Materials Science and Technology: Challenges for the Chemical Sciences in the 21st Century

Organizing Committee for the Workshop on Materials and Manufacturing, Committee on Challenges for the Chemical Sciences in the 21st Century, National Research Council

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CHALLENGES FOR THE CHEMICAL SCIENCES IN THE 21ST CENTURY

MATERIALS SCIENCE AND TECHNOLOGY

ORGANIZING COMMITTEE FOR THE WORKSHOP ON
MATERIALS AND MANUFACTURING

COMMITTEE ON CHALLENGES FOR THE CHEMICAL SCIENCES
IN THE 21ST CENTURY

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[1] Committee member until July 2001; subsequently the Board on Chemical Sciences and Technology (BCST) liaison to the committee in her role as BCST co-chair.

[2] Committee member until March 2002, following his retirement from DuPont.

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Preface

The Workshop on Materials and Manufacturing was held on June 13-15, 2001, in Washington, D.C. This workshop was the first in a series of six workshops that will make up the study Challenges for the Chemical Sciences in the 21st Century. The task for each of the workshops is defined as follows:

- Discovery: Identify major discoveries or advances in the chemical sciences during the last several decades.
- Interfaces: Identify the major discoveries and challenges at the interfaces between chemistry/chemical engineering and such areas as biology, environmental science, materials science, medicine, and physics.
- Challenges: Identify the grand challenges that exist in the chemical sciences.
- Infrastructure: Identify the issues and opportunities that exist in the chemical sciences to improve the infrastructure for research and education, and demonstrate the value of these activities to society.

The Workshop on Materials and Manufacturing brought together a diverse group of participants (Appendix D) from the chemical sciences who were briefed on a variety of issues related to the impact of and challenges for the chemical sciences as they relate to materials science and technology. These presentations served as a starting point for discussions and comments by the participants. The workshop participants were then divided into small groups who went into breakout sessions to develop these discussions further. Each group provided this feedback to the workshop as a whole.

This report is intended to reflect the concepts discussed and opinions expressed at the Workshop on Materials and Manufacturing. The report is not intended to be a comprehensive overview of all of the potential challenges that exist for the chemical sciences in the areas of materials science and technology. The organizing committee has used this input from workshop participants as a basis for the findings expressed in this report. However, sole responsibility for these findings rests with the organizing committee.

This study was conducted under the auspices of the National Research Council's Board on Chemical Sciences and Technology, with assistance provided by its staff. The committee acknowledges this support.

Klavs Jensen and Charlie Kresge, Co-chairs,
Organizing Committee for the Workshop on Materials and Manufacturing
Challenges for the Chemical Sciences in the 21st Century

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 (NRC's) Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making the 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 participation in the review of this report:

Robert Cava, Princeton University
Edwin Chandross, Bell Laboratories
Toby Chapman, University of Pittsburgh
Frank E. Karasz, University of Massachusetts
Lydia Sohn, Princeton University
Jack Solomon, Praxair Inc.
Joseph Wirth, GE Chemicals (retired)
Gregg A. Zank, Dow Corning Corporation

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 Dr. David C. Bonner, Cabot Corporation. 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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Executive Summary

CONTEXT AND OVERVIEW

Researchers in the chemical sciences synthesize and process materials by manipulating chemical reactions and physical transport. This ability to construct materials from molecular components, combined with the ability to manipulate materials for function, has blurred the line between chemistry and materials science. Similarly, as the chemical sciences have developed materials and devices to explore biological processes and used biologically inspired self-assembly to create materials from molecular building blocks, the boundaries with biochemistry and molecular biology have also been blurred. Advances in synthesis and processing of materials continue to have significant impact on emerging fields such as biotechnology, information technology, and nanotechnology.

Materials with tailored functionality (such as high strength, electronic, or optical properties) are critical to modern technologies. For example, high speed computer chips and solid state lasers are complex, three-dimensional composite materials built by organizing chemical entities with nanometer precision through the application of synthesis procedures. As advances on materials continue, chemical resolution on the nanometer scale will be required. As a result, better preparation of both new and existing materials is needed, along with preparations that are cost effective and have minimal environmental impact. Particularly in the field of nanotechnology, advances in synthetic techniques such as new vapor, liquid, and solid catalytic reactions will be needed. In addition, new self-assembly methods offer opportunities for “bottom up” synthesis of materials from their molecular constituents.

The ability of the chemical sciences to modify and predict molecular structures and the emerging understanding of self-assembly, promises a revolution in new materials with properties thus far only predicted by theory. Decisions about the development and implementation of new materials will ultimately be based on cost versus benefit for our society. A strong competitive advantage can be gained in materials development from an efficient iteration between molecular alterations of a chemical or material and the processes by which the chemical or material is "engineered" into the final product.

DISCOVERY

As new materials requirements become more complex, materials chemistry is increasingly turning toward the discovery of new materials and methodologies. Methodologies continue to take advantage of pure serendipity and trial and error approaches, but they are significantly enhanced by new approaches such as combinatorial synthesis, high-throughput screening, and molecular computations. In the past several decades, the chemical sciences have made large strides in the development of novel and useful materials. The development of thermoplastics and/or structural polymers has had an increasing influence on a range of applications, particularly in construction and national defense. New polymers have led to such devices as low current/low power polymer-based displays. Moreover, polymers for drug delivery and tissue engineering are beginning to benefit the biomedical field. Catalysis has been an especially fruitful area of research in the energy and transportation sector, with the catalytic converter being the ubiquitous example of novel catalysis benefiting society broadly through reduced air pollution. The development of metallocene catalysts is leading to high-strength polyethylene for multiple applications, ranging from grocery bags to light weight armor. Photoresist, a photochemically active polymer, has made it possible to define with nanometer accuracy the complex patterns that form the backbone of computer chip production. New advances are being made in organic-based electronics that might be useful in a variety of applications, including large-area displays, memories, sensors, and identification tags. Three-dimensional photonic crystals with complete photonic band gaps at optical telecommunication wavelengths are expected to result in revolutionary optically integrated photonic circuits for computers and telecommunication systems.

Materials chemistry is drawing on a wide range of means to develop new compounds and applications. Design by analogy is perhaps the most common method used to produce new materials. The development of new inorganic nanoscale materials by analogy with biological systems is just one example of this approach. Future materials technologies are going to require molecular structures of increasing complexity and precision composition that is greater than that possible today. Materials will have to be tailored from the molecular level to the macroscopic device in order to achieve the functionality required by advanced technological applications. Molecular self-assembly inspired by biological synthesis may hold the key to new routes useful to future technologies. Because most processes for synthesis by analogy presently remain imprecise, high-throughput methods of synthesis and analysis offer another promising alternative to conventional cycles of design, re-evaluation, and redesign. The rapid increase in computing power continues to have considerable impact on analytical and computational methods. Molecular simulations, previously limited by both computing power and accuracy, now enable scientists to understand and design complex systems at the molecular level. The development of new instrumentation is essential in both materials characterization and in exploring potential applications. For example, scanning probe microscopy has enabled greater understanding of materials at the nanoscale and has enabled materials of this size to become active components in functional devices.

The relative roles of "needs-driven" and "discovery-driven" research in materials science and engineering will always be an important consideration. While it may seem that "materials discovery" must lie in the latter area, there is considerable room for discovery in the fields of chemistry and chemical engineering on materials that have clear links to future technologies. The continued health of materials research will require fundamentally new insights into the behavior of materials (whether or not applications are identified at the outset) as well as developments driven by clearly articulated technological and market needs. Important research programs can mix these two kinds of objectives in many different ways, resulting in a broad spectrum of activities that is likely to lead to breakthroughs.

> **Finding: Materials discovery occurs via many routes. A diverse portfolio of interdisciplinary research efforts directed toward discovery of new materials systems is likely to produce significant advances in this field.**
>
> **Finding: Renewed and expanded emphasis on synthesis, catalysis, and processing methods will be essential to continuing advances in materials science and technology.**
>
> **Finding: Recent developments in combinatorial synthesis, high-throughput screening, and molecular-based computation of materials offer substantial promise as adjuncts or alternatives to more traditional programs of design, evaluation, and re-design.**

INTERFACES

Materials chemistry is interdisciplinary by nature. Cooperative efforts between materials chemistry and other disciplines have given rise to many of the synthetic materials introduced over the course of the twentieth century. Advances in new materials often result from work on a specific or perceived need in several different areas. As a result, materials chemistry is closely linked to materials science, physics, biology, medicine, along with many other fields. Work at the interfaces among these disciplines represents some of the most exciting and challenging areas of scientific inquiry today and raises expectations of significant technological impact in the future. Scientists and engineers of all backgrounds need to better understand the various disciplines—the language of each, how to work with each other, and how to fund and reward collaborative activities.

Work at the interface between materials chemistry and medicine over many decades has brought innumerable advances that we take for granted today. Materials that can be implanted into the body and remain for many years without adverse effects require understanding of the biological processes around the material and reactions that the material may undergo in the body once implanted. Collaborations at this interface have led to the development of special-purpose metal alloys and polymer coatings to prevent the body from rejecting prosthetic bone replacements. Materials chemistry has also had a significant impact on separations technologies such as hemodialyzers, blood oxygenators, intravenous filters, and diagnostic assays. Biocompatible polymeric materials have been developed for controlled delivery of drugs, proteins, and genes. Extensive work continues on new materials for medical diagnostics and particularly medical sensors. In the future, research in materials chemistry might include in situ drug production, cellular systems, and human integrated computing. It is certain that new sensors that take advantage of the latest developments in materials will be essential for health and national defense.

The role of chemistry is so embedded in structural materials that it is almost taken for granted. For example, the materials in modern cars and airplanes that make them safer, lighter, and more fuel efficient than their predecessors result from advances in materials synthesis and processing. Coatings on structural materials, whether to inhibit corrosion, protect, beautify, or serve some other purpose, are also the products of materials chemistry—as is the adhesion of these coatings to the base material. The identification of appropriate combinations of materials in a composite and optimization of processing conditions require a detailed understanding of the underlying chemical processes. In the future, structural materials will incorporate sensing, reporting, and even healing functions into the body of the material. Such "smart materials" will require integration of dissimilar materials, which can only be achieved through collaborations across the many disciplines involved.

Chemistry has had a tremendous role in developing the materials and processes forming the basis for advanced computing, information, and communications technologies. The modern chip fabrication facility is essentially a chemical factory in which simple molecular materials are transformed into complex three-dimensional composites with specific electronic functionality through the use of chemical processes such as photoresist, chemical vapor deposition, and plasma etching. Two exciting future directions are the migration of electronic and optical organic materials and realization of analogous control of light via photonic lattices such as what we have today in electronics. The development of photonic circuits and optical computing is yet another possible example of an area enabled by the chemical sciences that requires multidisciplinary approaches.

Dramatic progress will be required on many fronts, including materials chemistry, to achieve both improved quality of life and improved environmental quality. Life cycle engineering, the process of reducing excess waste throughout the production process, will require the development of environmentally benign materials as well as the development of sustainable processing and disposal methods. Materials chemistry will also continue to contribute to the safety of our food supply by the development of new packaging materials, which can be expected to incorporate sensors to indicate spoilage or unsafe storage conditions

Finding: Materials that are self-diagnosing, self-repairing, and are multifunctional would potentially be of great value in many applications.

Finding: Materials chemistry is basic to technological developments. Advances will require close interaction between scientists and engineers working in diverse fields.

CHALLENGES

Fundamental chemical research creates the infrastructure that enables technologies key to the health and well-being of our communities. Therefore, research must focus on future challenges and how solutions to those challenges will affect society as a whole. As the world's population continues to grow and the standard of living improves, environmental concerns in developing nations grow exponentially. In the drive to alleviate diminishing resources, a key challenge is to develop new technologies that enable affordable clean energy. Materials chemistry is already critical to the development of photovoltaics, solar cells, and fuel cells. The development of new recyclable and biodegradable materials will also become an important challenge as environmental concerns increase.

Another challenge is to use chemistry to create new materials utilizing the insights obtained by studying biological structures, by functionally integrating cells and bio-molecules into materials, for example. The results might include miniaturized, multifunctional biosensors and human-computer interfaces. We might also be able using living systems as a means to synthesize and process materials with intricate structures, such as the silicates made by marine species. Fundamental understanding will be necessary to control matter on all length scales (nano-, micro-, and macro-) as well as at all steps in the self-assembly processes. For any given application, knowledge of materials properties and function from the atomic scale to the macro-scale – 18 orders of magnitude in length and time scales is necessary.

Proper analysis of materials is essential in augmenting the field of materials science. The challenge is the development of instruments for high-resolution, three-dimensional, element-specific mapping that are non-destructive and provide real-time information on both hard and soft materials on multiple scales.

It is necessary to understand how technological advances and scientific breakthroughs relate to society in a global context. Technological developments must be increasingly efficient, considering issues such as the globalization of sourcing and manufacturing. Almost every technology that has been discussed or that can be envisioned is likely to have a direct impact on the future challenges facing mankind as a whole.

> **Finding: Advances in materials chemistry will be essential for simultaneously improving the standard of living and environmental quality.**
>
> **Finding: The design of tailor-made materials with defined performance attributes is a grand challenge.**
>
> **Finding: A grand challenge in materials chemistry is to create new materials utilizing the insights obtained by studying biological structures.**
>
> **Finding: New analysis techniques will be required to enable significant progress in materials chemistry.**

INFRASTRUCTURE

As research into new materials continues, it is important to recognize that today's problems represent a challenge to our current infrastructure. The benefits of a healthy infrastructure are numerous. A broader and more efficient research structure will serve to feed the competitive engine while developing new areas of research. Infrastructure also involves education at all levels. At the university level, it is important to note that fields of study are changing rapidly and that research in the chemical sciences, particularly on new materials, is becoming increasingly interdisciplinary. Providing students with the tools needed to learn about specific topics in other disciplines and to communicate effectively in these fields will be essential.

Effective investment in both instruments and maintenance, particularly in regional cooperation for instrument use, will help to limit redundancies in local research capabilities and ultimately may save money for the universities and businesses involved.

Basic research, applied research, development, and demonstration play a role at all levels in the development of new materials. If academic researchers develop an understanding of the needs for and applications of new materials in the marketplace, important problems are examined almost inevitably. If there is a tight feedback loop between discovery and the end user, research teams will be better able coordinate their efforts and see a higher rate of return on technology development.

Industry increasingly finds itself unable to support basic research. As a result, the health of the chemical sciences will depend largely on the basic molecular science done in universities and national labs. Great care must be exerted to ensure that truly novel, high-risk, yet high-quality works are supported at the federal level.

> **Finding: Instrumentation has always played an important role in materials research, and new tools for fabrication and analysis will continue to move the field forward.**

> **Finding: Chemical scientists are called upon increasingly to communicate with scientists in many other disciplines, and must learn to do so effectively.**

Introduction

Materials chemistry has contributed to the advancement of a number of technologies, including medicine and health, information and communication, national security and space, transportation, structural materials, arts and literature, textiles, personal hygiene, agriculture and food science, and the environment. The excitement of materials chemistry is amplified by its intimate connections with other disciplines and its impact on daily life. These interdisciplinary interactions between the chemical sciences and other fields in the development of new materials and their applications also require close interaction and clear communication between scientists working in diverse areas.

As the contribution of materials chemistry to other disciplines increases, it will become necessary for scientists of all backgrounds to better understand how to undertake collaborative activities with other disciplines. Although it is not feasible for scientists to master a vast body of scientific knowledge over many disciplines, scientists must gain the skills that will allow them to master specific topics.

The need for advanced materials becomes apparent when looking both at the contributions that this area of chemical research has already provided and at how advances in many areas of science are dependent on the development of new materials with increased capabilities.

The following report is a product of presentations and insightful discussions from a diverse group of scientists in the area of materials science and technologies. This report is not intended to be a comprehensive guide to either of these areas, but merely a reflection of challenges that were specified by the speakers and participants of the workshop.

1

Context and Overview

INTRODUCTION

Work in the chemical sciences on new materials offers many diverse opportunities; to detail all of them in a brief overview would be impossible. A few examples of technical challenges indicate the breadth of work in the chemical sciences on materials science and technology, particularly how these challenges relate to the need for interdisciplinary approaches between the chemical sciences and a number of other fields. These challenges should be viewed in a global, social context to perceive the full dimensions faced in meeting them.

TECHNICAL CHALLENGES

To define opportunities in the chemical sciences related to materials, it is necessary to determine where current scientific interest lies and what impact existing research and development has had on society. Three areas of great interest to the majority of scientists include bio-, information-, and nanotechnology. Although research in each of these fields has already offered great advances, remarkable opportunities remain for the discovery and application of new technologies.

Researchers in the chemical sciences form and manipulate materials at the atomic and molecular level. From this point of view, many modern materials are merely chemicals that have been "engineered" for use. Thus, for many materials, the differentiation between materials science and chemistry is blurred in a similar fashion to the manner in which chemistry and biology for many applications has become blurred (in the development of pharmaceuticals, for example).

Interfaces between the chemical sciences and other fields are always interesting, especially when these fields are experiencing explosive growth. Biology and information are two areas that interface with the chemical sciences, and should lead to exciting breakthroughs. Developments at the interface between engineered and nonbiological systems are anticipated in the long term. However, advances in the short term have been seen already. The broad goal of engineering the surfaces of materials to interface with biological systems, has led to breakthroughs such as the Dacron^{TM} heart patch, the heart valve, and the tricuspid valve. Other advances in this area include the use of materials for replacement joints and new fabrics for tissue growth, including artificial skin. All of these advances have led to significant improvements in the quality of life for many patients. In addition, these advances often reduce costs and environmental impact.

Advances in information technology center on smaller semiconductor features. These features are now approaching the molecular scale in size. Thus, exquisite control of materials properties is required to impact areas such as information storage technologies (Sidebar 1.1), consumer electronics (Sidebar 1.2), or quantum computing. To accomplish this requires better preparation of both new and existing materials. A multitude of materials will be needed for these applications.

For example, polymer synthesis is being applied in the drive to reduce feature size. Biopolymers and biomimetic polymers have several materials properties of interest. These materials have applications in the design and construction of nanoscale integrated circuits, laminated structural elements (smart sensor interiors in automobiles, planes, and trains), and in microsensors that can be embedded in persons or animals or placed on protective clothing.[1] (Advances in polymerization often rely on mimicking nature, increasing functionality, broadening particle size, and simplifying processes. The importance of this approach is reflected in the major effort at present in living free-radical polymerizations. See Sidebar 1.3).

Dielectric materials are used to insulate the microscopic wires between transistors on a chip. Materials with increasingly lower dielectric constants ($k < 2$) are needed to increase transmission for electronic devices that are becoming increasingly smaller and closer together. Polymer dielectrics have been an important advance for these applications. An important advance in the future may also be found using porous polymers.

Other opportunities exist in the area of nanotechnology. Carbon nanotubes

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[1] See, for example, J. Janata, M. Josowicz, P. Vanysek, and D. M. DeVaney. 1998. Chemical Sensors. Analytical Chemistry 70: 179R-208R. B.M. Paddle. 1996. Biosensors for Chemical and Biological Agents of Defence Interest. Biosensors and Bioelectronics 11: 1079-1113.

SIDEBAR 1.1
Information Storage Technology[a]

There is an apparently insatiable demand for increasing microelectronic performance and storage capacity. Storage capacity has doubled roughly every three to four months. However, in traditional magnetics technology, physical limitations of the bit size used for data storage are rapidly being reached. As a result, new technologies are necessary.

A novel project at IBM, the Millipede Project, addresses future ultra-high-density storage devices by using a thermal mechanical read-write strategy. This project uses an Atomic Force Microscope (AFM) based industrial-scientific-medical (ISM) band chip, which contains individual heated cantilevers (Figure 1.1). Contact of the heated cantilever tip with a thin polymer film produces a nanoscopic indentation or hole that can represent a bit of information (see Figure). Although potentially simple, if a single cantilever is used, an extremely slow read-write process results. Increased speed can be achieved by employing numerous AFM-ISM cantilevers in a highly parallel design, with each cantilever individually addressable. Using this technology, researchers have developed a 32 by 32 array of thermally heated AFM-ISM tips, yielding a total of 1,024 tips. Since each AFM-ISM tip operates independently, highly efficient and fast read-write operations can be achieved—hence the name Millipede.

A problem still remains, however, with the polymeric recording layer. A very thin film is required of which little is known about the behavior, stability of the nanometer-sized bits, and the underlying principles of the writing and erasing process. All of these fundamental materials questions are critically important since a useful operating device would require the ability to read and write repeatedly.

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[a] Craig J. Hawker, IBM, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

have received much attention due to their favorable electrical properties and strength. These materials may be thought of as rolled up sheets of graphite that can have different helical structures and can be singlewalled or multiwalled. It is difficult to predict the application of carbon nanotubes because of the current difficulty in reproducibly synthesizing and working with them. This may ultimately make silicon nanowires a more important technology. One area of particular difficulty is using nanotubes for electronic devices. Ideally, carbon nanotubes are unique, low-dimensional conductors with either metallic or semiconducting properties. In practice, however, these hollow cylinders have a strong tendency to agglomerate as they form, resulting in either large, multiwalled

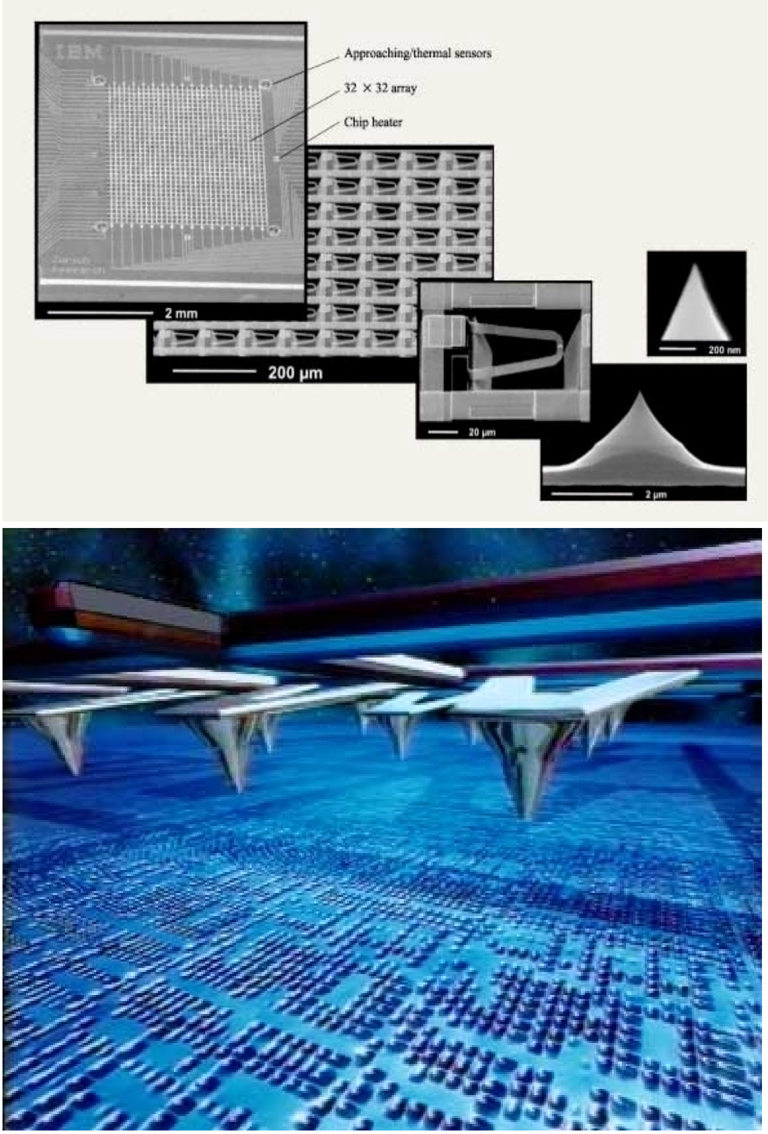

FIGURE 1.1 Contact of a heated cantilever tip with a thin polymer film to create a nanoscopic indentation. (Figure courtesy of IBM.)

SIDEBAR 1.2
Fundamental Technology Innovations: Replacement for the Barcode[a]

The barcode has become so ubiquitous in our consumer society that many overlook its impact. Since it came into common use roughly 20 years ago, the barcode has been added to such a large array of products that it is difficult to find an item that does not carry a code.

As useful as this system is, it does present some drawbacks. In a checkout line, the product barcodes are scanned serially. While this system is a vast improvement over manual entry of prices, it essentially still remains an advance of the earlier system. A fundamental change in the way items are purchased would be to eliminate this serial system at the end and replace it with a serial selection performed while the customer is shopping. With this system, the customer would simply select items that would then be tallied as he or she shopped. One possible innovation would be the development of a device that stores the information that is present on the barcode. This device could be powered externally through a small antenna. The actual circuit, which serves to store the barcode data, might have at least 10,000 transistors and a clock rate on the order of a kilohertz.

The true innovation would be in the nature of this device. The replacement for the barcode would contain no silicon and would operate using polymer-based organics. Production would be by printing rather than by photolithography, and the cost would be less than one cent per copy. The nature of this device and its mode of production would lead to its manufacture on a massive scale. Already, the production of transistors in the United States is on the order of 39 per second. Production of a printed organic polymer device would be expected to surpass this rate.

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[a] George M. Whitesides, Harvard University, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

nanotubes with many concentric carbon shells or bundles (ropes) of aligned singlewalled nanotubes. Both aggregates are complex composite conductors incorporating many weakly coupled nanotubes, each having a different electronic structure. This complexity remains the primary difficulty in both understanding and developing nanotube-based electronic devices.[2] Regardless, work on these

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[2] P.G. Collins, P. Avouris. 2001. Controlling the Electronic Properties of Carbon Nanotube Circuits. Ninth Foresight Conference on Molecular Nanotechnology. Santa Clara California.

SIDEBAR 1.3
Tailored Macromolecules and Nanoscopic Materials: Polymers and Free-Radical Processes[a]

Polymerization has traditionally been difficult to control. Living free-radical polymerization, which combines the best of traditional living polymerization and ionic chemistry, shows promise of changing this.[b] In living free-radical processes, a mediating radical sits at the end of a polymer chain. This chain is then activated by an external stimulus such as heat or the presence of a transition-metal catalyst. This can add a few monomer units. The mediator then returns and regenerates the dormant polymer chain. This process has increased the degree of polymerization by a limited number of monomer units, and the procedure can cycle, resulting in controlled growth of the polymer chain.

The mediator is absolutely critical. It is involved in every step of the polymerization. Its structure will determine to a great extent what polymerizations are possible. Using high-throughput methods, it is possible to screen many initiators of catalysts rapidly. The beauty of these systems is that they are compatible with a wide range of different monomers and functional groups. Therefore, polymer size can be controlled from very low molecular weights up to more than a hundred thousand. Polymer shape can also be controlled. Living free-radical polymerization is an elegant example of the transfer of organic chemistry to the polymer community.

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[a] Craig J. Hawker, IBM, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

[b] *Controlled/Living Radical Polymerization: Progress in ATRP, NMP, and RAFT,* Matyjaszewski, K., Ed.; American Chemical Society: Washington, D.C., 2000: Vol. 768.

types of materials requires new vapor, liquid, and solid catalytic reactions. These new classes of chemical reactions will open the door to fundamentally new kinds of materials.

The last 50 years have been described as the period of electronics, with the next 50 years expected to be the period of photonics. Information will travel and be stored using light (photons) rather than electrons. One of the major benefits in a change to photonics would be vastly increased bandwidth compared to electronic transmission. Bandwidth is the width of the range of frequencies that a signal occupies on a given transmission medium. Because the frequency of visible energy is so high (on the order of millions of megahertz), thousands or millions of signals can be impressed onto a single beam by means of frequency division multiplexing. In addition, a single strand of fiber can carry visible light at several different wavelengths, each beam having its own set of modulating signals. The opportunities in this area are simply enormous.

Just as semiconductors exclude electron propagation for certain energy bands and thus allow for the construction of circuits, photonic band gap materials—crystalline structures that exclude light transmission in all directions for specific wavelength ranges—are being developed in an attempt to build so-called circuits of light.[3] Photonic band gap materials are engineered three-dimensional diffraction gratings with interesting properties. An example would be a recently developed material with a negative index of refraction. This material is only a centimeter in length but operates in the centimeter radiation wavelength scale. Developing this amazing material to operate in the optical wavelength regime is an important challenge in the chemical sciences.

SOCIAL CONTEXT

It is necessary to understand how technological advances and scientific breakthroughs relate to society in a global context (i.e., what the rest of the world will be interested in as opposed to what will interest scientists). The development of most new technologies used to be in the hands of a few major world powers. This is no longer true. Scientists all over the world are working actively on technical innovations that affect citizens in their countries and beyond. For a country to compete in this global scientific marketplace, its technological developments must be increasingly efficient. Social factors are affected by, and determine the rate of technology adoption. For example, most of the information technology we have is still limited to the desktop. If that technology were put in a wristwatch or a cell phone, information access and portability would change dramatically.[4] Information technology would be even more powerful if interconnectivity were improved and portable devices were allowed to communicate with each other. Developments such as these raise interesting questions regarding the use of information stored in this manner.

Decisions about technology will often be made based on cost and benefit in our market-driven economy. One of the most important factors to consider is the

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[3] K. Busch, S. John. 1999. Liquid-Crystal Photonic-Band-Gap Materials: The Tunable Electromagnetic Vacuum. Physical Review Letters 83: 967-970.

[4] IBM Corp. has recently developed a prototype terabit memory that stores a trillion bits of data, or twenty times more than a current disk drive, in a square inch. IBM believes the Millipede device is a good match for mobile devices like cell phones, and that prototypes may lead to replacement chips that can plug into the same sockets as current flash memory chips, but with incredible storage capacity and only about 100 milliwatts power consumption. See http://www.eetimes.com/at/news/OEG20020611S0018.

impact of capitalism on innovation. Although innovation may arise directly from marketplace needs (i.e., information technology, health care, environmental needs), technological developments often will be driven by a cost calculation that requires a short time between commercialization and payback. The time from discovery to large-scale application of new materials can be very long (15 to 20 years). With the increasing ability to provide a valuable function by creating complex materials in which the juxtaposition of molecular components is carefully controlled (e.g., composites, semiconductor lasers), the role of chemistry in materials has moved from an analytical and bulk synthetic role to a more integrative approach of building the new material molecule by molecule or atom by atom. Much of the activity in what today is called nanotechnology reflects this change in perspective.

A strong competitive advantage in materials development (shortened development time, reduced cost, higher quality and functionality) can be gained if there is an efficient iteration between making molecular alterations in a chemical or material and the processes by which that chemical or material is “engineered” into the product. The greater the ability of the product development team members to appreciate and/or operate across a variety of scientific disciplines, the better the outcome will be. The education and training of the technical work force must include exposure to a spectrum of disciplines, if not actual hands-on experience in them.

Moore’s law (i.e., the observation that the number of transistors on a given piece of silicon would double every couple of years) is often quoted as a tribute to the innovations in materials and processing that have enabled the number of transistors in an integrated circuit to double every 18 months since about 1960. It is also quoted as the basis for predicting the limits of silicon technology in a few more generations. This development has led to exploration of new materials and clever device architecture and a push to create “molecular electronics” with even smaller critical dimensions. In turn, this has generated much work in the area of active organic electronic components and various assembly modes that avoid photolithography.

As a consequence of innovations in integrated circuitry, demand, and investment, the number of transistors produced is also rising exponentially (now 10^{18} per year). However, the total revenues have been rising at a much slower rate. In fact, the price per transistor has fallen from a dollar in 1960 to one millionth of a dollar in 2000. It is clear that it does not make sense to “go up against” silicon technology where silicon technology is adequate unless the functionality is substantially better (by a factor of 2 or greater) and the cost structure is much more attractive. No industrial firm will take a risk on new technology unless there is a major incentive. This does not mean that technologies such as organic transistors and nanoprinting should not be supported. This is work that can reveal new insights, molecular structures, or entirely new ways of molecular assembly and device construction. However, further development with targeted applications is likely to result in a significant return on investment.

Basic and applied materials science is not solely an outgrowth of ceramics, metallurgy, and automobile manufacturing, but instead is interdisciplinary. It combines chemistry, physics, biology, and other sciences. Breakthroughs in the development of new materials have repeatedly resulted through such interactions across disciplines. As new materials are developed in the future, attention must be paid to all of the sciences involved or opportunities will be missed.

Chemistry has a particular role to play in this effort. It has made major contributions to fields as diverse as agriculture, electronics, medicine, and environmental science, to name just a few. The fabrication of modern of device types such as microelectronics, photonics, designer drugs, and bioengineered species, involves chemical processing. In fact, an integrated circuit process or a printed wiring board process is really a chemical process.

One of the main characteristics of chemistry is that it involves small-scale manipulations of matter, atom by atom. The chemical sciences must continue to use this very basic characteristic to meet the needs and desires of science and society, which will result in limitless possibilities.

2

Discovery

INTRODUCTION

Development of new materials has followed a number of different pathways, depending on both the nature of the problem being pursued and the means of investigation. Breakthroughs in the discovery of new materials have ranged from pure serendipity, to trial-and-error approaches, to design by analogy to existing systems. These methodologies will remain important in the development of materials but as the challenges and requirements for new materials become more complex, the need to design and develop new materials from the molecular scale through the macroscopic final product will become increasingly important. The use of molecular modeling and the engineering of new materials into useable forms or devices are of particular importance.

BREAKTHROUGHS IN MATERIALS DEVELOPMENT

The chemical sciences have made great strides over the past several decades in the development of novel and useful materials. Although the following is not meant to be an exhaustive list of such breakthroughs, these examples point to the range of materials and their applications.

Polymers

Examples such as Teflon serve to show how the chemical sciences have contributed indispensable materials to everyday use. More recently, the development of thermoplastics and/or structural polymers has had an increasing influence on applications ranging from construction to national defense. New paints and coatings, clothing fibers, and photographic films have all benefited from the development of new materials.

There are newer polymeric materials whose commercial impact has yet to be realized. Work on semiconductive and conductive polymers have made great strides, but further work is necessary. Synthesis of amphiphilic dendritic block copolymers that are designed to form ultrathin organic films have also had major advances, but these materials also need further development. Other promising materials, from polymers for drug delivery to tissue engineering, have the potential to benefit the biomedical field but are still in a relatively early stage of development.

Catalysis

Advances in new materials for catalysis cover a wide range of applications. Zeolites and pillared clays have had a huge impact on the petroleum industry. New zeolites with specified properties continue to be developed with various utilities.

Ziegler-Natta catalysts allow the preparation of billions of pounds per year of organic polymers with controlled molecular structures and useful material properties. This method is also useful because it allows the synthesis of polymers that cannot be produced in a practical manner by any other method. Some examples of these are linear unbranched polyethylene and isotactic polypropylene.

In the energy and transportation sector, catalysis has been an especially fruitful area of research. As a result, supported gold catalysts have been developed. In addition, selective oxidation of carbon monoxide has been achieved and a gold-transition-metal oxide has been developed that provides very active NOx reduction as well as hydrocarbon oxidation. Perhaps no more ubiquitous an example of novel catalysis exists than the catalytic converter, which contains a porous ceramic coating embedded with palladium and rhodium. The platinum particles serve to complete the oxidation of hydrocarbons and carbon monoxide to carbon dioxide, while rhodium converts nitrogen oxides to nitrogen and oxygen.

Another important breakthrough in this field includes the development of metallocene catalysts, which are expected to revolutionize the polyethylene and polypropylene markets. The use of supramolecular organic templates containing appropriate surface functionalities to regulate the nucleation and growth of inorganic magnets, semiconductors, and catalysts is significant as well .

Electronics

This broad category has benefited from many breakthroughs in the development of new materials. Perhaps no recent advance has had a greater impact in this area than the creation of chemically amplified photoresist. Photoresist, resins containing photochemically active polymers, can be coated on a wafer and irradiated using photons (photolithography), electrons (electron-beam lithography), or X-rays (X-ray lithography). These developments have had considerable impact on computer chip production.

In the field of telecommunications, high-temperature superconductors and ceramic materials containing copper-oxide planes have potential uses in communications shielding. However, the commercial impact of these materials has yet to be demonstrated.

Instrumentation

The development of new instrumentation is essential both in characterizing materials and in exploring their potential applications. Scanning probe microscopes have enabled greater understanding of interfacial phenomena and are particularly important as work on new materials progresses on the nanoscale. Matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF), a mass spectrometry technique that uses laser light to ablate unfragmented polymer molecules mixed with an organic acid matrix into a time-of-flight mass spectrometer, is finding increasing application in the polymer community. Likewise, induction by coupled plasma mass spectroscopy has become a pervasive tool for analysis at materials interfaces.

METHODS OF DISCOVERY

As the areas and applications of materials discovery continue to expand, so too does methodology. The fields of materials chemistry and engineering are drawing on a wide range of resources to develop new compounds and applications.

Design by Analogy

Design by analogy is perhaps the most common method for producing new materials. As the range of available materials continues to grow and the community fully explores the behavior of existing materials, design by analogy will continue to be productive. Research into the development of new inorganic nanoscale materials by analogy with biological systems is just one example of this approach. For example, work in sensor design is progressing on “synthetic cells” that couple reactions much in the same way that living cells utilize metabolite channeling to localize reactions.

Chemistry and materials manufacturing technologies will be required to make structures of increasing complexity, hierarchically organized, and with a precision greater than what is possible today. Biological synthesis of such materials may hold the key to new routes that might be utilized for future technologies

(Sidebar 2.1). For example, the silica shell of a diatom illustrates the complexity of materials synthesis that biological systems can achieve.

Syntheses such as the silica shell of a diatom are remarkable in at least three respects. First, the precision with which the nanoscale structure of these biological materials is formed in many cases exceeds that of present human engineering. Second, the conditions under which these syntheses occur are very mild. These are physiological, low-temperature, ambient pressure processes occurring at neutral pH without the use of caustic chemicals. This is in marked contrast to human manufacturing of silica materials. Synthesis occurs on an enormously large scale, approaching gigatons of silica shells annually. Formation of these materials occurs at temperatures close to 0°C in the polar seas, indicating the presence of unique mechanisms of synthesis. The challenge for scientists is to identify these mechanisms in order to utilize their advantages.

Computer-Assisted Materials Design

A key goal in the development of any new material is to be able to design and construct materials with desirable and predictable properties. In order to meet this goal, researchers seek to design these new materials at the molecular and atomic level. Increasingly, this capability depends on materials design facilitated by computer modeling and simulation. The increase in supercomputing calculating power allows researchers to move design of materials properties from the macroscopic to the quantum-mechanical level.

It is possible to determine the properties of new materials by utilizing density functional theory. As computing power has increased, density functional theory—first postulated in the 1960s—has had an enormous impact on the design of new materials. Greater computing power combined with greater accuracy, now makes it possible to understand complex systems at the molecular level. For example, density functional theory combined with a self-consistent field theory for polymers has been applied to reveal new self-assemblies in which both particles and polymers organize into mesoscopically regular patterns. In particular, researchers have begun to delineate conditions in which polymer nanostructures can drive filler particles to self-assemble into nearly continuous nanowires.[1] Computer modeling will continue to have a large impact on both chemical synthesis and theoretical applications as computational power at the desktop level increases.

Combinatorial Synthesis and High-Throughput Screening

Since most processes for synthesis by analogy remain imprecise, high-throughput methods offer another promising alternative to conventional cycles of

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[1] David Jasnow, "Nanoengineered Materials: From Polymer Composites to Structured Adsorbents," NSF Partnership in Nanotechnology Conference, January 29-30, 2001, Arlington Virginia.

SIDEBAR 2.1
Nanostructured Biological Materials Reveal New Routes to Synthesis[a]

The mother-of-pearl of the abalone shell, composed of the microlaminate of nacre, is a high-performance composite with a fracture toughness 3,000 times greater than that of the mineral alone. While its structure is only about 1 percent protein by weight, these proteins are responsible for the control of the structure and thus its high performance.[b]

Studying this material presents significant challenges because to get the proteins it is necessary to literally pull biomolecules out of a rock (the limestone of the shell), usually with low yields. About 50 different proteins exist in the mineral composite of nacre. Some of these proteins lie between crystals, and many of them are occluded within crystals.

Extraction of occluded proteins from the calcite, which forms a primer layer, and the aragonite that grows upon it shows that these are different families of proteins. In reconstruction experiments *in vitro*, it was shown that the proteins determine both the nanostructures and the hierarchical organization of the two different mineral layers.

The key is to isolate enough of the protein to analyze part of its structure. Once this is accomplished, it becomes possible to clone the DNA that codes for the protein. The protein is then produced by genetic engineering with *E. coli* bacteria. With much more of the protein in hand, it is possible to study the mechanism of synthesis of the microlaminate.

The results from this approach led to a break from the paradigm that had governed the field for a number of years. The prevailing model was that a self-assembling organic template first serves as the surface upon which nucleation of the crystals takes place and that this process is simply repeated many times. Investigators learned that although such a process could make an artificial microlaminate, it does not produce the remarkable enhancement of fracture toughness found in the natural material.

Organization of the proteins and minerals forming the mother of pearl of the abalone shell in nature proceeds via multiple mechanisms operating to control structure and assembly, each working at a different length scale. These mechanisms operate contemporaneously. Small proteins interact with the growing crystals by specifically binding to certain step-edges or crystal faces. This determines polymorph selection, atomic lattice orientation, and morphology of the crystals. An unanticipated mechanism of molecular stenciling guides the growth of the crystals from one layer to the next to generate the microlaminate structure.

Research into the biosynthesis of these materials indicates that this process is quite complex, far beyond a simple linear synthesis. A genetic switch between one polymorph and the other governs one of the key steps. This switch turns off the synthesis of one family of proteins that

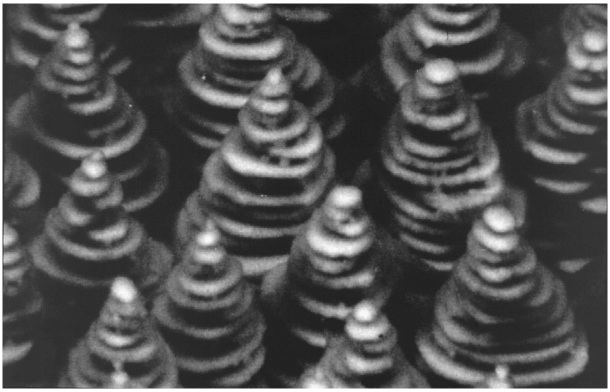

FIGURE 2.1 Crystal lattices of aragonite.

directs the synthesis of calcite and turns on the synthesis of a second family of proteins that synthesize aragonite. A very different and even more complex mechanism is responsible for the hierarchical organization of the crystal plates. The crystal lattices of aragonite grow in the form of tapered conical stacks of flat plates, resembling the tapered and layered shapes of pagodas (Figure 2.1). Atomic force microscopy revealed that each stack consists of a single crystal, even though protein sheets apparently separate the layers from which it is made. The underlying conclusion is that the protein sheets must be fenestrated, providing a path for communication and growth of the crystals through these sheets. Further work subsequently confirmed that there are nanopores in the protein sheets separating the crystal layers and that these act like molecular stencils. Because the pores are distributed randomly, the growth of the crystals from one layer to the next is randomly offset, which generates the interdigitation of the crystals that contributes to the remarkably enhanced fracture toughness.

Elucidation of these mechanisms relied extensively on the development of advanced instrumentation. Six different inventions that modified and improved the capabilities of atomic force scanning probe microscopy were required to successfully solve this system.

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[a] Daniel E. Morse, University of California, Santa Barbara, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

[b] For further details on this subject, see D.E. Morse, *et al., Nature 371*: 49-51, 1994; *Proc. Royal Soc. London, B 256*: 17-23, 1994; *Chem. Matrls. 8:* 679-690, 1996; *Nature. 381*: 56-58, 1996; *Acta Mater. 46*: 733-736, 1998; *Curr. Opin. Colloid Interface Sci. 3*: 55-62, 1998; *Chem. Mater. 9*: 1731-1740, 1997.

design, evaluation, and redesign. Work in the chemical sciences on the development of new materials is now integrating methodology developed in the pharmaceutical industry. Specifically, materials companies are beginning to use combinatorial synthesis in their research (Sidebar 2.2).

By creating large collections of chemically diverse materials, called libraries, and screening these libraries and materials simultaneously for desirable performance, enormous quantities of information regarding reaction conditions and potential target materials can be generated at a vastly accelerated pace. The challenges of implementing such methods include creating screens for target properties and developing software for interpretation of the data streams that emerge from high-throughput experimental programs.

Reaction scale is a further advantage of the combinatorial process. As opposed to traditional multi-gram reactors, combinatorial reactions can be performed at milligram concentrations. This enables large numbers of experiments to be performed with minimal use of reagents, lab space, and waste generation. This methodology does, however, require diversity of the substructure of reactants and a wide variety of synthetic routes. The importance of process conditions must be considered. In addition, an efficient automation screening and data storage analysis system must be in place.

SUMMARY AND FINDINGS

The roles of "needs-driven" and "discovery-driven" research on materials in the chemical sciences will always be an important consideration. Although it may seem that "materials discovery" must lie in the latter area by definition, there is considerable room in the fields of chemistry and chemical engineering for discovery of materials that have clear links to future technologies. The continued health of materials research will require fundamentally new insights into the behavior of condensed matter (whether or not applications are identified at the outset), as well as developments driven by clearly articulated technological and market needs. Important research programs can mix these two kinds of objectives in many different ways. This broad spectrum of activities is most likely to lead to breakthroughs.

> **Finding: Materials discovery occurs via many routes. A diverse portfolio of research efforts directed toward the discovery and development of new materials systems is likely to produce significant advances in the field. Renewed and expanded emphasis on synthesis, catalysis, and processing methods will be essential to continuing advances for new materials.**

The chemical sciences are distinguished by their emphasis on synthesis. Synthetic chemistry may claim a critical role in the development of new materials and in the creation of entirely new classes of materials. Realization of the technological impact of early advances also required skills in areas such as processing and analysis. Highly efficient and selective catalytic transformations are especially promising. As chemical synthesis of new materials proceeds into the twenty-first century, new methodologies will be adapted and incorporated into the complement of synthetic approaches.

As the chemical sciences begin to expand their use of high-throughput screening for the development of new materials, it is likely that researchers will look to the lessons learned in the pharmaceutical industry in the use of combinatorial synthesis. Discovery efforts must therefore encompass not only new products, but new processes as well.

> **Finding: Recent developments in parallel synthesis and high-throughput screening of materials offer substantial promise as adjuncts or alternatives to more traditional programs of design, evaluation, and redesign.**

Instrumentation has always played an important role in materials research. New tools for fabrication and analysis will continue to move the field forward. However, changes in instrumentation needs are to be expected, driven in part by increased emphasis on nanoscale science and engineering and partly by developments in neighboring fields such as microfluidics and robotics. The materials chemistry and chemical engineering community must position itself to contribute to these developments and to exploit such advances in the discovery and refinement of materials and materials systems. Continuing developments in areas such as scanning tunneling microscopy and atomic force microscopy are examples of instrumentation that will have an impact on nanotechnology research and development (see Sidebar 5.1 for others).

> **Finding: Exploitation of high-throughput experimental designs will require development of new instrumentation, new methods for analysis of high-volume data streams, and testing of key properties on very small amounts of material.**

SIDEBAR 2.2
Combinatorial Materials Synthesis: Homogeneous Catalysis[a]

A homogeneous catalyst consists of a metal center with stabilizing ancillary ligands, usually organic ligands, and a vacant coordination site at which the reaction takes place. Performance properties of the catalyst site can be varied dramatically depending on the choice of ligands, the choice of metal, the process conditions, the activation conditions, and the conditions under which the reaction is run. Within the field of polyolefin catalysis, it is currently not possible to predict which new metal-ligand combinations will lead to active catalyst classes and which will have low or no activity. Even for a well-studied catalyst, small changes in the ligand structure can have dramatic and unpredictable effects on catalyst performance. Olefin polymerization catalysts therefore represent good candidates for the application of high-throughput approaches.

An integrated high-throughput workflow for the discovery of new catalysts offers enormous advantages over conventional methods of catalyst discovery. A high-throughput screen can identify catalytically active systems rapidly and also identify and reject inactive systems, which is important. Additionally, the ability to generate sufficient quantities of meaningful catalyst performance data can provide comprehensive structure-property relationships. Conventionally, a Ph.D.-level researcher and a technician can only perform one experiment in the morning and one experiment in the afternoon. Using high-throughput methods, a primary screen can typically run a thousand polymerization experiments a day with four people to perform the screening. In the secondary screening, typically a hundred experiments are performed a day.

A high-throughput program to discover new polyolefin catalysts requires large numbers of ligands that express suitably diverse electronic and steric properties as well as efficient methods of attaching the ligand to the metal to form the catalyst candidates. Furthermore, efficient activation methods, suitable rapid screening techniques, efficient automation, and a data storage and analysis system are also required (see Figure 2.2). The number of experiments rapidly increases. For instance, consider the situation with 6,000 ligands in the ligand archive and 40 metal precursors. With five complexation routes, five activation conditions, and three process conditions, the number of experiments approaches 20 million!

The high-throughput workflow includes the design of libraries using custom-made computer software, automated delivery of metal precursors and ligands into the reactors using a liquid-handling robot, and a rapid primary screen that serves to assess the potential of each metal-

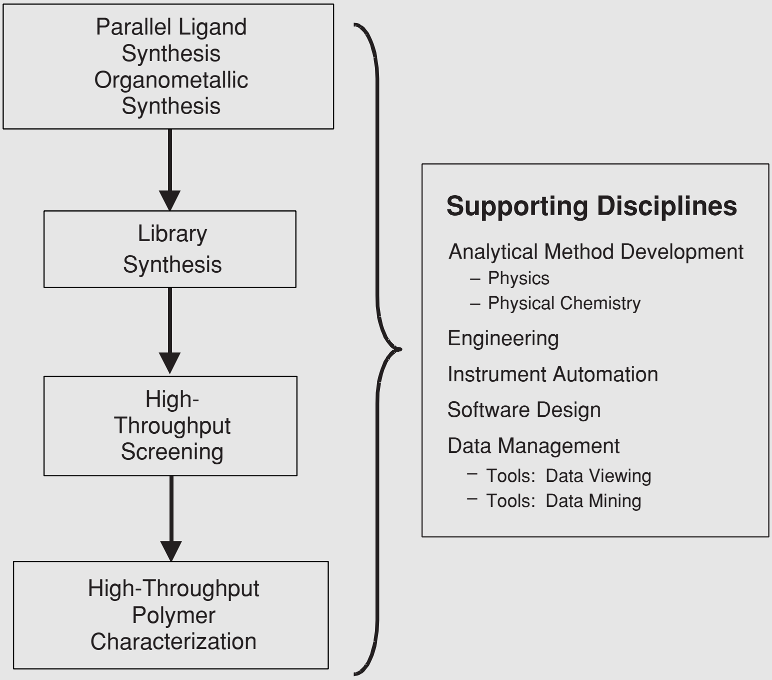

FIGURE 2.2 Workflow and supporting disciplines for a high-throughput polyolefin catalyst discovery program.

ligand-activator combination as an olefin polymerization catalyst. “Hits” from the primary screen are subjected to secondary screens using a 48-cell parallel polymerization reactor.

Individual polymerization reactions are monitored in real time under conditions that provide meaningful information about the performance capabilities of each catalyst. The primary and secondary screens are supported by rapid polymer characterization techniques and sophisticated data-handling software.

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[a] W. Henry Weinberg, Symyx Technologies, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

3

Interfaces

INTRODUCTION

Materials chemistry and engineering are interdisciplinary by nature, and have given rise to many of the synthetic materials that were commonly used over the course of the twentieth century. Advances in the development of new materials often result from work on a specific or perceived need in a host of different areas. As a result, materials chemistry and engineering is closely linked to physics, biology, medicine, metallurgy, ceramic engineering, along with many other fields. Work at the interfaces between these disciplines is some of the most exciting and challenging scientific inquiry today and raises expectations of significant technological impact in the years to come. This chapter provides some illustrative, but by no means exhaustive, examples of the impact of materials chemistry on different disciplines and endeavors, as well as some thoughts on areas in which future technological impact is likely.

MATERIALS CHEMISTRY AND MEDICINE

Many decades of work at the interface between materials chemistry and medicine has brought innumerable advances that are now taken for granted. Developing materials that can be implanted in the body and remain for many years without adverse effects requires understanding of the biological processes that occur around the material and reactions that may occur once implanted in the body, especially if they can have harmful consequences. For example, this type of detailed knowledge has led to the development of special-purpose metal alloys and polymer coatings to prevent the body from rejecting prosthetic bone replacements.

Many other new materials are also used in medical applications where they must adhere to bone, mimic color, flex like natural tissues, and/or keep their form under conditions of use. Today these implantable materials are largely passive and provide structural integrity, such as a hip replacement.

In addition to these implantable materials, materials chemistry and engineering has also had a significant impact on separations technologies used in medicine. Examples of these applications include hemodialyzers, blood oxygenators, leukofilters, intravenous filters, apheresis filters, and diagnostic assays.

One area in which the use of new materials for separations is particularly important is in the development of new biocatalysts. The development of low-cost bioseparations systems has been the focus of much work in the effort to make them competitive with classic organic and inorganic catalysts. Another example is the use of "PS Gel," a resin used to obtain high-purity blood serum. This material allows for more efficient and accurate clinical testing than is possible using conventional separation techniques.

Developments in materials chemistry and engineering have led to significant improvements in drug delivery systems. Biocompatible polymeric materials have been developed that allow for the controlled delivery of drugs, proteins, and genes. Copolymer networks are being developed that form a mesh-like structure and are potential delivery systems for drugs. By varying the monomers that make up these copolymers, it may be possible to tailor the dosage and time over which these drugs are delivered to the body.

Materials research in the biomedical field has included extensive work on new materials for medical diagnostics, particularly medical sensors. Strained-layer semiconductor superlattices allow scientists to tailor the electrical and optical properties to design materials and devices with targeted properties. These enable the development of new lasers with potential applications to medical diagnostics. Novel polymeric systems are also utilized in devices, instruments, or implants for medical diagnostics.

The interface between materials chemistry, engineering, biology, and medicine presents a number of challenges that must be overcome. One overarching issue is the integration of biocompatible materials into living systems. This includes areas such as bone scaffolding, artificial organs, and tissue engineering. Research on biocompatible materials will emphasize an active role in sensing and responding to stimuli in such areas as the development of neuroprostheses or synthetic muscles. Such functions are likely to be achieved only by highly heterogeneous materials. In the future, research in the chemical sciences related to materials may include such esoteric areas as in situ drug production, nanocellular systems, and human integrated computing. It is almost certain that as research in the biomedical field advances, better sensors that take advantage of the latest developments in new materials will be essential. Success in any of these areas will require detailed understanding of the interactions between the material and the human body, knowledge of the chemistry between the various constituents of the heterogeneous composite, and understanding of how to control the properties of the composite to produce the desired response.

STRUCTURAL MATERIALS

The role of chemistry is so embedded in structural materials that it is almost taken for granted. An example is in the differences in properties of iron and steel alloys. Materials in modern cars and airplanes, including polymers and polymer composites, make them safer, lighter, and more fuel-efficient than their predecessors as a result of advances in materials synthesis and processing. Progress in the development of structural materials takes many forms, including research, inexpensive production methods, fire resistant materials, materials that are easily recycled, and the incorporation of existing materials in new environments. In all of these areas, significant contributions have been made by chemistry and engineering.

Coatings on structural materials, whether to inhibit corrosion, protect, beautify, or serve some other purpose, are the products of all chemical sciences. So, too, is the science behind the adhesion of these coatings to the base material.

Over the past several decades, composite materials that typically involve the intricate mixing of different materials (metals, ceramics, and/or polymers) in a controlled manner, have come into use as structural materials due to their unusual combinations of properties—for example, immense strength or toughness and light weight. The identification of appropriate combinations of materials in a composite and the optimization of the processing conditions needed to give optimal properties require a detailed understanding of the chemical processes that govern the synthesis route.

In the future, structural materials will incorporate sensing, reporting, and even healing functions into the body of the material. A likely area of development to produce these materials will be multicomponent materials that combine properties of both plastics and ceramics. In addition, sensing materials almost certainly will require tailoring of material properties on a scale that has yet to be achieved for the large amounts of material required for most structural applications. Widely dissimilar materials may have to be controllably integrated, which is an area of research that is well within the domain of the chemical sciences.

INFORMATION TECHNOLOGY AND COMMUNICATIONS

The tremendous advances in computer, information, and communications technologies made over the last few decades have made profound changes in everyday life. The tremendous role that materials chemistry has had in enabling these changes is less obvious. The modern computer chip fabrication facility utilizes chemical processes in manufacturing. The deposition on and removal of material from silicon wafers during processing along with the control and measurement of impurities to incredibly low levels all require tremendous understanding of the many chemical processes involved.

The transmission of light through long stretches of optical fiber has historically been limited to two wavelength regions in the infrared spectrum. These two regions are separated by a region in which trace amounts of hydroxyl incorporated into the fiber during fabrication absorb light and prevent its long-distance transmission. Recent advances in controlling the chemical processes at work during fiber fabrication have reduced the amount of hydroxyl in the fiber to the point where long-distance transmission of these formerly unavailable wavelengths of light is now possible. This is a boon to multiplex technology, which uses many closely spaced wavelengths and requires high-quality fiber with properties that are substantially independent of wavelength.

Two exciting future directions in information technology and communications will rely heavily on materials chemistry for success. The first of these is the migration of electronic and optical functions that historically have been performed in inorganic materials (e.g., semiconductors, silica-based fibers) to newly developing organic materials. Prototypes utilizing organic semiconductors in applications such as electronic paper are favorable indications that these materials may have a significant commercial application (Sidebar 3.1).

The second direction is in the development of the control of photons via photonic lattices analogous to that for electrons and holes (Sidebar 3.2). This requires control of materials structure at the length scale of the wavelength of the light to be controlled.

NATIONAL SECURITY

One of the areas of particular concern in national security is the aging and reliability of materials found in systems ranging from weapons to air, land, and sea transportation or combat vehicles. As these various components of our national security apparatus remain in service long beyond their original design life, concern increases about subtle changes in their chemical and structural nature. In order to understand these changes and their implications, it is critical to have the analytical tools and chemical knowledge that allow us to understand the chemical reactions that take place under realistic service conditions. This knowledge in turn gives confidence in the integrity of the system and allows predictive determination of when component replacement or retirement is needed. Future directions may include the development of materials or material systems that report their condition or even repair themselves. Such developments will require the tailoring of materials on a molecular scale.

ENVIRONMENT

Achieving improved quality of life and achieving improved environmental

SIDEBAR 3.1

Organic Materials Synthesis: Inspiration and Driver of Organic Semiconductor Devices[a]

Organic semiconductor development is a highly multidisciplinary effort, encompassing specialists ranging from synthetic chemists to electrical engineers. A main driving force for studying organic-based electronic devices is the potential lower fabrication cost compared to silicon. Organic transistors might be useful in a variety of applications, including large-area displays, memories, sensors, and identification tags, where the low cost is of paramount importance.[b] Other potential applications are less cost-driven. For example, the use of organic materials increases the opportunity to integrate an electronic device covalently with molecules or biomolecules. Organic materials require only moderate temperatures during processing. This allows the use of applications integrating components or materials of limited thermal stability. Organic materials also enable the production of semiconducting devices on flexible substrates or in nonconventional or nonplanar geometries.

An organic semiconductor film, which generally consists of a crystalline film of conjugated aromatic monomers, oligomers, or polymers (Figure 3.1), can be incorporated into a field-effect transistor, a device that enables charge to flow across a channel in a controlled manner. An applied voltage controls the amount of charge that can travel through this channel and can turn the charge flow on or off. Optimizing the mobility—the speed with which a charge will move in a given electric field—of this semiconductor material is one way to enhance the performance of this kind of device.

In order to control the properties (on-off ratio, mobility) and hence the function of organic semiconducting devices, the properties of the films formed by the organic molecules must be controlled. Molecular design and synthesis have played vital roles in the emergence of this technology. A variety of aromatic ring systems and sequences of aromatic rings have been used as the active cores of semiconducting film-forming molecules. Furthermore, an almost limitless array of side chains distinguished by length or functionality can be appended to these cores. The figure below presents some representative examples of organic semiconductor molecular structures. Self-assembly properties, charge carrier energy levels, and environmental robustness are some of the properties that can be optimized through variation of the molecular structure.

There are many other aspects to the chemistry of organic semiconductors. The film's substrate can be modified to ease deposition, minimize current leakage, and even provide additional function such as charge storage. The film formation process must be controlled in order to obtain morphologies that allow a charge to be transferred easily among

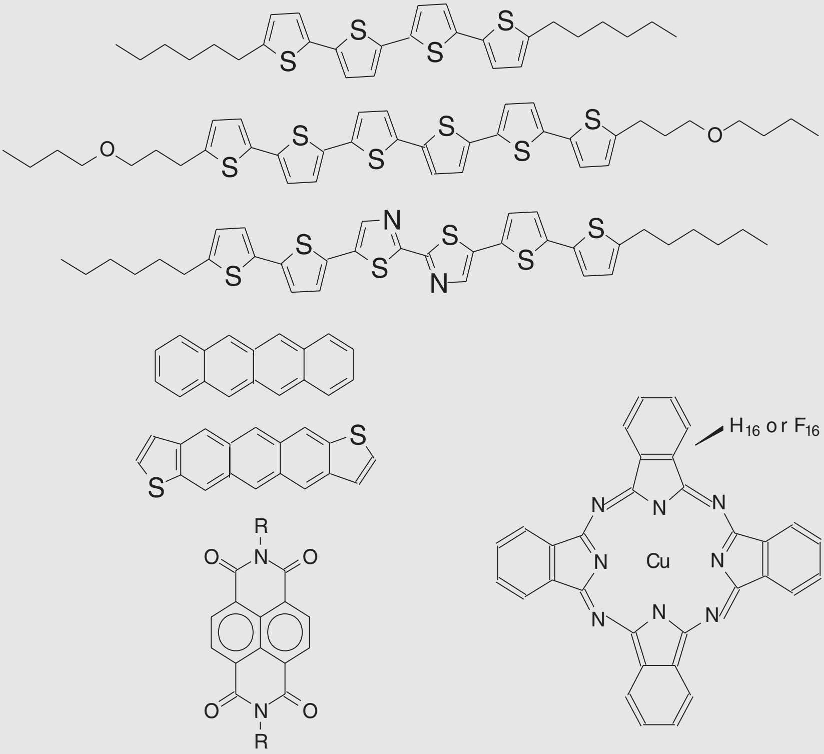

FIGURE 3.1 Examples of organic semiconductor molecular structures.

neighboring molecules and current flow to be continuous from one end of the device to another. Our present understanding of the film assembly process is minimal, and much opportunity remains for studying the process dynamics and molecular tuning.

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[a] Howard Katz, Lucent Technologies, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

[b] Z. Bao, "Organic and Polymeric Materials for Thin Film Transistor Applications," in B. Hsieh, Y. Wei, M. E. Galvin, Eds., *Semiconducting Polymers*, American Chemical Society, Washington, D.C., 1999.

SIDEBAR 3.2
The Race for the Photonic Chip[a]

Three-dimensional photonic crystals (PCs) with complete photonic band gaps at optical telecommunication wavelengths have generated much interest in the last few years (Figure 3.2). Devices founded on this new class of materials have the potential to revolutionize future photonic technologies. This kind of research may pave the way to future information technologies based on optically integrated, highly compact microphotonic crystal devices, chips, computers, and telecommunication systems.[b]

One approach to moving these synthetic three-dimensional Si-PCs to envisioned photonic technologies hinges on the ability to conduct wafer-scale patterning of single-crystal silica colloidal crystal templates called opal-patterned chips. These templates enable the chemical replication and coupling of photonic crystal lattices—inverse opals—in high-refractive-index semiconductors such as silicon and germanium, to optical waveguides to create photonic crystal devices. In this context, recent and exciting research involves the discovery of the opal-patterned chip. The chip is composed of single-crystal micron-scale features of silica colloidal—opals—that have controlled thickness, area, topography, and orientation and are embedded within an oriented single-crystal silicon wafer. Production of this chip is a straightforward, rapid, and reproducible chemical procedure that is easy to integrate into existing chip fabrication facilities, which makes it amenable to mass production.

Opal-patterned chips may provide an enabling technology for engineering photonic crystal lattices, photonic band structures, designed functional defects, and internal light sources in three-dimensional PCs that have complete photonic band gaps operating around 1.5 micrometers.

quality are inherently in conflict in current society. In order to reach both goals simultaneously, dramatic progress will be required on many fronts, including materials chemistry. Catalytic conversion, which allows the conversion of environmentally harmful chemicals in exhaust streams to relatively benign ones, has already had a dramatic impact on local environmental quality while enabling us to increase our reliance on internal combustion engines. Life-cycle engineering, in which the waste stream is minimized from the production of an initial material to the eventual reclamation and recycling of the product, is becoming widespread in Europe and is attracting increased interest throughout the world. Putting this concept into practice requires materials chemistry at every step. This involves the selection and design of environmentally benign materials, the development of environmentally friendly materials processing methods, and the disassembly of materials into new products or harmless waste.

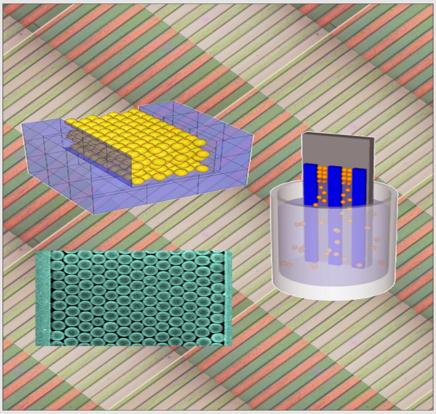

FIGURE 3.2 Three-dimensional photonic crystals.

These advances in three-dimensional photonic crystals, if reduced to practice, could pave the way to an amalgamation of microphotonic crystal devices with optical waveguides on chips for future optically integrated photonic circuits, computer, and telecommunication systems.

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[a] Geoffrey A. Ozin, University of Toronto, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

[b] Y.S. Ming, and G.A. Ozin, "The Race for the Photonic Chip, Opal-Patterned Chips", Adv. Funct. Mater., 11:1-10, 2001.

AGRICULTURE AND FOOD SERVICES

The current productivity of our agricultural enterprise would not be possible without the developments in fertilization, pesticides, and herbicides made by the chemical sciences. The unprecedented safety of our food supply is largely due to refrigeration (enabled by Freon© and its more environmentally benign successors), clean food-processing conditions, and the development of new generations of packaging materials and technologies. Future developments may include the incorporation of sensors into packaging materials to indicate spoilage or unsafe storage conditions. Developing materials for such sensors and integrating them into packages, will involve the tailoring of materials at the molecular level to achieve the desired combination(s) of properties.

ART AND LITERATURE

Works of art and literature are usually designed to endure for generations if not millennia. Unfortunately, chemical changes in the paper, paint, canvas, film, or stone over the centuries damaged some works. The chemical sciences have contributed to art and literature by allowing the stabilization or restoration of great works of the past. Chemistry has also contributed to the formulation of archival quality supplies for these "traditional" media. The variety of media available is exploding with the growth of electronic and optical media and communication. One new medium is the flat-panel display, which is becoming ubiquitous in the home, workplace, and even outdoors as its cost drops. Liquid crystals, the materials at the heart of many of these displays, are the creation of materials chemists. The molecules in a liquid crystal display tend to align with neighboring molecules even though they are in a liquid state and do not have the long-range translational order of a solid. The chemical sciences are an integral part of the search for the electronic, optical, and/or magnetic archival media of the future.

SUMMARY AND FINDINGS

The nature of the interaction between chemistry and other sciences is driven by the nature of the problem. For example, the problem of developing protein templates draws on the ability of chemists to perform complex syntheses on many different scales. The chemical sciences have had significant impact on advances at the scientific interface, including research into the superparamagnetic effect that has led to a higher storage density as well as advances in micro- and nanofabrication that have enabled the development of new materials.

Finding: Self-diagnosing, self-repairing, multifunctional materials would be of great value for applications in structural components, military equipment, and materials integrated into living systems.

Finding: Progress in materials chemistry faces a series of scientific and technical challenges. These include understanding interfacial science related to materials, multiscale modeling and prediction, and controlled synthesis and controlled assembly.

However, these challenges also show opportunities where skills and expertise could be developed, and where education can be made available for those entering the field.

As the examples in this chapter show, materials chemistry is a central part of many technologies that we take for granted. It will also play a critical role in developments that are poised to improve our lives in the not-too-distant future.

4

Challenges

INTRODUCTION

The chemical sciences provide the underpinnings for most, if not all advanced technologies that we use today. Fundamental chemical sciences research creates the infrastructure that supports technologies that are key to the health and well-being of our communities. Just as our current research efforts are built on the knowledge gained by our predecessors, tomorrow's innovations will be based on today's research. (Sidebar 4.1).

MAJOR RESEARCH CHALLENGES

Fundamental chemical science research efforts can be linked to several areas that can immediately be seen to impact each individual, namely, water, energy, food, and air. Coupled to these necessities, development of chemistry to address environmental concerns is a significant grand challenge. As the standard of living improves worldwide, environmental concerns in developing nations grow proportionately. Chemistry could provide the means to decouple environmental impacts from this growth in the standard of living. Examples of areas in which the chemical sciences research can play a role include the following:

- Allocation of diminishing resources
- Remediation of existing environmental problems
- Finding or developing replacements for strategic materials
- Decentralization of power supplies

SIDEBAR 4.1
Turning Lead into Gold[a]

The dream of making valuable things from cheap ones dates back thousands of years and has lost none of its appeal in modern times. Many important advances in modern materials science can be described in such terms, and many can be traced to new methods of chemical synthesis and new methods of catalyzing chemical change. A half-century ago, Karl Ziegler in Germany discovered a Ti/Al catalyst and Giulio Natta in Italy found that it could convert cheap, gaseous ethylene or propylene into valuable solid materials that are now made in quantities of billions of pounds per year. More recently, revolutionary advances in transition metal chemistry have made the olefin metathesis reaction—previously unpredictable and difficult to control—an important route to valuable polymers and specialty chemicals. New developments in controlled free-radical chemistry are providing new routes to specialty polymers, with commercial impact just a few years away. In all of these examples, the ability of chemists to devise new catalysts has been essential.

Biocatalysis—especially catalysis by protein enzymes—has long been a special source of inspiration for chemists, since living systems routinely accomplish difficult chemical reactions under the mildest of conditions. An especially exciting recent development is the possibility of engineering these systems to perform reactions that do not occur naturally. Chemists are already developing synthetic schemes that exploit the power and selectivity of natural enzymes, but result in materials that could never be obtained in a direct means from nature.

One of the most appealing aspects of using biocatalysis is the prospect of making materials that are not only tough and durable, but also carry information. We're already good at the first part—we can make bulletproof vests—but we're a long way from encoding the human ge-

For instance, research in the chemical sciences is critical to the development of new materials technologies that might enable affordable clean energy. This could be accomplished through the design and development of a high-capacity reversible energy storage medium or the identification and development of alternative energy sources. Chemistry is unquestionably critical to the development of photovoltaics and hydrogen-based fuel cells. In the area of nuclear energy, it is also chemistry that must lead in the design of new processes for improved handling of nuclear wastes.

Another issue related to the environment is the development and implementation of sustainable routes to materials and the development of new recyclable and biodegradable materials. In addition, the concepts of energy and materials nome into a piece of plastic. Macromolecular systems (systems that consist of long molecular chains) have the capacity to carry information at very high density and to read information in and back out. DNA works by encoding information in the sequence of its monomeric building blocks. An important challenge for chemistry is to devise synthetic materials systems that can carry information at high density. Exciting progress has been made in recent years in devising molecular systems that can serve as switches and thereby move us toward information storage at the molecular level. There's a long way to go before this approach will be practical, but the early signs are encouraging.

Still another way to create valuable materials systems from inexpensive building blocks is to "teach" them how to sense their environment and respond to it in some useful fashion. Such systems are often described as "smart" materials (a term that by analogy would make the information-laden systems discussed above into "educated" materials). In a recent development of this kind, an inexpensive epoxy matrix was engineered to carry microcapsules filled with a healing agent.[b] As a crack propagates through the matrix, the microcapsules open and mix the healing agent with a catalyst, causing rapid polymerization in the crack. Materials of this kind regain most of their initial toughness, without any "active" repair, following fracture. Such "self-healing" materials might add greatly to the safety of transportation and other systems that are subject to catastrophic materials failure.

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[a] David A. Tirrell, California Institute of Technology, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

[b] S. R. White, N. R. Sottos; P. H. Geubelle; J. S. Moore; M. R. Kessler; S. R. Sriram; E. N. Brown; S. Viswanathan. Nature 409:794–797, 2001.

efficiency must be pervasive. The use of toxic materials and the emission of harmful materials must be minimized to the greatest extent possible.

The efficient use of limited natural resources must be maximized. It is only through the application of fundamental principles and insights of the chemical sciences that environmentally benign materials and applicable manufacturing process technologies can be developed.

A major research challenge in materials chemistry is to create new materials utilizing the insights obtained by studying biological structures. Could cells and biomolecules be functionally integrated into materials? As a first step, we must understand how to both spatially and temporally control chemical systems. We are just beginning to understand how molecules self-assemble on short-length scales. This understanding must be extended to appreciate how to design molecules and facilitate self-assembly on a macroscopic scale. Such spatial and temporal control of chemical systems might enable one to envisage and build a multifunction sensor in just one step.

The concept of self-assembly could be broadly looked at as the seamless manipulation of matter and information from molecular to macro scales through understanding of interconnects, synthesis, and dynamics. There must be understanding of interconnection issues between materials at all length scales coupled with understanding of how materials properties change in the transition from the nano- to the micro- and the macroscales. These transitions must be modeled to provide understanding and facilitate materials design from the molecular level up. To control matter at all length scales, there must be fundamental understanding of all steps in the self-assembly processes. This includes the mechanisms for self-assembly and crystallization, non-equilibrium steps or structures, protein folding, and how to control macromolecules.

Although the importance of self-assembly processes to biological systems is generally understood, their impact on advanced technologies such as electronics and communications is likely to be equally significant. Active and passive photonic materials are the cornerstones of the telecommunications infrastructure. For any given application, the goal is to design and build the desired material through fundamental knowledge of materials properties and function from the atomic scale through the macroscale. Such understanding and control requires the development of requisite process control methodologies and the ability to predict materials properties from the nano- to the macroscale. Molecular-level structure or property process control is an absolute requirement. Even the smallest defects and impurities must be identified. Developing a tool for high-resolution, three-dimensional element-specific mapping that is nondestructive and provides real-time information on both crystalline and noncrystalline materials on multiple length scales would be a worthwhile research challenge. In the area of analysis, diagnostic tools that allow for in situ process control are critical for future materials manufacturing.

Having the design and synthesis methodologies in place along with advanced analytical capabilities allows the next question to be addressed, namely, what should be made. The answer requires accurate design of materials with a road map of how to make them, not only on a laboratory scale, but more importantly on the manufacturing scale. On some level, the latter will be driven by cost, but through theory and modeling come an understanding of structure (at all length scales) and concomitant ability to develop affordable materials for a given technology application. Figure 4.1 schematically shows the interplay between each of the above components.

As we move further into the twenty-first century, many of the most exciting developments are occurring at the interfaces between disciplines. Ever more frequently, chemical scientists and engineers work with biologists, physicists, elec-

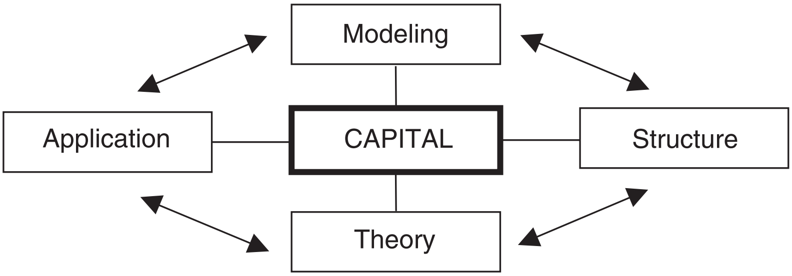

FIGURE 4.1 The interplay of competing interests in the design of new materials.

trical or mechanical engineers, device engineers, and/or computer scientists to address significant scientific and technological challenges. It is these interchanges that will create new opportunities in the chemical sciences.

Significant research efforts focus on improving the health and well-being of our society. Much of the ongoing biomaterials research is aimed at restoration and enhancement of the function of living materials. Such efforts encompass not only work aimed at restoring lost organ function and expression of the human genome but also the development of miniaturized, multifunctional biosensors and human-computer interfaces. Researchers, while maintaining their own specific expertise, must increasingly be trained to work in multidisciplinary environments. New device concepts require precise design of materials at the molecular level as well as fabrication processes that allow for complete control of structure and defects. For biosystems, understanding of biological function and how materials designs will either influence or be influenced by the environment is critical.

Although only a few examples of multidisciplinary research problems have been presented, each of these relates to high-performance materials developed for specific functionalities. (For example, see Siedebar 4.2.) A design methodology that effects ease of processing and scaling must be developed. Conceivably, such materials will also be bio-inspired.

Additional interfaces that will create challenges for the chemical scientist, relate to the development of analytical or characterization methodologies. Some examples are the detection of hydrogen in metal or local analysis of materials; identifying and understanding the effects of "impurities" in alloys and metals; and developing accelerated test methods. Are all critical to the development of advanced materials technologies and manufacturing methodologies. The ability to visualize nanoscale interactions between chemical systems could greatly advance miniaturization of devices, whether electronic, photonic, catalytic, or biologically compatible. The ability to visualize or characterize nanoscale interactions could in turn lead to the development of principles and theory for the self-assembly of materials and thus ultimately allow the truly rational design of materials with defined functionality.

SUMMARY AND FINDINGS

Finding: Advances in materials chemistry will be essential to improving our standard of living while also improving environmental quality.

Almost every materials- and chemistry-related issue and technology that has been discussed or can be envisioned is likely to have a direct impact on environmental challenges. As a result, environmental concerns must remain at the center of developing new materials and manufacturing technologies. New materials technologies are also needed to enable affordable clean energy, such as energy storage media, and materials to enable the use of alternative energy sources.

Finding: Major research challenges for the chemical sciences include the design of tailor-made materials with defined performance attributes, such as synthetic materials systems that can carry information at high density, utilizing the insights obtained by studying biological structure to design and make new materials.

To achieve complete control of material properties, knowledge of the processes that affect spatial and temporal control of chemistry is required. Resources are needed to explore self-assembly processes that could lead to the seamless manipulation of matter and information from the molecular through the macromolecular scale. For example, high-density information systems may be devised using DNA encoding as a model, where information is built up on the macromolecular scale through monomeric building blocks (Sidebar 4.2). Interconnection issues between materials at all length scales must be understood, and this understanding must be coupled to an understanding of how materials properties change in the transition from nano- to micro- to macroscales.

The acquisition of biomimetic approaches to materials design and synthesis will both lead to an understanding of natural processes and provide insight into value-added ways to design materials with new functionalities and enhanced performance. In effect, a “tool box” is required that will provide understanding and facilitate materials design from the molecular level up, where that design will be for an intended technology application.

Finding: New analysis techniques will be required to enable significant progress in materials chemistry.

Methodologies are required to visualize nanoscale interactions between chemical systems; these could greatly advance the miniaturization of devices—whether those devices are photonic, electronic, catalytic, or biologically compatible. This ability could in turn lead to the development of a set of principles and theory for self-assembly of materials and thus ultimately allow truly rational design and manufacture of materials with defined functionality.

SIDEBAR 4.2
Materials Needs for Defense and Energy[a]

In responding to the needs of both the Department of Defense (DoD) and the Department of Energy (DOE), researchers are often called upon to develop new materials and novel applications for existing materials. Materials needs for DoD consist of structural materials, materials for energy and power, electronic and photonic materials, and functional organic as well as biological materials. All of the services desire complete defense systems based on materials that require less maintenance. In order to develop these materials to meet long-term DoD needs, a wide range of scientific advances will be necessary.

Meanwhile, DOE has sought breakthroughs in materials research to address issues related to its missions—the stewardship of an aging arsenal of nuclear weapons, nonproliferation of weapons of mass destruction, and issues related to the supply and management of energy.

While a new material or process may be very promising in the laboratory it may be completely inappropriate for mission needs because it is not manufacturable. Materials and process scientists must ensure that production of the material or component can be scaled to a level appropriate for its end use. Yield must be high and defect density low, so there is little or no waste or inefficiency. The end product must be able to be inspected and characterized either through rigorous process-based quality approaches or via more standard inspection. The product must also be manufacturable at an acceptable cost.

As the demand grows for increased functionality at lower volume, weight, and cost, the need to understand and develop new materials on the molecular scale will increase. Strategies must be developed to incorporate nanomaterials into structures, to use self-assembly to build structures with order on multiple length scales, and to develop nanotechnology into a manufacturable technology.

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[a] Nancy B. Jackson, Sandia National Laboratories, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

5

Infrastructure

INTRODUCTION

As research into new materials continues, it is important to recognize that today's problems represent a challenge to our current infrastructure. Infrastructure involves far more than the identification of research priorities followed by targeted funding. Several key issues can be noted. A combined approach to research that addresses most or all of these issues will likely help to ensure a healthy infrastructure:

- Integration of research and teaching
- Broadened participation of underrepresented groups
- Improved infrastructure for research and education
- Demonstrated value of research to society
- Return on investment
- Correlation between investment and economic progress
- Feedback between the chemical industry and university research
- The effects of university research on industrial competitiveness, maintaining a technical workforce, and developing new industrial growth

Although all of these factors are not addressed in detail here, it is clear that all of them relate to how research breakthroughs can be transitioned to the "real world" and how the positive impact of these developments can be assessed and improved.

INFRASTRUCTURE ISSUES: UNIVERSITY RESEARCH AND TEACHING

Problems in understanding issues related to science often involve the public at large. It is therefore in the best interest of all scientists to ensure that further outreach to these audiences is made to inform the public of the problems, opportunities, and challenges that effect the scientific community. At the university level, it is important to note that fields of study are changing rapidly. As noted earlier, research on materials and the chemical sciences in general is becoming increasingly interdisciplinary. Important problems addressed by researchers in the chemical sciences are no longer strictly limited to physical chemistry or organic synthesis. In 1995, *Chemical and Engineering News* identified "emerging or growing technologies expected to affect chemistry, the need for chemists, and the way that chemists work. The broad areas identified are biotechnology, environmental chemistry, catalysis, materials science (including polymers, electronics, and photonics), information (including communication, computer technology, and computer molecular modeling) and energy." As new challenges in the chemical sciences arise, the ability of chemists and chemical engineers to overcome barriers in communicating with scientists in a host of other disciplines will become more important.

Although it is essential that future chemists and chemical engineers be conversant in other scientific disciplines, it is not feasible for students to master a vast body of scientific knowledge over many disciplines. Providing students with the tools needed to learn about specific topics in other disciplines and to communicate in areas outside their discipline is, however, not only useful but also essential. Such real-world skills as public speaking, effective writing, and teamwork through activities such as teaching, mentoring, or leadership programs can provide students the necessary means to quickly adapt and converse in a scientific field outside their degree discipline.

Education at the undergraduate and graduate university level as well as in the classroom and the research laboratory must reflect the changing nature of scientific advances. Research at the university level will have to be increasingly interdisciplinary if it is to reflect trends in the chemical sciences.

University Instrumentation Facilities

There are distinct advantages to having an instrumentation facility with an effective investment in both instruments and maintenance (Sidebar 5.1). With experts on-site, it is possible to train students, faculty, and others to operate and interpret results. It is of particular importance to have an on-site expert to confer with when an unusual experimental result is found. Small facilities—those with capitalization costs of at least $1 million and operating costs of about $200,000 per year—have a large impact on science. The issues described above apply di-

SIDEBAR 5.1
Instrumentation Infrastructure for the Materials and Chemical Sciences[a]

Instrumentation is essential in all areas of chemistry, but it is of particular importance in the development of new materials. Nowhere is this more evident than in the use of instrumentation to visualize nanomaterials. The use of imaging such as electron microscopy enables the researcher to get an idea of what is or is not possible. While the development of new materials draws on a range of instrumentation facilities, of particular importance are the issues facing small- and medium-scale research facilities, which are very critical to those in the chemical sciences who are working on new materials.

For work in the chemical sciences on materials, key instrumentation enables visualization. This encompasses diffraction, microscopy, and spectroscopy. Synthesis and processing are also important. Crystal growth, thin film deposition, and the ability to manipulate atoms are all necessary tools. Of course, instrumentation for characterization is also required, encompassing the testing of mechanical, magnetic, optical, and transport properties. As an example, research on nanostructures requires the ability to observe materials on an animated scale. Tremendous revolutions have taken place in the development of probe microscopy. It is now possible with scanning probes to move atoms on a surface, watch them move on the surface, and also observe the electronic states associated with dopants in a semiconductor.

Larger-scale facilities with X-rays have worked to develop tools such as the hard X-ray advanced proton source at Argonne National Laboratory. It is now possible to focus down to the order of 30 nanometers, or less. As a result, it is now possible to obtain diffraction information from individual structures at the nanoscale level with this X-ray nanoprobe.

This tool is just one in a series of complementary methods for performing diffraction. Electron diffraction can obtain signals from incredibly small volumes with single-atom sensitivity. However, this method produces highly dynamic scattering, making it difficult to interpret structure. Scattering is weaker with X-rays, allowing for structural analysis. In studying magnetism, neutrons have a number of attractive features.

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[a] J. Murray Gibson, Argonne National Laboratory, presentation to Challenges for the Chemical Sciences in the 21st Century: Workshop on Materials and Manufacturing, National Research Council, Washington, DC, 2001.

rectly to these types of facilities. In addition, key issues for these facilities include operating costs, balance, and specialization. To avoid duplication of effort, it is logical for facilities to specialize and to initiate regional cooperation.

INFRASTRUCTURE ISSUES: ACADEMIC-INDUSTRIAL INTERFACE

Although many academic researchers have a solid technical approach to their work and enjoy working on interesting problems, a clear understanding of the market need for materials developed in the university laboratory is often lacking. Attention to the market almost inevitably leads to the examination of important (as well as interesting and technically demanding) problems. Various consequences of an academic research program closely tied to the needs of industry may include the following:

- Research that is more relevant to students
- A demonstrated value to society
- Increased industrial and government investment in the academic research infrastructure
- Potential for economic return on industry investment.
- Improvement of competitiveness and development of new industrial growth

However, it is important to note that the nature of this interaction is extremely important. Industrial-academic partnerships in which past or present problems are the main focus will most likely not succeed. On the other hand, partnerships that look at problems four or five years in the future are much more compatible with the timeframe of a Ph.D. thesis.

Infrastructure and Technology Development

The traditional method of technology development leads to very inefficient use of resources. Research by competing individuals working in isolation leads to large number of potential technologies and discoveries, only a fraction of which are ever combined to form useful new products and/or processes.

Materials development is typically highly empirical, and rarely are appropriate experiments and/or modeling performed early enough in the research process to answer critical questions that an end user might have. The disconnect between researcher and application engineer is reflected in the amount of time it takes, for example, to build a reliable part out of a known alloy (at least 36 months). This is short compared to the time it takes to change ship steel (7-10 years), apply lightweight composites (15+ years), or develop ceramics for engines (20+ years). By contrast, system design is well integrated with established testing protocols that lead to much shorter insertion times (e.g., it takes only 30 months to go from a clean sheet of paper to a completely new engine design).

A road map to research is not always an appropriate answer, however. Although there are several advantages, such as providing direction and defining distances as well as a path around obstacles, it does not provide a complete explanation of how research should be done. For example, a road map assumes a common starting point and a fixed destination (i.e., one where there is no competition). A roadmap also may serve to stifle creativity. In addition, this approach provides no time information.

By first defining the desired product or process and the anticipated technology needs, research teams can better coordinate their efforts in order to obtain a higher rate of return on technology development. The results of fundamental research are tied to the needs of technologists who then build on this information to create further knowledge. Basic research, applied research, development, and demonstration play a role at all levels in the process since there is a tight feedback loop between discovery (whether planned or serendipitous) and end use. Continued academic/industrial consortia are expected to strengthen this feedback.

To be successful in universities, a funding organization that plays a more proactive role will be required. For example, the funding agency must provide a clear need (i.e., priorities, well-defined goals). This organization must understand both government and societal needs and be able to mix strategic (global) and tactical (directed) R&D. This means the appropriate combination of basic research, applied research, development, and demonstration (i.e., a "mixed-risk" approach).

Technical and the fiscal flexibility to review and change funding between and among scientific and engineering disciplines is required with this type of approach. By making connections between research groups and fostering an atmosphere of collaboration, government program managers could provide a very valuable service through technology transfer. This would not involve commercialization of technologies per se, but rather ensure a free flow of knowledge from those that generate it to those that may ultimately need it.

INFRASTRUCTURE AND FEDERAL SUPPORT OF RESEARCH

While corporate funding of academic research is a continuing and growing source of support, federal grants still are the predominant form of underwriting for this work. An examination of the academic-federal interface, particularly in light of the relationship between academic research and industry, indicates areas in which adjustments may be in order.

Over the past decade or so, a paradigm shift has occurred regarding federal support for research. Presently, there is almost universal support in this country for federal funding of scientific research for medicine and defense. However, it is not clear if there is a similarly large base of support for government funding of research in science and technology outside of these applications. As a result, it is imperative that researchers continue to point to the societal impact of the work they do. The incredible growth in federal support for medical research over the last 30 years can be accounted for in part because the general public has become aware of the impact of this work on their lives. Research on new materials tends to be oriented more toward industrial and/or commercial applications. This being said, it is also important to keep in mind that industry increasingly finds itself unable to support the level of basic research it had been supporting. The health of the chemical sciences and the ability of the field to continue moving forward partly depend on the type and quality of basic molecular science done in universities and national labs. Given that there is not likely to be a level of public funding commensurate with the number of requests from university researchers, great care must be exerted to ensure that truly novel, high-risk, yet high-quality work is supported at the federal level.

Presently, many aspects of the academic-federal interface are working well. Industrial-academic-national lab internships and graduate fellowship programs expose students to a wide range of research environments and provide a relatively inexpensive means to both train the next generation of scientists and to help them formulate their career paths. Similarly, junior faculty awards have been a crucial means of support to assistant professors at the start of their careers. Support for research centers and major instrumentation laboratories is strong at the federal level, as is funding for academic departmental instrumentation.

Although many positive aspects exist in the relationship between federal funding agencies and academic researchers, there are difficulties to be overcome. In terms of funding maintenance, there is concern that the time line for funding is too long whereas the funding cycle is too short. The result of this situation for many researchers is that large amounts of time that would be devoted to research is instead spent on maintaining funding. As noted in Sidebar 5.1, while instrumentation and facilities are well supported by federal funding, inefficient use of these facilities leads to underutilization. Finally, although there is a general consensus in the chemical sciences community that the number and caliber of new chemical scientists produced by U.S. universities is sufficient, the overwhelming percentage of these new scientists are foreign nationals. There is a demonstrable lack of U.S. graduate students. Attracting U.S. students to the chemical sciences at the graduate level is a challenge in all areas of research: federal, academic, and industrial.

SUMMARY AND FINDINGS

Researchers work on problems that have an impact on society. Focused efforts, solving problems that are seen as incredibly important, are the ones that will capture the public's imagination and gain public support.

The benefits of a healthy infrastructure are numerous. A greater range of possible research, and more research in a given time frame, will serve to feed the competitive engine, as well as help to develop new areas of research. For the graduate student, improvements in infrastructure can conceivably reduce the time necessary to earn a degree. For the general public, the benefits of a better understanding of science and technology would produce a new generation of analytically thinking people in the work force regardless of whether they choose the sciences as a career.

> **Finding: Chemical scientists are now and will increasingly be called upon to communicate with scientists in many other disciplines, and must learn to do so effectively.**

Many advanced technologies have been enabled by the chemical sciences, yet they have required input from many different disciplines. Increasingly, fundamental ideas and innovative approaches to broad technical challenges that face society are being developed at the interfaces between these disciplines. Providing for innovation in an effective and timely manner requires seamless interaction between chemical scientists, engineers, biologists, physicists, electrical or mechanical engineers, device engineers, and computer scientists. It is the interactions and the interfaces between these previously perceived disparate disciplines that will create new opportunities for the future.

Appendixes

A

Statement of Task

The Workshop on Materials and Manufacturing is one of six workshops held as part of "Challenges for the Chemical Sciences in the 21st Century." The workshop topics reflect areas of societal need—materials and manufacturing, energy and transportation, national security and homeland defense, health and medicine, information and communications, and environment. The charge for each workshop was to address the four themes of discovery, interfaces, challenges, and infrastructure as they relate to the workshop topic:

- Discovery—major discoveries or advances in the chemical sciences during the last several decades.
- Interfaces—interfaces that exist between chemistry/chemical engineering and such areas as biology, environmental science, materials science, medicine, and physics.
- Challenges—the grand challenges that exist in the chemical sciences today.
- Infrastructure—infrastructure that will be required to allow the potential of future advances in the chemical sciences to be realized.

B

Biographies of the Organizing Committee Members

Klavs F. Jensen (Co-chair) is Professor of Chemical Engineering and Materials Sciences at the Massachusetts Institute of Technology. His research area is processing and characterization of advanced inorganic materials, including chemical vapor deposition of semiconductors and metals, laser-assisted processing and fabrication of inorganic composites; synthesis and characterization, as well as mathematical models. He received his M.Sc. from the Technical University of Denmark, 1976, and his Ph.D. in chemical engineering from the University of Wisconsin-Madison in 1980.

Charles Kresge (Co-chair) is the Global R&D Director for the Chemical Sciences Capability, Corporate Research & Development, of The Dow Chemical Company. His expertise is in the area of catalytic synthesis, characterization, and applications. He received his bachelor's degree in chemistry from Swarthmore College and his Ph.D. in physical chemistry from the University of California.

Tobin J. Marks is Charles E. and Emma H. Morrison Professor of Chemistry at Northwestern University. He is an inorganic chemist with research interests in transition metal and f-element organometallic chemistry, catalysts, vibrational spectroscopy, nuclear magnetic resonance, synthetic facsimiles of metalloprotein active sites, and carcinostatic metal complexes. He received his B.S. degree from the University of Maryland and his Ph.D. from the Massachusetts Institute of Technology. He is a member of the National Academy of Sciences.

Julia M. Philips is currently at Sandia National Laboratories. Her research area is development and implementation of models of materials and processes that link the processing of materials with their performance via their microstructure, development and deployment of models for extraction of information during materials processing. She received her Ph.D. in applied physics from Yale University.

Elsa Reichmanis is Supervisor of radiation, sensitive materials and applied groups at Lucent Technologies. Her research specialty is chemistry, properties and application of radiation sensitive materials, particularly as they relate to resists and other materials for lithographic applications electronic materials. She received her Ph.D. in organic chemistry from Syracuse University. She is a member of the National Academy of Engineering.

David A. Tirrell is Ross McCollum-William H. Corcoran Professor and Professor of Chemistry and Chemical Engineering; Chair of the Division of Chemistry and Chemical Engineering at the California Institute of Technology. His areas of research are in the development of new polymeric systems of controlled molecular and supramolecular architectures, specifically, artificial proteins and flexible polymeric nanowires and nanotubes. He received his B.S. from the Massachusetts Institute of Technology in 1974, and his Ph.D. from the University of Massachusetts at Amherst in 1978.

C

Agenda

Workshop on Materials and Manufacturing Challenges for the Chemical Sciences in the 21st Century

National Academy of Sciences
2101 Constitution Ave., N.W.
Lecture Room
Washington, DC 20418

Wednesday, June 13

7:30	Breakfast
Session 1:	**Context and Overview**
8:00	Introductory remarks by organizers. Background of project.
8:00	**Douglas J. Raber**, National Research Council
8:05	**Ronald Breslow**, **Matthew V. Tirrell**, Co-chairs, Steering Committee on Challenges for the Chemical Sciences in the 21st Century
8:20	**Klavs F. Jensen**, Co-chair, Materials and Manufacturing Workshop Committee
8:30	**George M. Whitesides**—*Harvard University*
9:05	Discussion
9:25	**Angelo A. Lamola**—*Rohm and Haas*
10:00	Discussion
10:20	Break
10:50	**Craig J. Hawker**—*IBM*
11:25	Discussion
11:45	Lunch
Session 2:	**Discovery**
12:45	**W. Henry Weinberg**—*Symyx Technologies*
1:35	Discussion

1:55 **Daniel E. Morse—University of California, Santa Barbara**
2:20 Discussion

2:40 Breakout Sessions
Breakout questions: What major discoveries or advances related to materials have been made in the chemical sciences during the last several decades? What is the length of time for them to show impact? What are the societal benefits of research in the chemical sciences? What are the intangible benefits, for example, in health and quality of life? What problems exist in the chemical sciences? Has there been a real or sustained decline in research investment in either the public or the private sector? Has there been a shift in offshore investment?

3:45 Break
4:00 Reports from breakout sessions (and discussion)
5:00 Reception
6:00 Banquet—Dinner Speaker: Diane A. Jones, U.S. House of Representatives Subcommittee on Science

Thursday, June 14

7:30 Breakfast

Session 3: Interfaces
8:00 **Howard Katz**—*Lucent Technologies*
8:25 Discussion
8:45 **Geoffrey A. Ozin**—*University of Toronto*
9:10 Discussion

9:30 Breakout Sessions
Breakout questions: What are the major discoveries and challenges related to materials at the interfaces between chemistry or chemical engineering and such areas as biology, environmental science, materials science, medicine, and physics? How broad is the scope of the chemical sciences in this area? How has research in the chemical sciences been influenced by advances in other areas, such as biology, materials, and physics?

10:45 Break
11:00 Reports from breakout sessions (and discussion)
12:00 Lunch

Session 4: Challenges

1:00 **Nancy B. Jackson**—*Sandia National Laboratories*
1:25 Discussion
1:45 **David A. Tirrell**—*California Institute of Technology*
2:10 Discussion

2:30 Breakout Sessions
Breakout questions: What are the materials-related grand challenges in the chemical sciences and engineering? How will advances at the interfaces create new challenges in the core sciences?

3:45 Break
4:00 Reports from breakout sessions and discussion
5:30 Reception (light refreshments)

Friday, June 15

7:30 Breakfast

Session 5: Infrastructure

8:00 **J. Murray Gibson**—*Argonne National Laboratory*
8:25 Discussion
8:45 **Lawrence H. Dubois**—*SRI International*
9:10 Discussion

9:30 Breakout Sessions
Breakout questions: What are the materials-related issues in the chemical sciences, and what opportunities and needs result for integrating research and teaching, broadening the participation of underrepresented groups, improving the infrastructure for research and education, and demonstrating the value of these activities to society? What returns can be expected on investment in chemical sciences? How does the investment correlate with scientific and economic progress? What feedback exists between chemical industry and university research in the chemical sciences? What are the effects of university research on industrial competitiveness, maintaining a technical work force, and developing new industrial growth (e.g., in polymers, materials, or biotechnology)? Are there examples of lost opportunities in the chemical sciences that can be attributed to failure to invest in research?

10:45	Break
11:00	Reports from breakout sessions (and discussion)
12:00	Wrap-up and closing remarks **Charles Kresge**, Co-chair, Materials and Manufacturing Workshop Committee
12:15	Adjourn

Executive Session of the Organizing Committee

12:15	Working lunch: general discussion
1:00	Develop consensus findings
1:45	Develop consensus recommendations
2:30	Develop action items, follow-up steps, and assignments
3:30	Adjourn

D

Participants

CHALLENGES FOR THE CHEMICAL SCIENCES IN THE 21ST CENTURY: WORKSHOP ON MATERIALS AND MANUFACTURING

June 13-15, 2001

Richard A. Adams, University of South Carolina
Joseph A. Akkara, National Science Foundation
Richard C. Alkire, University of Illinois
Ronald D. Archer, University of Massachusetts
Susan J. Babinec, Dow Chemical Company
Mark T. Bernius, Dow Chemical Company
Ronald Breslow, Columbia University
Robert A. Brown, Massachusetts Institute of Technology
Michelle V. Buchanan, Oak Ridge National Laboratory
Leonard J. Buckley, Naval Research Laboratory
Donald, M. Burland, National Science Foundation
Manoj K. Chaudhury, Lehigh University
Helena L. Chum, National Renewable Energy Laboratory
Oliver Chyan, University of North Texas
Geoffrey W. Coates, Cornell University
Khershed P. Cooper, Naval Research Laboratory
Dady Dadyburjor, West Virginia University
Patricia Dehmer, U.S. Department of Energy
Lawrence Dubois, SRI International
M. Samy El-Shall, Virginia Commonwealth University
Hicham Fenniri, Purdue University
Mary E. Galvin, University of Delaware
Andrew Gewirth, University of Illinois, Urbana-Champaign
J. Murray Gibson, Argonne National Laboratory

Greg Gillette, GE Corporate R&D
Louis C. Glasgow, E.I. du Pont de Nemours and Company
David S. Green, National Institute of Standards and Technology
Mihal E. Gross, Agere Systems
Esin Gulari, National Science Foundation
Arnold M. Guloy, University of Houston
Paula T. Hammond, Massachusetts Institute of Technology
Craig J. Hawker, IBM Almaden Research Center
Chris W. Hollinsed, E.I. du Pont de Nemours and Company
Nancy B. Jackson, Sandia National Laboratories
Wyn P. Jennings, National Science Foundation
Klavs F. Jensen, Massachusetts Institute of Technology
Diane A. Jones, U.S. House of Representatives Subcommittee on Science
Howard Katz, Bell Laboratories, Lucent Technologies
Steven W. Keller, University of Missouri
Charles Kresge, Dow Chemical Company
Angelo Lamola, Rohm & Haas Company
Jorn Larsen-Basse, National Science Foundation
John W. Larson, Lehigh University
L. James Lee, Ohio State University
Andrew J. Lovinger, National Science Foundation
Toni G. Marechaux, National Research Council
Tobin J. Marks, Northwestern University
Krzysztof Matyjaszewski, Carnegie Mellon University
Richard McCullough, Carnegie Mellon University
Tyler D. McQuade, Massachusetts Institute of Technology
William S. Millman, U.S. Department of Energy
Tyrone D. Mitchell, National Science Foundation
Daniel Morse, University of California, Santa Barbara
Ralph G. Nuzzo, University of Illinois, Urbana-Champaign
Geoffrey A. Ozin, University of Toronto
Charles H. F. Peden, Pacific Northwest National Laboratory
Julia M. Phillips, Sandia National Laboratories
Thomas B. Rauchfuss, University of Illinois, Urbana-Champaign
William Rees, Georgia Tech
Elsa Reichmanis, Lucent Technologies
Don Rohr, GE Corporate R&D
Rodney Ruoff, Northwestern University
Alan J. Russell, University of Pittsburgh
Lynn F. Schneemeyer, Agere Systems
Jeffrey J. Siirola, Eastman Chemical Company
Rick Sisson, Worcester Polytechnic Institute
Paul H. Smith, U.S. Department of Energy

Jack Solomon, Praxair, Inc.
Lawrence R. Sita, University of Maryland, College Park
Judy Stein, GE Corporate R&D
Johannes Swank
David A. Tirrell, California Institute of Technology
Matthew V. Tirrell, University of California, Santa Barbara
Carole Trybus, Concurrent Technologies Corporation
Richard Uriate, GE Corporate R&D
Dion Vlachos, University of Delaware
Paul F. Walters, American University
W. Henry Weinberg, SYMYX Technologies, Inc.
Robert Wellek, National Science Foundation
George M. Whitesides, Harvard University
Younan Xia, University of Washington
Peidong Yang, University of California, Berkeley
Gregg A. Zank, Dow Corning Corporation

E

Reports from the Breakout Session Groups

A key component of the Workshop on Materials and Manufacturing was the breakout sessions that allowed for individual input by workshop participants on questions and issues brought up during the presentations and discussions. Each color-coded breakout group (red, yellow, green, and blue) was assigned the same set of questions as the basis for its discussions. The answers to these questions became the basis for the data generated in the breakout sessions. After generating a large amount of suggestions and comments, the breakout groups attempted to organize and consolidate this information, sometimes voting to determine which topics the group decided were most important. After each breakout session, each group reported the results of its discussion to the entire workshop.

The committee has attempted in this report to integrate the information gathered in the breakout sessions and to use it as the basis for the findings contained herein.

SESSION 1: CONTEXT AND OVERVIEW

No Breakout Session was held.

SESSION 2: DISCOVERY

Breakout questions: What major discoveries or advances related to materials have been made in the chemical sciences during the last several decades? What is the length of time for them to show impact? What are the societal benefits of research in the chemical sciences? What are the intangible benefits, for example, in health and quality of life? What problems exist in the chemical sciences? Has there been a real or sustained decline in research investment in either the public or the private sector? Has there been a shift in offshore investment?

Red Breakout Group

- Communications and information technologies are based on chemical processes or reactions and materials (microelectronics, photonics):

    Optical fibers and materials, $LiNbO_3$, erbium-doped amplifiers
    Optoelectronic polymers
    Compound Semiconductors
    Magnetic materials
    Photoresists
    High critical temperature (T_c) semiconductors
    Chemical vapor deposition, etch processes
    Ultrapure materials

- Engineering materials for advanced performance have been impacted by chemical processes and syntheses:

    Composites
    Paintings, coatings, and adhesives
    Teflon, polyolefins
    Silicones
    Block copolymers
    Living polymerization products and methods
    Metal complexes for polymerization
    Fibers—clothing

- Advances in processing technologies have led to new materials and formulations:

    Combinatorial materials discovery
    Supercritical processing
    Cryogenic processing
    Genetic engineering

- Electrochemical processes and devices underlie advances in energy and power systems:

    Electrochemical materials
    Batteries
    Fuel cells

- New materials and fabrication proceses have enabled new sensors and technologies for rapid analyses.

Yellow Breakout Group

Polymers

- Conductive polymers (no commercial impact yet: products are being developed)
- The discovery of plastic and crystalline materials that have promising transistor properties will likely impact future electronics (1972: conducting organic crystals; 1997: conducting polymers; 1990-ish: transistor sexithiophene)
- The discovery of light-emitting diode (LED) properties in conjugated polymers and organic molecules will probably impact new low-cost electronics (~1972: conducting organic crystals; ~1977: conducting polymers; ~1990 polymer LEDs)
- Semiconducting polymers: show promise for printable plastic electronics (not yet commercial)
- Chemically modified conductive polymers, optimized as gas sensors (impact: still small, prototype and R&D stage)
- Chemically processible conjugated polymers for semiconducting properties ("discovered": 1991; impact: poised 2001-2002; "commercial": 2002-2003; ~+13 years)

Catalysis

- Mesoscopic materials (e.g., the mesoporous molecular sieve MCM-41) discovered by Mobil in the early 1990s, many microporous materials developed over the last decade
- Zeolites have had an important impact on the chemical industry, and they hold significance as hosts for growth of opticoelectronic materials—zeolite catalysts in petroleum processing
- Nanostructured catalysis (e.g., zeolites, pillared clays, monodispersed metal particles [impact: zeolites for cracking of oil]), discovery: ~1970s, technical implementation: ~10 years (new fluidized-bed reactor technology
- Metallocenes give better control of polyolefins and higher productivities.
- In 1986, industrial chemists were almost mocking the oligomerizing olefin catalysts being developed, now we have new plants based on these metallocence catalysts.
- The catalytic converter has had a major impact on the quality of life.
- Supported gold catalysis for low-temperature oxidation of CO was discovered in approximately 1930 but its relevance was not appreciated. It was

picked up by the Haruta group in the 1980s-early 1990s. The technical impact on a commercial scale was seen in the 1990s.

Biomedical Applications

- Advances in chiral synthesis allow manufacture of entantiopure pharmaceuticals with reduced side effects.
- Drug exploration using combinatorial synthesis
- Encapsulation has allowed controlled release for drug delivery systems.
- Biodegradable materials as drug delivery devices (1997)
- Polymers for biomedical applications (drug delivery, tissue engineering)
- Tissue engineering—the combination of engineering, polymer chemistry, and medicine—has rapidly advanced from a pure scientific curiosity to the market and may replace tissue, skin, etc. New synthetic methods in polymer chemistry have led to a huge array of new materials (cross-coupling radical control).

Instrumentation

- Scanning probe microscopy has enabled understanding of interfacial phenomena.
- Scanning tunneling microscopy was discovered in ~1984 and showed impact in the 1990s (~10-15 year time line).
- The inductively coupled plasma mass spectroscopy has become a pervasive analytical tool with broad impact.
- Giant magnetic resistance (GMR) for spin-sensitive memory (information techonology) was discovered in ~1990 (?) and implemented in ~3-4 years, with impact around 1995.
- Materials processing: molecular beam epitexy (diode lasers)

Electronics

- Photonic band gap materials for photonics. Not yet commercialized due to no processing methods
- Photoresist-enabled integrated circuit and computer technology.
- Chemically amplified photoresists, discovered in 1979, had commercial implementation in the 1990s. It is fundamentally important for the large-scale manufacturing of microelectronic devices with smaller feature sizes (continuation of Moore's law).
- The concept of "chemically amplified resists" was developed in ~1980 and first implemented ~1990. It was accepted in general manufacturing around 1995.
- Low-*K* dielectric materials were identified as a need in the 1990s and

were implemented in 2001-2002. These were required for the continuation of Moore's law.

- Soft lithography—imprinting: early 1990s; commercial implementation: 2002 (?); cheap way to make integrated circuits

Combinatorial Chemistry

- Combinatorial chemistry has revolutionized drug discovery and catalyst development.
- Combinatorial chemistry has revolutionized drug discovery in the pharmaceutical industry.

Macromolecules

- Buckyballs—quantum dots and wires
- Carbon nanotubes—no commercialization because no cost effective processing
- Dendrimers—discovered in 1985, commercialization in 2000; synthetic globular macromolecule as a scaffold-template for sensors (Army), magnetic resonance imaging (MRI) agents, porous structures

Computational/Modeling

- Density functional theory (DFT) allows understanding of reactivity at the atomic level, for complex systems; this was previously limited by computer power and accuracy.
- Computational capability and software have enabled molecular design in organic synthesis.
- Molecular modeling over the last decade enables materials characterization and understanding of materials growth mechanisms previously limited by lack of reliable intermolecular potentials and computer power.

Superconductors/Telecommunications

- High-T_c superconductors, discovered mid-1980s; no impact yet
- High-T_c superconductors in communication shielding; benefits: cell phones
- High-purity optical fibers (erbium-doped optical fibers)
- "Sol-gel" processing for telecommunication-optical fiber applications; initial research ~1985 (?); implementation: ~2000

Other

- Manhattan Project—the basic chemistry of plutonium (redox, separation, materials, etc.) enabled the nuclear age.
- Self-assembly materials (surfactants, block polymers, etc.)
- Synergistic properties of multiple components of material system (i.e., composites)
- Supercritical CO_2 processing; discovered in the 1980s; facilitates the synthesis of fluoropolymers (2000).

Green Breakout Group

- Low volatility organics and adhesives

  Volatile organic compounds and water-based
  1950-1960s: emulsion polymerization
  Particle engineering
  Coatings, surface treatments
  Weatherability
  Paints
  Reflective powder paints
  Adhesives

- Inorganic electronic materials

  Zone refining-1950s; semiconductors
  Hydrothermal synthesis—1950s and 1960s
  Picoelectric
  Thermoelectric materials
  SiO_2 dielectrics
  Optoelectronics
  Other inorganic electronic materials and applications

    Self-assembly processing
    Microcontact printing for use in lab on a chip
    Self-assembled monolayers: microcontact printing
    Spatially addressable synthesis has spawned Symyx, Affymax, Affymetrics
    Copper processing techniques for ICs (deposition, patterning, etching); impact: late 1990s
    Porous silicon nanocrystalline behavior; research 1990s
    Metelorganic chemical vapor deposition (MOCVD) processes for materials—GaAs, InP

Sol-gel glass research: early 1980s; commercialization: late 1990s (~15 years)

Nanocrystalline TiO_2 —sunscreen

GMR read heads for high-density data storage; impact: 2000

Gallium nitride epitaxy-ready on sapphire for blue lasers; commercialization: ~ 10 years (~2000)

Semiconductor lasers wide-band gap

High-quality low-loss silica optical-fiber manufacturing; impact: telecommunications

Thermoelectrics: refrigerants, energy for space probes, portable coolers

- Active organic materials

Liquid crystals: 1800s
Conducting polymers 1970s
Organic semiconductors—transistors
Low LED displays: 1990s +
Other active organic materials and applications

Liquid-crystal polymers (e.g., zylon); impact: late 1990s

Polymer LEDs for displays; impact: today

Organic LEDs; commercialization: ~2000; impact: lower cost, better visual display

- Reinforced composites

Fiber-reinforced composites; basic work on carbon and composite fibers

- Electrochemical devices

ferrocenes
lithium-ion and lithium-polymer batteries; impact: 1990s

- Homo- and heterogeneous catalysis

Organometallic chemistry-1950s
1950s—mesoporous materials (e.g., MCMs)
Catalytic converter
Other catalysts

Metallocene catalysts, ~1990

Living polymerization has been used to make block copolymers and other materials previously inaccessible:

Glycopolymers
Peptide polymers

Site-selective porous inorganics (zeolites) for control of catalytic activity; impact: petroleum and plastics industry

Organometallic chemistry, 1950s: first homogeneous catalysis; 1950s-1970s: catalysis with asymmetric induction-chiral drugs

Well-defined homogeneous living polymerization catalysis: ring opening metathesis polymerization and atom transfer radical polymerization

Catalysis for olefin polymerization at low pressure; Ziegler-Natta: 1950s, single-site metallocene: 1990s; designer polyolefins—better garbage bags and car bumpers, etc.—could replace polyvinyl chloride (PVC) in many areas

- Thin films and coatings

Chemical vapor deposition (CVD)

1950s Diamond-like carbon thin films
1970s Chemical vapor deposition widespread (thin films, coatings, coatings for memory)

Plasma chemical vapor deposition
Combustion chemical vapor deposition

1980s Wear resistance
1990s Heat dissipation (thin films, coatings)

Other Thin Films and Coatings
- CVD diamond
  - 1970s—Russia, Japan
  - 1990s—Impact
- CVD coatings
  - Magnetic disk/tribology
- Diamond-like carbon coatings for low friction
- Diamond-like films; impact: coating of tools, thermal management

- High critical temperature superconductors

1911 Low temperature superconductors – magnets 1960s

1986-1988 High critical temperature cuprate superconductors
- Processing
- Volume, scaling

1990s Filters: niche power applications

2000s Transformers

- Other breakthroughs or advances

Scaffolds for tissue engineering

Chlorofluorocarbons (CFCs)
Utility as refrigerants
Demonstrate that chemists response to environmental challenge

Substitutes for Freon (new chlorofluorocarbons)

Refrigeration, air conditioning, cleaning solvents
Benefit: efficiency of Freon without the environmental impact

Advanced positive photoresist (I-line, deep ultraviolet, etc.)

Photolithography (chip production)
~1980 for fundamental work
~1990 for I-line use
1995 for deep ultraviolet
Benefit: computing

Power and computer-active memory increases that have enabled powerful personal computers and servers, liquid crystal displays

Quasi-crystalline metal films (hard, corrosion-resistant coatings); impact: late 1990s

Advanced ion-exchange resins

Original work 1950s, but improvements continue today
Benefits: cheap clean water, water pure enough for semiconductor manufacture
Longer-lived boilers, catalysts

Polymerase chain reaction (PCR) and related molecular biology techniques have been used to engineer organisms to overproduce commodity polymers (polyhydroxylalkanoates) as well as produce highly organized peptide materials.

Catalytic converters for autos, 1970s; impact: cleaner air

Single-walled nanotube

Blue Breakout Group

- Analytic techniques—enablers for miniaturization

Instrumentation
  Nuclear magnetic resonance (NMR)
  Synchrotron
  Spot profile analysis (SPA), atomic force microscopy (AFM)—1980 to now

Emissions control—also relied on new chemical understanding of the impact of emissions on air quality, etc.

- Materials

Intrinsically conducting polymers: around 1971
Nylon—invented: 1933; commercialized: 1939; impact: 1944
Teflon—invented: 1938; impact: 1945
Electrochromic materials: late 1970s
Polyethylene, high-density polyethylene
Thermoplastics— Lexan, etc.: about 20 years from innovation to profitability
Alloy development—shape memory, superalloys
Photographic film; phosphors; organic light-emitting polymers
Catalysts—homo, hetero, zeolites, organic templates
Block copolymers
Quantum materials: quantum dots, buckyballs
Composites

- Processing and synthesis

Sol-gel processing
Semiconductor metallization—electrochemical processing
Petroleum refining, catalytic cracking
Direct process for synthetic rubber; silicone polymerization
Synthesis of inorganic solids (mesoporous oxides, zeolites)
Hydrothermal solid-state synthesis
Ziegler-Natta catalysts
Single-site catalysis
Living polymerization
Total synthesis
Combinatorial approaches
Self-assembly

Purification of (elemental) silicon: led to silicon-based electronics

Photolithography; first mention: 1880s, with chromate; 1960s, practical for microelectronics

Controlled morphology

SESSION 3: INTERFACES

Breakout questions: What are the major discoveries and challenges related to materials at the interfaces between chemistry or chemical engineering and areas such as biology, environmental science, materials science, medicine, and physics? How broad is the scope of the chemical sciences in this area? How has research in the chemical sciences been influenced by advances in other areas, such as biology, materials, and physics?

Red Group

- Chemistry   Biology, Medicine

Met: Implantable devices
Implantable power
Separation technologies
Commodity production of biocatalysts, monomers, polymers
To meet: Devices for functional metabolism
In situ drug production
Artificial organs (lungs, skin, ligaments, etc.)
Nanocellular systems
Human integrated computing

- Chemistry   Materials Science

Need: Ultrahard materials
Cementitious materials (not CO_2 producing)
High temperature materials for power and propulsion
Multifunction materials
Construction
Energy production
Technology to reduce corrosion losses

- Chemistry   Physics

To Meet: Quantum computing
Magnetic computing
Photonic computing

Self-organization of structures
Biomolecular structure organization

Yellow Group

- Multifunctional materials

  Self-reporting materials
  Smart materials and learning materials
  Self-healing materials
  Interdisciplinary materials
  Multicomponent compounds with properties of ceramics and plastics

- Environment

  Low volatile organic compound materials and coating
  Solvent-free catalysis—green catalysis
  Membranes—water purification
  Disassemble or disable and recycle materials
  Self-cleaning materials
  Green chemistry for materials synthesis
  Link behavior of biocatalysts and inorganic catalysts
  New catalysts for a cleaner environment
  Environmentally friendly materials

- Health

  Medical and environmental diagnostics
  Materials for improved human performance
  Biocompatible materials
  Materials for human-computer interface
  Artificial organs
  Tissue engineering and adding biological functions to materials

- Supporting technologies

  Controlled architecture of multicomponent materials
  Harnessing biological systems to prepare nonnatural materials
  Chain folding of polymers
  Prediction of materials properties from structure
  Better multiscale modeling

- Other suggestions

  Photovoltaics
  Better portable power
  Understanding mobility of charge carriers
  Advanced chemical power sources
  Fuel processors for fuel cells
  Nanomagnetic materials
  All-optical network
  Materials for computing
  Corrosion-resistant structural materials
  Macroglobal-scale issues
  Replacements for metals—high-performance materials, microfluidics

Report to Plenary Session

- Why invest in materials?
- Materials that improve health
  - Tissue engineering
  - Biosensors
  - Biofunctional materials
  - Living materials
- Materials that improve environment
  - Disassemble (e.g., tires)
  - Permanence (e.g., concrete)
- Materials that perform multiple functions
  - Failure reporting and triggered healing
  - Biosensing—responses

- Barriers – areas of science and technology that if addressed would enable the above

Interfacial science
Multiscale modeling and prediction of structure and architecture
Controlled synthesis of predictable structured materials (e.g., photonics)
Incorporating the power of biology, biosynthesis of materials, and synthesis of biomaterials

Green Group

- Medicine and health—biocompatible materials (implants, dental, neuroprosthesis, synthetic muscles); sensors, diagnostics (instrumentation, contrast agents)

- Structural materials—alloys-metallurgy, housing, roads, coatings, concrete and asphalt, composites, polymers-rubber, corrosion inhibition, amorphous materials, sealant, composites, recycled materials, transparent materials, insulation, functional materials, self-repairing and diagnosing materials, amorphous materials, fasteners

- Art and literature—e-paper, inks/paints, conservation, paper science, coatings, archival media, entertainment, displays

- Agriculture and food services—delivery, packaging, sensors, animal health diagnostics, bioengineered materials, processing or separations, soils, refrigeration

- Space and national security—lightweight materials, sensors, high-temperature materials, multifunctional materials, reliability and robustness, electronic materials, armor, advanced textiles, coatings, energetic materials

- Textiles—synthetic fibers, waste reduction, dyes, fibers or plastics, coatings (multifunctional), composites, Gortex, synthetic elastomers, superabsorbents (diapers), velcro and fasteners, processing

- Personal hygiene—shampoos and conditioners, soaps and detergents, hair sprays, sunscreen, diapers, cosmetics, tooth brushes and toothpaste, colorants

- IT and communication—optical fibers and coatings, optoelectronics, microelectronics, displays, RF and microwave, portable communications, storage, hard copy and printing, packaging, processing, personal electronics, reduced waste stream in processing, amorphous materials

- Environment—PVC pipe, water purifications, catalytic converters, waste treatment, sensors, fuel cells and photovoltaics, coatings, green processing and green materials, nuclear waste separation and containment

- Transportation—tires, roads, lightweight materials, coatings, corrosion-resistant or reflective paints, ceramics, strength-temperature-wear, sensors, fuels

Blue Group

- Biology-Medicine

  Biomedical engineering
    - Tissue engineering
    - Bone scaffolding
    - Biomimetics
    - Protein engineering
    - Biofabrication

  Biosensors
    - Medical diagnostics
    - Medical imaging
    - Rapid DNA screening

  Microfluidics
    - Solid-phase synthesis
    - Templating
    - Genomics
    - Genetically modified organisms

- Physics

  Liquid crystals
  Surface chemistry (monolayers)
  Spin glasses
  Electron-phonon coupling

- Materials

  Ceramics
  Magnetic materials
  High-temperature materials
  Semiconductors
    - Conducting polymers
    - High-temperature superconductors

  Microphotonics
    - High temperature sensors
    - Imaging
    - Quantum devices
    - Nonlinear optics
    - Data and storage

Theory and modeling

How broad is the scope of the chemical sciences in this area? The nature of the interaction is driven by the nature of the problem.

- Superparamagnetic effect: higher storage density
- Molecular electronics: new modes of logic
- Materials design from first principles and modeling
- Biological sensing detection: advanced imaging
- Complex synthesis (many different scales): protein templates
- Advanced micro- and nanofabrication
- Crystal growth and engineering
- Combinatorial synthesis
- Protein folding
- Self-assembly

How has research in the chemical sciences been influences by advances in other areas? Dynamics of processes:

- Selective catalyst design
- “Impossible” materials
- Global climate change
- Energy of recapture
- Advanced battery and fuel cells (alternative energy)
- Emergence
- Transport phenomena
- Funding

SESSION 4: CHALLENGES

Breakout questions: What are the materials-related grand challenges in the chemical sciences and engineering? How will advances at the interfaces create new challenges in the core sciences?

Red Group

- Understanding and manipulating chemistry at interfaces

Solid-solid
Solid-liquid
Functional integration of linking cells and biomolecules to materials

- Sustainable routes to materials

Energy efficiency
Materials efficiency (e.g. recycle—whole polymers or component monomers)
No toxics
No emissions or greenhouse gases
Also: maximization of limited resources; molecular recycling

- Materials by design

Process control and property prediction across 18 orders of magnitude in length and time

Also: modeling to design; structure and property process control at molecular level

- Materials for energy generation, storage, and conservation

Hydrogen, solar, photovoltaics
Improved handling of materials for nuclear fuel-power cycle

- Diagnostic tools for intelligent processing: instrumentation for real-time, atomic-level resolution, high-sensitivity, high-chemical-specificity, nondestructive analysis

- Infrastructure issues—education funding, interfaces within chemistry departments, communicating between disciplines

- Also: large parallel synthetic matrix experiments

Yellow Group

Grand Challenges

- Address:
    - Water
    - Energy
    - Food
    - Air

(Must be revolutionary)

1. Use chemistry to decouple environmental impact from a worldwide standard of living.

    - Alleviate diminishing resources.
    - Remediate existing environmental problems.
    - Find replacements for strategic materials.
    - Decentralize the power supply.

2. Apply chemistry to harness the power of biology for materials science.

3. Spatial and temporal control of chemistry

    - Self-assemble on a macroscale
    - Build a multifunction sensor in a single step.

Dot Votes for Challenges

Pill to stop AIDS (7 votes)
Miniaturization of medical sensor systems (5 votes)
High-performance materials—easy to process (4 votes)
Self-scaling materials (bio-inspired vs. biomimetic) (4 votes)
Safe storage of H_2 (4 votes)
Make materials disassembly friendly (3 votes)
Optical computing, photonic circuits (2 votes)
Room-temperature fixation of N_2—100 percent selective catalysts (2 votes)
Scaling (understanding, manufacture) (2 votes)
Chemistry-materials alleviation of diminishing resources

Green Group

What are the materials-related grand challenges in the chemical sciences and engineering? How will advances at the interfaces create new challenges in the core sciences?

Three Challenges

1. Putting it together (and processing)
    - Arrangement at the atomic and other length scales
    - Control (kinetic versus thermodynamic)
      Weak bonding
      Assembly (directed, templated, mechanical)

    - Hierarchical construction with feedback
      Bioinspired
      Catalysis

2. Analysis
    - Understanding what we make
      Structure (over all length scales)
      Function (over all length scales)
    - Defects and impurities
    - High resolution 3-dimensional element-specific mapping
        Nondestructive, real time
        Noncrystalline, multiple length scales

3. What to make

Modeling

Application Driven

Capital

Structure (length scales)

Theory

- Accurate a priori design of materials and a road map of how to make them

Blue Group

Seamless manipulation of matter and information from molecular to macrosize scales: (1) interconnects (2) synthesis (3) dynamics:

- Interconnections at all length scales

  Understanding and modeling transitions between nano- and microscales
  Nano- or micro fabrications in all dimensions
  Photonic materials
  Transition from electronics to photonics

- Control matter at all scales

  Harness capabilities and power of nature
  Self-assembly and crystallization
  Understanding nonequilibrium steps and structures
  Understanding all steps in self-assembly
  Understanding protein folding

- Materials that enable unlimited clean energy

  High-capacity reversible energy storage
  Alternative energy sources—unlimited
  New recyclable and biodegradable materials

- Restoration and enhancement of function of living materials

  Nanostructures and bioapplications
  Expression of human genome
  Restoration of lost organ function
  Human computer interface

- What are the challenges for the next few decades?
  Particle science and engineering
  Understanding complexity
  Understanding scale-up
  Investigation of larger-scale, more realistic systems
  Influence of fields
  Detecting hydrogen in metals (local analysis)
  Effects of "impurities" in alloys and metals
  Understanding scattering effects
  Accelerated testing methods

Visualizing nanoscale interactions
Miniaturization
Developing principles and theory for aggregation (self-assembly) of materials
Broadened parallel investigations
Increased computational power and tools

- Other answers that were not completely related:

Redefining the scientific method
Student education
New instrumentation: development and access

SESSION 5: INFRASTRUCTURE

Breakout questions: What are the materials-related issues in the chemical sciences, and what opportunities and needs result for integrating research and teaching, broadening the participation of underrepresented groups, improving the infrastructure for research and education, and demonstrating the value of these activities to society? What returns can be expected on investment in chemical sciences? How does the investment correlate with scientific and economic progress? What feedback exists between chemical industry and university research in the chemical sciences? What are the effects of university research on industrial competitiveness, maintaining a technical work force, and developing new industrial growth (e.g., in polymers, materials, or biotechnology)? Are there examples of lost opportunities in the chemical sciences that can be attributed to failure to invest in research?

NOTE: There was no Blue Group for the last Breakout Session.

Red Group

What parts of the infrastructure *ARE* working well?

- Industrial/academic/national lab internships
- Major instrumentation laboratories
- Quality of the graduate students and their love of science
- Steps toward interdisciplinary research
- Research centers (where they exist)
- Startups or options for graduate students
- Technology transfer (at large universities)
- Motivation and incentives

- National Science Foundation (NSF) Grant Opportunity for Academic Liaison with Industry (GOALI)-type programs

What parts of the infrastructure are *NOT* working well?

- Support for research centers
- NSF funding for university research
- Servicing of funding
- Lack of long term research funding (>5 years)
- Outreach
- Science education structure (K-12)

What payoffs are expected from having a healthy infrastructure?

- Laypersons' better understanding of science and technology
- Improved quality of life
- Science education feeds a logically thinking workforce
- Feed the competitive engine
- Development of new areas of research, new fields
- Defense

Yellow Group

Infrastructure elements

- Instrumentation—maintenance funding, extent of utilization, staffing issues (considered service jobs), poor support for "medium" size
- Buildings—age of manufacturing plants, decaying infrastructure
- Academic department and tenure structure
- Legal system—intellectual property limitations, intellectual property benefits
- People—right number, right skills, chores of professional staff, refocusing of chemistry undergrads from chemistry
- R&D funding system

Good and bad

- People

Good: Industry is getting the people it needs; universities are sustaining themselves

Bad: Shortage of number of people in some areas
Unnecessary and trivial responsibilities for professionals

Changing goals of students
Lack of training in some areas

- Instrumentation and faculty issues

Good: Centers pool resources and enable larger investment; research centers foster collaboration, provide bridge between disciplines

Bad: Funding for maintenance and staffing
Underutilization
Support for "medium" size

- Payoff of (good) infrastructure

Greater range of possible research
Greater amount of research possible in given time
Shorter time from idea to product
Shorter time to degree

Green Group

What works (numbers refer to votes)

Center grants (7)
Major user facilities (7)
Graduate fellowship programs (6)
Private donations to universities (6)
Number and quality of graduate students and graduates (4)
Funding for single principal investigators (PIs) and departmental instrumentation (4)
Junior faculty awards (4)
Single PI system (2)
Postdoctoral fellowships
Connectivity
Database access
Research parks (industry-university)
Startups are generating jobs
Peer review system
Multiple funding sources

Problems

Timeline for funding too long; funding cycle too short (8)
Capitization (7)

Education—K-12 and undergraduate (6)

Too few U.S. students (5)

Traditional academic department structure (5)

Top universities—diversity of faculty and graduate students and mentoring (5)

Grants not able to support enough personnel (2)

Too few graduate fellowships (2)

Major user facilities—need to inform prospective users and make user friendly (1)

Not enough support for centers (1)

Globalization of R&D and manufacturing

Lack of databases (e.g., thermodynamics and kinetics)

Entrepreneurial initiative

Intellectual property—university-industry interface