, recyclability, and more, is urgently needed. Creative approaches for funding materials research toward sustainability goals should be developed by NSF, DOE, and other agencies.

Chapter 3
Findings and Recommendations

- **Finding:** Sustainability and environmental impact have special import in the domain of polymer materials research owing to the dual factors of the massive accumulation of discarded polymeric materials in the environment and the unique challenges to polymer recyclability.
- **Recommendation:** The massive accumulation of discarded polymeric materials points to several needed actions, namely, stimulating and executing further research on environmental degradability of polymers, better methods of separating incompatible polymers out of waste streams, research toward recycling without separation, and fundamental research in green chemistry possibilities within polymer research.

DEMAND FROM THE ULTIMATE APPLICATIONS

- **Key Finding:** Many of the real-world challenges and opportunities in materials research occur at the intersections among traditional disciplines, and at the interfaces between fundamental and applied research. Pure science often benefits from proximity to applied research. Collaboration and information transfer among different disciplines and among academia, industry, and government laboratories greatly increases the likelihood of successfully meeting these challenges and capitalizing on these opportunities.
- **Key Recommendation:** Government agencies, led by the Office of Science and Technology Policy (OSTP), should work with high priority to foster communication among materials research stakeholders through the support of interdisciplinary research and the development of modalities for freer flowing interactions among universities, private enterprise (including start-up ventures), and national laboratories.

INFRASTRUCTURE NEEDS

- **Key Finding:** Infrastructure at all levels, from midscale instrumentation for materials characterization, synthesis, and processing with purchase costs of $4 million to $100 million in universities and national laboratories to large-scale research centers like synchrotron light sources, free electron lasers, neutron scattering sources, high field magnets, and superconductors is essential for the health of the U.S. materials science enterprise. Midscale infrastructure, in particular, has been sorely neglected in recent years, and the cost of maintenance and dedicated technical staff has increased enormously.
- **Key Recommendation:** All U.S. government agencies with interests in materials research should implement a national strategy to ensure that university research groups and national laboratories have local access to develop, and continuing support for use of, state-of-the-art midscale instruments and laboratory infrastructure essential for the advancement of materials research. This infrastructure includes materials growth and synthesis facilities, helium liquefiers and recovery systems, cryogen-free cooling systems, and advanced measurement instruments. The agencies should also continue support of large facilities such as those at Oak Ridge National Laboratory (ORNL), Lawrence Berkeley National Laboratory (LBNL), Argonne National Laboratory (ANL), Stanford Linear Accelerator Center (SLAC), National Synchrotron Light Source II (NSLS-II), and National Institute of Standards and Technology (NIST)—and engage and invest in long-range planning for upgrades and replacements for existing facilities.

INFRASTRUCTURE NEEDS

- **Key Finding:** Progress in three-dimensional (3D) characterization, computational materials science, and advanced manufacturing and processing have enabled an increasing digitization across disciplines of materials research and has in some cases dramatically accelerated and compressed the time from discovery to inclusion in new products.
- **Key Recommendation:** Federal agencies (including NSF and DOE) with missions aligned with the advancement of additive manufacturing and other modes of digitally controlled manufacturing should by 2020 expand investments in materials research for automated materials manufacturing. The increased investments should be across the multiple disciplines that support automated materials synthesis and manufacturing. These range from the most fundamental research to product realization, including experimental and modeling capabilities enabled by advances in computing, to achieve the aim that by 2030 the United States is the leader in the field.

INFRASTRUCTURE NEEDS

- **Key Finding:** The Materials Genome Initiative, and the earlier Integrated Computational Materials Engineering approach, recognized the potential of integrating and coordinating computational methods, informatics, materials characterization, and synthesis and processing methods to accelerate the discovery and deployment of designer materials in products. The translation of these methodologies to specific industries has resulted in numerous successful applications that have reduced the development time with corresponding cost savings.
- **Key Recommendation:** The U.S. government, with NSF, DOD, and DOE coordinating, should support the quest to develop new computational and advanced data-analytic methods, invent new experimental tools to probe the properties of materials, and design novel synthesis and processing methods. The effort should be accelerated from today's levels through judicious agency investments and continue over the next decade in order to sustain U.S. competitiveness.

Chap 5 – National Competitiveness

This subject is complex, and though part of our charge, it presents issues (e.g. economic and geopolitical) that involve more than science and engineering and that are beyond the expertise of the committee. It deserves further study.

- The creation and control of materials is critical to any advanced economy – prediction of importance to GDP
- America dominated materials science and engineering for most of the post-war period, but it no longer does
- Other countries, the European Union, Japan, Korea, and particularly, the emerging giant China now threaten our leadership.
  - They are investing heavily in state-of-the-art facilities like synchrotrons, centers for neutron scattering, etc.
  - They have centralized industrial policies designed to improve their economic competiveness, and they often tailor research support with this goal in mind.

How Should US Respond

- Strong and sustained support for fundamental and applied research is essential; includes development and maintenance of research infrastructure – important for both fundamental research and product development – e.g. neutron scattering
- Nurture international collaboration
- But an environment that brings new technology to the market place is also needed.
- In the global economy, enterprises get the technology they need wherever it is – example of GE’s additive manufacturing. How important is local production? Transfer of US technological innovation to foreign production?
- iMac and no screws (NY Times, Jan. 29, 2019)

NATIONAL COMPETITIVENESS

- **Key Finding:** Intense competition among developed and developing nations for leadership in the modern economic drivers, including smart manufacturing and materials science, will grow over the coming decade.
- **Recommendation:** The U.S. government, with input from all agencies supporting materials research, should take coordinated steps beginning in 2020 to fully assess the threat of increased worldwide competition to its leadership in materials science and in advanced and smart manufacturing. The assessment program, which should be established on a permanent basis, should also define a strategy by 2022 to combat this threat.
- **Recommendation:** The U.S. government should fund and pursue a strategy-based permanent program of robust investment focused on materials science and smart manufacturing that will allow us to maintain our position as a world leader in materials science and not to fall behind our many competitors.

Findings/Recommendations

Finding: International scientific collaboration and science diplomacy is vital to U.S. success in fundamental and applied materials research. In some cases, scientists are forbidden to travel between countries. While many U.S. researchers understand how to protect sensitive material, with the increasing prevalence of cyber espionage, this understanding needs to be updated.

Recommendation: In order to maintain international collaborations, the United States must allocate funds to develop methods to educate our researchers on how to be vigilant in maintaining security both while traveling abroad and when welcoming international colleagues to the United States. Such education would also be crucial for maintaining industrial security within the United States.

Case Studies

- Flat Panel Liquid Crystal Displays
- Additive Manufacturing in Aerospace
- Permanent Magnets
- Photovoltaics
- Lithium Ion Batteries

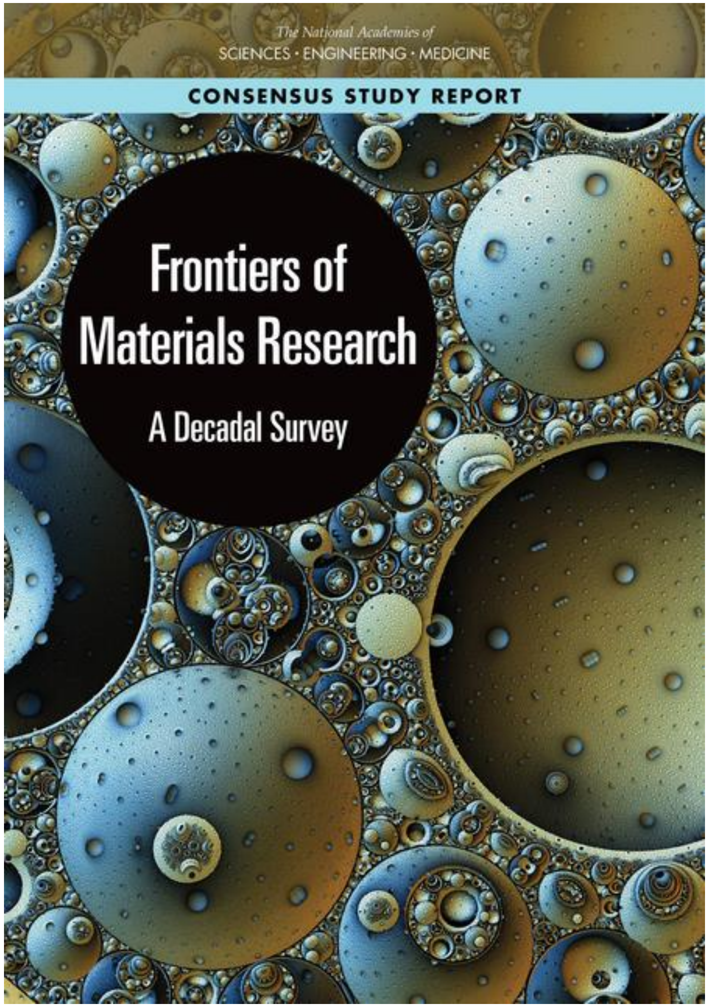
These studies illustrate the international nature of discovery, of industrial search for new materials, and the unpredictable paths of ideas to profitable products.

Recent Advances in MR

Exciting times for MR: Paradigm-changing advances in MR have accelerated the pace of discovery

- Computational Science: new algorithms, AI and machine learning, Big Data
- New tools: materials characterization, synthesis and processing, computational modelling
- New materials: 2D, vitrimers, high-entropy alloys, metamaterials
- New Theory: Topological insulators, quantum computing

Recent past has been a good time (many committee members say it has been the best time) for MR. Future possibilities looks even brighter.



Questions?

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