The National Science Foundation's Program in Materials Science: New Frontiers, New Initiatives, New Programs, and New Prospects

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IN WASHINGTON, REPORTS ARE PLENTIFUL. Most of them are on important topics and reflect careful analysis by well-informed, thoughtful people. But there are too many: with few exceptions, these reports conclude with a request for new programs and more money from agencies, departments, and legislators that hear the same litany over and over again; only the supplicants change. Rarely, a report commands major attention and holds it over some period of time. Praveen Chaudhari and Merton Flemings produced a report that has received the attention it deserves. *Materials Science and Engineering for the 1990s* (*1*), published by the National Research Council in 1989, has been the foundation for planning on a coordinated and sustained level not often seen in Washington, outside of major national efforts such as the space program or the superconducting supercollider.

The importance of materials science in tomorrow's world cannot be overstated. Technologies from microelectronics and nanostructures to spacecraft and biomedical prostheses depend absolutely on amazing materials created through the ingenuity of scientists and engineers. Kevlar composites, high-temperature superconductors, and buckeyball-based structures did not exist a short time ago. But we are already on the edge of an even more astonishing materials fixture: Just in the past few years, we have developed techniques to assemble materials molecule by molecule and atom by atom; we literally have the ability to move single atoms and place them where needed. Imagine the possibilities that power brings to the design, synthesis, and processing of newer, "smarter" materials for applications we have not yet considered. Truly, the opportunities are not only mind-boggling, they are also only mind-limited.

The socioeconomic impact of materials in the United States is no less staggering. The eight industries of aerospace, automobiles, biomaterials,

†Deceased

chemicals, electronics, energy, metals, and telecommunications—all critically dependent on materials—together generate $1.4 trillion in sales (1987 figures) and employ 7 million people. No wonder that *Materials Science and Engineering for the 1990s* attracted such attention!

Robert White, chair of the Federal Coordinating Council for Science, Engineering, and Technology (FCCSET) Committee on Industry and Technology, has already discussed the materials research and development activities of 10 federal departments and agencies that were coordinated into a coherent, cross-agency 1993 Presidential Initiative known as the Advanced Materials and Processing Program (AMPP). The AMPP Initiative as proposed for fiscal year 1993 was roughly a $2 billion enterprise, including both the existing base and the proposed 1993 increases. This section will focus on implementation of the AMPP at the National Science Foundation (NSF).

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Early Precursors to AMPP at NSF

Although the NSF has had a Division of Materials Research (DMR) and has supported a network of materials research laboratories (MRLs) since 1972, additional recognition of the emerging opportunities on the molecular scale in materials science prompted a 1984 workshop at the NSF. Sponsored by NSF's Divisions of Chemistry and Materials Research, the conference explored the scientific opportunities and programmatic needs in the area of materials chemistry (MC), roughly defined as the region of overlap between the macroscopic frontier of chemistry (the molecular science) and the microscopic frontier of real materials (a macroscopic science). Out of that workshop report grew a small but catalytic program to support collaborative projects involving both chemists and materials scientists or engineers, trying to bridge the gap between the colligative and molecular worlds. The role of chemists in materials science is now as it was then: To synthesize next-generation materials atom by atom, the chemist must understand all dimensions of molecular interactions and their impact on macroscopic properties in order to know which atoms to put where. Moreover, synthesis is the heart and soul of chemistry. Physicists, mathematicians, and engineers analyze, characterize, and process materials; chemists synthesize them.

Materials chemistry proposals were jointly reviewed and split-funded, and in 1987 and 1988, 33 cooperative research projects were initiated. In 1989, the partnership was expanded to include the Division of Chemical and Thermal Systems (NSF's home for chemical engineering), and the program was renamed Materials Chemistry and Chemical Processing (MCCP). In 1989, 1990, and 1991, each of the three participating NSF divisions invested about three-quarters of a million dollars in additional projects, most of which were later mainstreamed into existing program rubrics, and a high fraction of which have been successfully renewed.

The total 5-year investment in the materials chemistry programs (MC and MCCP) was more than $18 million. That number might be considered modest, but MC–MCCP accomplished two things: (1) it initiated about 60 collaborative research projects in the chemistry research community, where individualism was the overwhelming norm; and (2) it established within NSF a paradigm for interdivisional cooperation in the review and funding of interdisciplinary research.

NSF's 1992 Materials Synthesis and Processing Initiative

During 1990–1991, while the FCCSET Committee on Industry and Technology was carrying out the extensive analysis, coordination, and planning necessary to implement a Presidential Initiative, the NSF was carrying out its own component of this analysis. An inventory of support for materials science and engineering at NSF (1991 actual expenditures) includes the following:

- $216 million for materials research and development (R&D) research project support, principally in DMR, the Engineering Directorate (ENG), and the Chemistry Division (CHE)
- $31 million (additional) for national user facilities (nanofabrication, synchrotrons, magnet labs, and supercomputers)
- materials research laboratories (nine) and groups ($47 million)
- science and technology centers (7 out of 25 have materials as their focus)
- engineering research centers (6 out of 18 have materials as their focus)
- industry–university cooperative research centers (15 out of 26 have materials as their focus)

Recognizing the criticality of materials science and engineering, the NSF moved to get a head start on the materials programs being planned through FCCSET by establishing its own Materials Synthesis and Processing (MS&P) Initiative for fiscal year 1992. An increment of $25 million was requested in the 1992 budget as the first phase of a 5-year effort to strengthen research in materials synthesis and processing. The 1992 MS&P Initiative had two aims: (1) molecular-level approaches to the design and synthesis of new materials based on fundamental principles and a developing base of molecular structure–property–performance relationships; and (2) new and improved processing methods, including reactor design, kinetics, and applications to manufacturing, looking to produce materials with improvements in efficiency, properties, and quality.

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The MS&P Initiative was launched as planned in 1992, although the 1992 congressional appropriation was less than requested. Features of the program (*2*) included the following:

- They focused on synthesis and processing (including relevant theory and characterization).
- They included five eligible materials classes, two favored (electronic–photonic and biomolecular) and three others (structural, magnetic, and superconducting materials).
- They included single- and multidisciplinary projects.
- They accepted proposals from single investigators and groups.
- Nine NSF divisions cooperated in review and funding.

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Biomolecular materials were defined as those substances, natural or synthetic, with novel materials properties that use or mimic biological phenomena. A sample menu of ideas was generated to provide some sense of the envisioned scope of the MS&P program:

Electronic and Photonic Materials

- new materials with unique properties (semiconductors, superconductors, insulators, and composites)
- methods for deposition and growth (films, layered structures, bulk crystals, and fibers)
- low-temperature synthesis and preparation
- combining materials growth and processing techniques
- laser, electron, ion, and plasma-assisted processing
- real-time, in situ diagnostics

Biomolecular Materials

- genetic modification of natural synthetic pathways
- biomolecular self-organization and phase behavior
- novel catalyst, sensor, and transducer materials
- materials aspects of in vivo biopolymer processing
- synthetic structures mimicking natural composites
- biodegradable or biorecyclable materials

Structural Materials

- new metallic alloys, polymers, ceramics, and composites
- origin and evolution of phases, defects, and microstructures
- solid-state behavior controlling multiphase materials properties (phase transformations and grain boundaries)
- processing methods (particle consolidation, sol–gel conversions, rapid solidification, and powder synthesis)

- direct conversion of precursors to finished forms (reaction bonding and injection molding, microwave sintering, and net-shape manufacturing)

Magnetic Materials

- design and synthesis of new magnetic materials
- artificially structured multilayer magnetic materials
- enhanced properties in hard and soft magnets, thin films, and magneto-optics
- surface and two-dimensional magnetic behavior
- new processing methods for magnetic materials

Superconducting Materials

- superconduction in bulk materials, thin films, and reduced-geometry structures
- low-temperature, in situ processing and fabrication methods
- improved structure–property relationships and theory
- single-crystal growth of superconducting materials
- properties of surfaces and interfaces: connections, contacts, and passivation
- crystal structure, microstructure, and morphology

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All multi-investigator proposals were due by November 1, 1992, because it was anticipated that the large majority of them would have to be co-reviewed and co-funded by two or more disciplinary NSF divisions. Single-investigator proposals were accommodated within regular programmatic boundaries and guidelines. A matrix-managed review procedure was established. Proposals were to be addressed to the NSF division appropriate to the principal technical thrust of the proposal (its "center of gravity"), where a divisional coordinator carried out preliminary screening for suitability, negotiated with other divisions where required for joint review, and then managed the review itself. To a large extent, each NSF division used its usual review procedures, although several divisions reviewed all MS&P proposals with specially assembled review panels instead of using ad hoc mail review.

Approximately 700 proposals were received in response to the MS&P announcement in fiscal year 1992; some divisions had no deadlines for individual investigator proposals, so this inventory was not complete until the end of the 1992 fiscal year. The breakdown between collaborative proposals from groups and those from single investigators was approximately 2:1. About 50% of proposals had a center of gravity in the DMR (principally solid-state chemistry, polymers, and electronic materials) and were managed by DMR. Another 33% were managed by five engineering divisions, 12% by chemistry, and 5% by two biosciences divisions. As expected, most of the proposals fell into the categories of electronic and optical or photonic materials; fewer proposals than expected were received with a biomolecular materials focus.

Data for proposals and awards in which the Division of Chemistry was involved are as follows:

- Reviewed 122 out of 700 proposals; managed 82; 52 were single investigators; 70 were groups; 92 required interdisciplinary review; 30 were reviewed within CHE.
- Focus was on electronics (48%) and photonics (25%); biomaterials was 10%; magnetic was 8%; structural was 7% of the proposals.
- Funded 26 awards (21%), $3.1 million; 13 were single investigator; 13 were groups; 16 out of 26 were co-funded with four different divisions.

Data for proposals and awards in which the Division of Materials Research was involved are as follows:

- Reviewed 351 out of 700 proposals.
- Funded 57 awards and co-funded 28.
- Total investment was $6.4 million in 85 grants (16% success rate).
- Award distribution was as follows: 40%, electronics; 23%, optical–photonics; 18%, structural; 3%, biomolecular; 9%, magnetic; and 7%, superconducting.

What has been learned from MS&P about multidisciplinary program management? Program management must be kept simpler by taking a "varietal wine" approach to the labeling and review of proposals. It is quite cumbersome to matrix-manage a large number of proposals. In the future, NSF will have to assign proposals to a given program on the basis of the scientific "center of gravity", have that program solicit assistance as needed, but make review and award decisions more locally.

Looking Ahead to the AMPP

The AMPP is a coordinated interagency effort to exploit opportunities in materials research and development to meet significant national goals and to extend U.S. leadership in materials-dependent critical technologies. The goal (*3*) is "to improve the manufacture and performance of materials to enhance the Nation's quality of life, security, industrial productivity, and economic growth". To achieve this goal, a set of strategic objectives was established:

1. maintain U.S. leadership in advanced materials and processing
2. bridge the gap between innovation and application of technologies

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3. support agency mission objectives to meet national needs
4. encourage university and private sector R&D related to AMPP

Implementing priorities were also established:

1. support strategic objectives through R&D effort
2. plan federal programs to incorporate needs of strategic, industrial, and social sectors
3. promote applications through university–industry–Government cooperation in generic, competitive technology development
4. support the human resource base to meet future needs
5. maintain healthy infrastructure (e.g., facilities)
6. focus R&D on materials and processes that are most important to achieving AMP strategic objectives

Although the AMPP is an R&D program, its purpose goes well beyond curiosity-driven research. Success is going to be measured not only by new discoveries, but also by successful application of new knowledge and technology. Thus, a significant ambition within AMPP is to strengthen productive interaction between the Government, industry, and academic sectors. All participating federal agencies share the same AMPP goals and objectives consistent with their missions. NSF's mission is the generation and dissemination of fundamental knowledge and the training and development of scientists and engineers.

The AMPP has three conceptual tiers: (1) an inventory of current materials R&D; (2) targeted program enhancements; and (3) conceptual opportunities for technical breakthroughs. The inventories are by agency, by materials class (the terms are familiar to chemists), and by program component. AMPP has four program components: (1) synthesis and processing; (2) theory, modeling, and simulation; (3) materials characterization; and (4) education and human resources. National user facilities are included in the inventories, but they are not a program component in the sense of being subject to the same priority-setting practices.

The priority-assigned program components increase roughly as their applicability to the national needs identified in the AMPP program goal. Within synthesis and processing, process integration takes a higher priority than basic research; similarly, application-specific theory, modeling, or simulation takes precedence over more fundamental research. Bigger budgetary increments were proposed for synthesis and processing than for materials characterization. These priorities are for the overall interagency program. In synthesis and processing, for example, process integration may be emphasized at the National Institute of Standards and Technology (NIST), and basic research would be emphasized at NSF. Or, even within NSF, process integration and applied research may be centered in ENG, and basic synthesis is centered in CHE or DMR.

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The prioritization of research objectives and classes is is not necessarily what a "curiosity-driven" researcher likes to hear. However, these are Government-wide priorities. They apply to all participants in the AMPP, but not all agencies have exactly comparable missions. AMPP research carried out with NSF support will probably have a more fundamental flavor, on average, than R&D sponsored by a mission agency. Objectives for 1993 within the NSF component are

- synthesis of advanced materials
- fundamental physics and chemistry of materials
- links between synthesis and processing and materials structure, properties, and performance
- development of novel processing and manufacturing methods
- creation of linkages with industry for knowledge and technology transfer
- emphasis on academic research for education and training

The AMPP represents a major response to the needs and opportunities spelled out in the materials science and engineering (MS&E) report (*1*). Major opportunities exist for scientific breakthroughs in materials science, and many of them, perhaps most, will need chemists for the key finding or concept. Everyone who thinks about chemistry and materials can generate her or his own list. Some ideas and possibilities that seem particularly challenging and ripe for plucking by chemists are in the areas of polymers, biomolecular materials, and electronics–photonics.

New "natural" polymers based on synthesis from renewable resources, improved recyclability based on retrosynthesis to reusable precursors, and molecular "suicide switches" to initiate biodegradation "on demand" are the exciting areas in polymer science. In the area of biomolecular materials, new materials for implants with improved durability and biocompatibility, light-harvesting materials based on biomimicry of photosynthetic systems, and biosensors for analysis and artificial enzymes for bioremediation will present the breakthrough opportunities. Finally, in the field of electronics and photonics, the new challenges are molecular switches, transistors, and other electronic components; molecular photoaddressable memory devices; and ferroelectrics and ferromagnets based on nonmetals.

Although the AMPP represents a set of real opportunities—both intellectual and financial—for chemists, two important constraints must be recognized. The first constraint is also financial: The federal budget will not be everything the scientific community might hope for. Congressional spending caps and competition among many different funding demands will restrict budget growth. In some situations, agency or program budgets may not exceed those of 1992. At the NSF, at least, the AMPP will move ahead in 1993 at some level, because chemists and engineers are seizing on the fundamental intellectual challenges and basic questions posed by materials problems, whether or not funds are "set aside". In all three divisions that are the principal supporters of the chemistry aspects of materials, materials chemistry and chemical engineering have already been identified as major intellectual frontiers in long-range planning exercises. Hence, the AMPP represents an intellectual thrust as well as a fiscal one.

The other constraint is that AMPP is a goal-oriented research program. Even at the NSF, it is not quite "business as usual". Policy issues at the national level are pushing the NSF to take a broader view of its mission in education and research, relating those traditional strengths to national needs, especially in the area of economic competitiveness. NSF will increasingly look for opportunities to contribute to the nation's priorities through its unique programs. NSF, for example, is particularly well-suited to support fundamental research at academic institutions because that activity couples the research and education missions; that is, NSF is contributing to the nation's human resource infrastructure through research support.

However, NSF is also moving to contribute to more effective partnership in research between Government, industry, and academia. This partnership is important to speed knowledge transfer from the basic research laboratory to application and commercial development, and maps well onto the strategic priorities of the AMPP. For example, some quantitative measures of performance have been proposed to exist in monitoring the effectiveness of NSF programs and activities, such as the number of interdisciplinary research projects, the number of industry–university collaborations, the number of centers and groups, and the number of Memoranda of Understanding or Cooperative Research Agreements with other Government agencies.

The number of interdisciplinary projects supported is a useful indicator because it is in keeping with the AMPP goal to bridge the gap between different disciplines. An increase in the number of industry–university collaborations might speed knowledge transfer between those research sectors. The very existence and purpose of a fair number of centers hinge on industry–university partnerships. Extending the partnership concept from industry–university to include Government research laboratories is important to get maximum return on investment from these national treasures of scientific talent; that step, too, is already underway. Such criteria are not substitutes for the old standbys of important results and education of tomorrow's students, but they may be viewed as value-added measures for some situations.

Within the Division of Chemistry, several initiatives to improve intersectoral cooperation have already been established. New in 1992 were (1) a cooperative program with the Electric Power Research Institute on electrochemical synthesis: joint review and joint funding; and (2) a coopera-

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tive program with the Council for Chemical Research (CCR) on environmentally benign chemical synthesis and processing. In this CCR–NSF activity, university-based research projects are required to have industrial intellectual partnership in order to speed knowledge transfer and to ensure applicability of the research to real-world problems. Other new and experimental ventures are likely to follow. Many of today's important fields of chemistry grew out of basic research carried out in the years after World War II to answer important practical questions. Those applications of chemistry to the real world made chemistry the central science that it is today. The AMPP will be an important force for renewing existing links between basic research and application and for building the new ones for chemistry's tomorrow.

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