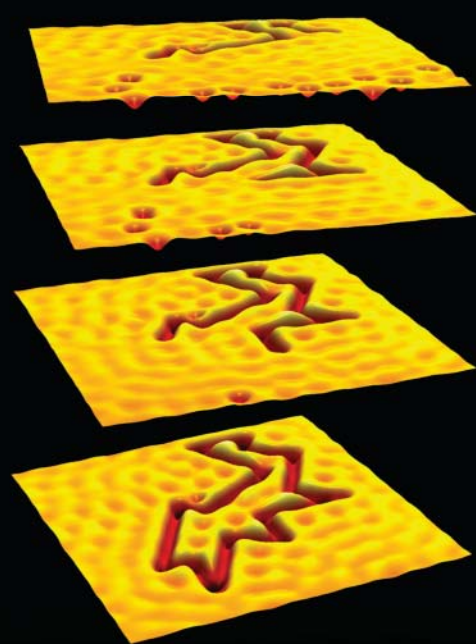
Materials by Design

Report of the
National Nanotechnology Initiative Workshop
June 11–13, 2003



About the Nanoscale Science, Engineering, and Technology Subcommittee

The Nanoscale Science, Engineering, and Technology (NSET) Subcommittee is the interagency body responsible for coordinating, planning, implementing, and reviewing the National Nanotechnology Initiative (NNI). NSET is a subcommittee of the Committee on Technology of the National Science and Technology Council (NSTC), which is one of the principal means by which the President coordinates science, space, and technology policies across the Federal Government. The National Nanotechnology Coordination Office (NNCO) provides technical and administrative support to the NSET Subcommittee and supports the subcommittee in the preparation of multiagency planning, budget, and assessment documents, including this report.

For more information on NSET, see http://www.nano.gov/html/about/nsetmembers.html.

For more information on NSTC, see http://www.ostp.gov/cs/nstc.

For more information on the NNI, NSET, and NNCO, see http://www.nano.gov.

About this document

This document is the report of a workshop held under NSET Subcommittee auspices in June 2003 seeking input from the research community on the NNI research agenda related to one of the original NNI "grand challenge" topics, "Nanostructured Materials by Design." The findings from this workshop were used in formulating the NNI Strategic Plan, particularly the Nanomaterials Program Component Area described in that plan. The meeting was jointly sponsored by the U.S. National Science Foundation (in particular the Division of Materials Research) and, through the NNCO, the other member agencies of the NSET Subcommittee.

Cover and book design

Book design and layout are by Roan Horning, Geoff Holdridge, and other NNCO staff members. Cover design is by Kathy Tresnak of Koncept, Inc., and Kanako Yamamoto of Affordable Creative Services, Inc.

Front cover: This sequence of images shows different stages in the construction of a "boundary" of carbon monoxide molecules on the surface of a copper crystal. Dualities abound. The scanning tunneling microscope used to build the structure is also used to image it. Electrons at the copper surface have many particle-like characteristics, such as discrete charge and mass, but behave like waves when bounded by the carbon monoxide molecules or tunneling to the tip of the microscope. The chemical and electronic properties of the constituent materials—copper and carbon monoxide—are critical to the fabrication process, while detailed comparisons of the final structure and another closely related structure enable a description of the finest details of these properties, down to the quantum-mechanical phase of the surface electrons. This is an important advance—using our ability to fabricate nanostructures from the "bottom up"—in understanding and manipulating the behavior of these structures in nanoscale size regimes, where quantum effects are dominant. The work, which was supported by the National Science Foundation, the Department of Energy, and the Office of Naval Research, may have important applications in quantum computing, nanoelectronics, and the science of spectroscopy, and has connections to other disparate fields ranging from the musical sounds of drums to the physics of higher dimensional string theories (courtesy of Hari Manoharan, Stanford University; for more information see *Science* **319**, 762-767).

Back cover: Micrograph of a FAST-ACT® particle—a proprietary formulation of nanoscale powders composed of magnesium, titanium, and oxygen—capable of absorbing and destroying toxins. Research funded by the National Science Foundation led to the discovery of these materials, which have enormous surface area that allows them to adsorb and rapidly decompose a wide range of toxic chemicals (e.g., sulfuric acid) as well as chemical warfare agents such as VX nerve gas (courtesy of Kenneth Klabunde, Kansas State University, and NanoScale Materials, Inc.).

The background graphic at the bottom of the entire cover is courtesy of L. J. Whitman, Naval Research Laboratory.

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Materials by Design

Report of the National Nanotechnology Initiative Workshop
June 11–13, 2003, Arlington, VA

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Sponsored by

National Science and Technology Council
Committee on Technology
Subcommittee on Nanoscale Science, Engineering, and Technology

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Report Credits

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Thanks are due to all the participants in the June 11–13, 2003, workshop held in Arlington, VA (see Appendix B). The presentations and discussions at that workshop provided the foundation for this report.

Credit is due to Paul Lagasse of WTEC for report editing; to Steve Miller, who assisted in editing the executive summary; and to members of the NNCO staff who helped format and proofread the report: Clayton Teague, Geoff Holdridge, Cate Alexander, Philip Lippel, and Stephen Gould.

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PREFACE

This report on *Materials by Design* is one of a series of reports resulting from topical workshops convened during 2003 and 2004 by the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the National Science and Technology Council's Committee on Technology through the National Nanotechnology Coordination Office (NNCO). The workshops were part of the NSET Subcommittee's long-range planning effort for the National Nanotechnology Initiative (NNI), the multiagency Federal nanotechnology program. The NNI is driven by long-term goals based on broad community input, in part received through these workshops. The NNI seeks to accelerate the research, development, and deployment of nanotechnology to address national needs; enhance our nation's economy; and improve the quality of life in the United States and around the world through coordination of activities and programs across the Federal Government.

At each of the topical workshops, nanotechnology experts from industry, academia and government were asked to develop broad, long-term (ten years or longer), visionary goals and to identify scientific and technological barriers that once overcome will enable advances toward those goals. The reports resulting from this series of workshops inform the respective professional communities as well as various organizations that have responsibilities for coordinating, implementing, and guiding the NNI. The reports also provide direction to researchers and program managers in specific areas of nanotechnology research and development regarding long-term goals and hard problems.

This particular report is the result of a workshop held under NSET Subcommittee auspices in June 2003 seeking input from the research community on the NNI research agenda related to one of the original NNI "grand challenge" topics, "Nanostructured Materials by Design." The findings from this workshop were used in formulating the NNI Strategic Plan, particularly the Nanomaterials Program Component Area described in that plan. This report was also co-sponsored by the National Science Foundation's Division of Materials Research to provide input to its particular research agenda within the overall NNI program.

This report identifies opportunities for advanced research in nanostructured materials and recommends the establishment of "nanofoundries" to develop the knowledge, methods, and instruments for the fabrication of nanoscaled materials that will enable economically viable applications with broad benefit for industry, technology, the economy, the environment, human health, and society.

On behalf of the NSET Subcommittee, we wish to thank Prof. Robert Hull for his role in conducting an outstanding workshop and in preparing this report, as well as the staff at the National Science Foundation's Division of Materials Research for their leadership in organizing the workshop. We also thank all the speakers, session chairs, and participants for their time and efforts to join the workshop and to make their individual contributions to the discussions at the workshop and to this report. Their generous sharing of the results of their research and their insights ensure that this document will serve as a valuable reference for the NNI.

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EXECUTIVE SUMMARY

Nanomaterials are the engine that drives the nanotechnology revolution. Advances and discoveries in nanomaterials are pervasive throughout all fields of nanoscience and nanotechnology, providing major new scientific advances and enabling broad new technological applications. New nanomaterials are continually being discovered, providing entirely new properties and functionality by virtue of their ultra-small dimensions or due to the new methods by which they can be assembled and integrated. These breakthroughs can be expected to continue. Fundamental research in this field in the coming decade can be expected to fuel revolutionary advances in electronics, computation, telecommunications, data storage, energy storage/transmission/generation, healthcare, transportation, civil infrastructure, military applications, national security, and the environment.

The extraordinary progress in the field of nanomaterials in the past several years, largely enabled by the National Nanotechnology Initiative, provides the platform for these advances. Scientists have already demonstrated the ability to assemble, modify, and measure a wide range of materials at the atomic and molecular levels. Nanomaterials and nanotechnology have enabled substantial advances in products with a wide range of applications, including catalytic acceleration of chemical reactions, magnetic data storage, electronics, self-cleaning coverings and fabrics, thin-film coatings, and biomedicine.

The potential impacts of nanomaterials on technology, economics, and society, however, are only starting to be realized. Currently, the critical barrier impeding utilization of the full potential of nanomaterials is the inability to economically manufacture these materials in sufficient quantities with adequate control and precision. The next major advance in nanotechnology will be development of improved manufacturing methods built on recent progress in synthesis and design of nanomaterials.

This report summarizes the discussions, findings, and recommendations of a workshop held in Arlington, Virginia, June 11–13, 2003, to assess progress to date and to determine the major challenges in the field of nanomaterials over the next decade and beyond. Workshop participants concluded that the major scientific and technological challenge facing nanotechnology is the ability to develop, apply, and scale advances in nanomaterials to the stage where multiple new practical applications can be realized. This will require major advances in several fields of fundamental understanding:

- Control of materials properties and phenomena at the nanoscale
- Methods for atomic- and molecular-scale measurements of structure, chemistry, and properties
- New computational tools and theory for understanding, modeling, and simulating materials at the nanoscopic, molecular, atomic, and subatomic levels
- New methods for externally guided self-assembly of nanomaterials

Successfully overcoming these fundamental challenges is critical to realizing the potential of nanotechnology.

This report discusses five areas of research priority**:** assembly and patterning of materials, new tools for developing nanomaterials, materials for computation and information storage, virtual materials, and new properties and functionalities at the nanoscale. Four areas of application that are expected to impact society are highlighted**:** energy, information technologies, healthcare, and infrastructure and transport technologies. Cross-cutting issues of education and societal implications are also discussed.

The workshop participants summarized the most important mission for the next decade of research in nanomaterials as the development of effective “nanofoundries.” By this is meant developing the knowledge, methods, and instruments for fabrication of nanoscaled materials that enable economically viable applications with broad benefit to industry, technology, the economy, the environment, health, and society.

Workshop participants developed a “twelve-point plan” for realizing this mission:

1. Support high risk, high payoff projects, emphasizing discovery of new nanomaterials and properties and invention of new techniques and instruments for nanoscale fabrication, measurement, and synthesis.
2. Emphasize research that addresses understanding and exploiting interfacial properties between dissimilar media such as interfaces between organic and inorganic materials, nanoscale fillers and matrices, and heterogeneous biomaterials.
3. Develop new techniques for synthesizing and refining nanomaterials in large quantities.
4. Invent, develop, optimize, and control new methods for self-assembly of materials based on both biological and nonbiological methods.
5. Develop methods for realization of controlled hierarchical structures with multiple length scales down to the nanoscale.
6. Emphasize materials, methods, and instruments for harnessing subatomic properties such as electron spin and quantum interactions, with potential for revolutionary advances in electronic logic, data storage, and computation.
7. Improve instruments and techniques for structuring and patterning materials at increasing levels of precision.
8. Develop techniques to measure the structure, properties, and chemistry of materials with full three-dimensional addressing at the atomic scale (in essence, a nanoscale global positioning system—a “nano-GPS”).
9. Develop computational methods, algorithms, and systems—both classical and quantum—to enable realistic simulation of processes over all relevant length and time scales.
10. Emphasize the interface between nanomaterials and biological systems to enable widespread improvements in human health. In parallel, the potential toxic effects of “nano-sized” particles on living systems and the environment should be fully investigated.
11. Focus on fundamental understanding of fault tolerance, that is, the degree of perfection necessary in nanoscaled systems to attain desired functionality, and the degree of perfection allowed in such systems by the fundamental laws of nature.
12. Develop internal sensing methods for use in assembling or operating systems to optimize synthesis, evolution, and adaptation.

In addition to the twelve points listed above, the workshop generated several broad-based, cross-cutting recommendations to enable nanotechnology to achieve the advances described above:

- Create a vigorous educational program addressing the nature and potential impact of nanomaterials, encompassing all segments of society and all levels of the educational spectrum
- Expand research in the field of structural materials to provide the foundations for new breakthroughs at the nanoscale in this important field
- Expand programs designed to support the operation of medium-sized specialized instruments for nanoscale science and engineering, and to develop more affordable instruments
- Strengthen the interactions between industry, academia, and government laboratories

Realization of the twelve-point plan could ultimately enable broad societal benefits. For example, major advances in healthcare may include applications in prevention, diagnosis, and therapy, such as the ability to repair vision, treat paralysis, and locally diagnose and treat cancers. Increasingly sensitive instruments will improve medical imaging resolution, enabling earlier detection, diagnosis, and treatment of tumors and other diseases. Miniaturization of surgical instruments has the potential to revolutionize procedures, reducing invasiveness and risk. Advances in miniaturized electronics that are biocompatible, coupled with nanoscale precision in drug delivery, are expected to allow remote monitoring and targeted dosimetry for highly individualized healthcare.

In the field of information technology, new generations of computers could combine petaflop speed with ultra-low power consumption and the ability to boot up instantly. Current “top-down” chip manufacturing is likely to integrate with “bottom-up” molecular assembly to enable entirely new paradigms for electronics and communications. Quantum computers may enable entirely new fields of computation and simulation.

To help address growing energy needs, increases in the efficiency of chemical catalysis coupled with greatly improved materials for power storage, conversion, and generation hold promise for revolutionizing energy usage. Nanostructured materials design could significantly reduce worldwide energy consumption. Sensors based on novel nanomaterials are expected to improve process monitoring, leading to real-time analysis to enhance energy efficiency and minimize waste in manufacturing operations and to help reduce environmentally harmful emissions.

Improvements in the safety and reliability of civilian infrastructure, transportation systems, and consumer products may include new nanostructured materials and composites for vehicles, buildings, bridges, and roads with greatly enhanced functionality and durability. With embedded sensors, new systems are possible with capabilities for self-diagnosis, self-correction, and self-healing. Together, such advances would enable major improvements in safety, quality, and reliability. In combination, these changes can result in substantial improvements in human health, the environment, the economy, and our standard of living, and they can help address other major challenges facing our nation and planet.

1. Introduction

PROGRESS IN THE PAST DECADE AND CHALLENGES FOR THE NEXT DECADE

There has been an extraordinary confluence of new capabilities in computation, synthesis, and measurement that has expanded knowledge of nanomaterials over the past decade, with further revolutionary advances promised in the coming decade. These capabilities offer the potential for engineering and design of materials, structures, and systems with unprecedented precision—that is, they promise the ability to assemble structures from blocks that approach the dimensions of single molecules or even single atoms. This will in turn lead to greatly improved, even entirely new, functional properties of nanomaterials.

Examples already exist that illustrate how the ability to mass-produce nanoscale objects with extraordinary precision has enabled new or greatly improved technologies. The increasing miniaturization of individual features in electronics has brought computational power to desktops that would have been unimaginable a decade ago. Transduction of magnetic to electrical signals in multiple metallic layers just a few atoms thick—the phenomenon of giant magnetoresistance (see sidebar 1)—has made possible the explosion in magnetic storage capacity at the consumer level. Industrial processes based upon chemical conversion are being driven by nanoscale engineered materials whose surface reactivity enormously accelerates the constituent chemical reactions. Each of these technologies is driving industries with annual sales of tens to hundreds of billions of dollars. Emerging markets include the use of precisely controlled slurries of nanoparticles for planarization of surfaces in the microelectronics and other industries, stain-resistant surfaces for clothing, pigmentation materials for paints, and the use of ultraviolet absorbing nanoparticles for cosmetics and sunscreens.

The future promise of nanomaterials is that these successes can potentially be replicated across an enormous range of applications, providing technology innovations for industries that have existed for centuries, such as construction; new technologies that have only recently evolved and enabled new industries, such as optical telecommunications; technologies that are currently only imagined, such as quantum computing; and technologies that have yet even to be conceived.

The most significant challenge to realization of this potential is to develop the ability to structure materials systems with the necessary precision over all relevant length scales, from atomic or molecular dimensions to objects as large as airplane wings or bridges (see examples in sidebar 2). Further, such materials and systems should be manufacturable in sufficient quantity and at sufficiently low cost that broad new technological applications become commercially viable. The assembly processes for these structures—as well as the materials themselves—should have a degree of "intelligence," that is, the ability to assemble in ways that are responsive to or optimized for the system's environment or its application needs.

Over the past decade—largely due to momentum developed through the *Materials by Design* Grand Challenge in the initial five-year implementation of the National Nanotechnology Initiative—extraordinary progress has been made in the ability to synthesize, control, manipulate, and address objects at the nanoscale. The forward-looking mission is to extend these capabilities to design and assembly of functional systems whose performance is optimized by the properties and interactions of components at the nanoscale. Nature has provided ninety-two elements and a set of bonding mechanisms with which to connect atoms and molecules. As the methods for building from these fundamental blocks are developed, the possibilities become limitless.

In response to this mission, this report identifies five crucial research and development (R&D) target areas where materials scientists should aim:

- Beyond conventional lithographic patterning and assembly
- Beyond equilibrium materials
- Beyond materials for binary logic
- Towards virtual materials
- To emerging developments at the nanoscale

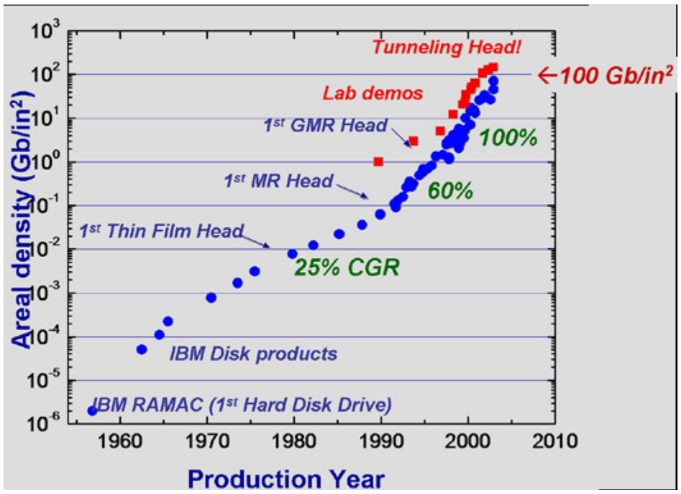
Nanomaterials R&D themes emerging from the above areas include:

- The need to control the size, distribution, placement, orientation, coherency, properties, and addressability of nanoscaled objects in diverse structures and environments, including biological media
- The need to effectively span length and time scales in both experiment and computation
- The ability for materials properties and systems to optimize, adapt, and reconfigure according to changing environment or evolving need
- The need for nanoscale tomographic (three-dimensional) measurement of structure, chemistry, and properties
- The ability to mass-produce nanostructured materials that can operate in extreme conditions, e.g., of temperature, pressure, or acidity

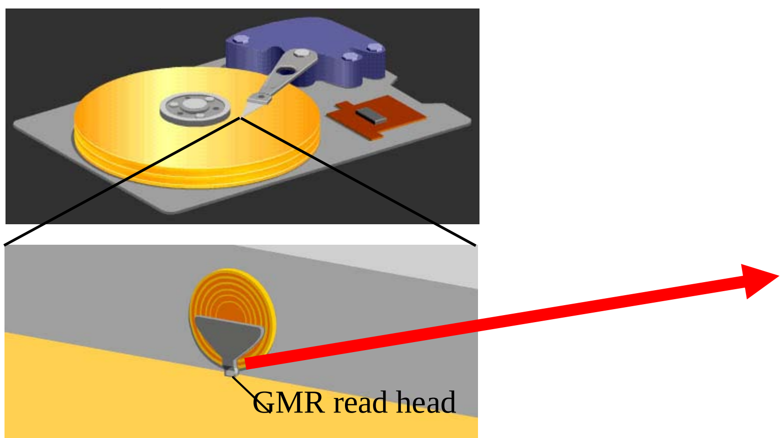
Workshop participants surveyed four areas of potential technological and economic impact for nanomaterials:

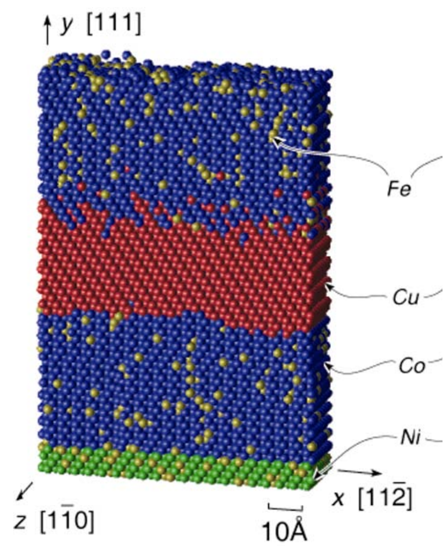
- Information technologies
- Health and medical technologies
- Energy technologies
- Civil infrastructure and transportation

The results of this exercise reemphasized the need to address the scientific priorities and R&D themes described in the preceding paragraphs and identified additional specific problems and barriers to overcome.

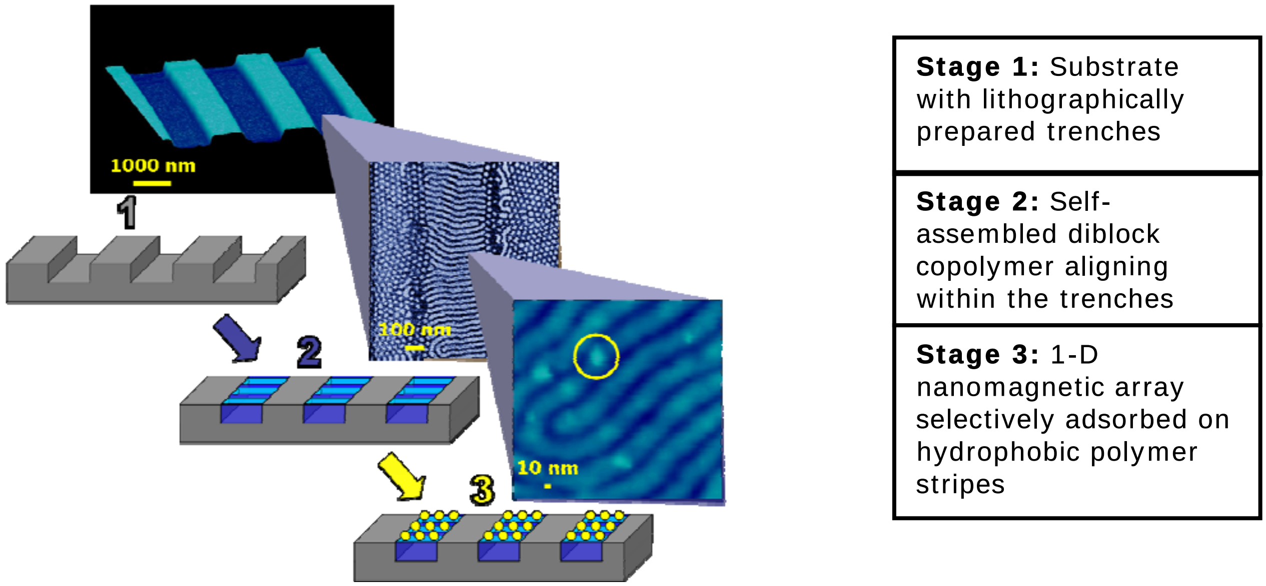


Top left: Evolution of hard drive storage capacity vs. year first in production (image courtesy of S. Parkin, IBM). Bottom left: Schematic image of a magnetic disc drive. Bottom right: Atomistic simulations of a giant magnetoresistive layer structure (image from X. Zhou et al., Acta Mater. ***49****, 4005 (2001); reprinted with permission from Elsevier).*

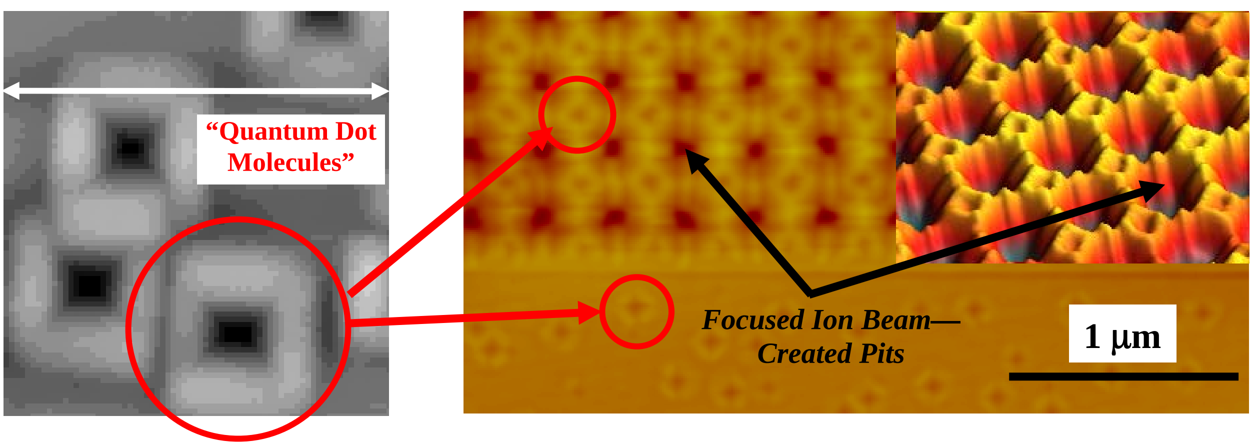




Sidebar 1: Giant Magnetoresistive Materials—A Fast Track from Fundamental Science to Economic Impact. Nanostructures formed from atomically thin layers of ferromagnetic and nonferromagnetic metals, for example, Co/Cu/Co, can be engineered to display very large changes in electrical resistance in small magnetic fields—the so-called giant magnetoresistance (GMR) effect—thus providing exquisite sensors of tiny magnetized regions in magnetic layers. These sensors, named spin valves, depend on spin-dependent scattering of electrons at the interfaces between the nonmagnetic and ferromagnetic materials. By engineering these interfaces on the atomic scale, the magnitude of the effect can be dramatically increased. Such sensors are at the heart of every magnetic recording disk drive manufactured today. Since their introduction at the end of 1997 by IBM, they have enabled a several hundred-fold increase in the capacity of disk drives even as the cost of these drives has decreased enormously. The phenomenon of GMR was originally a scientific curiosity discovered in 1988 at low temperatures (4 K) and large magnetic fields (20 K Oe) in single crystalline Fe/Cr multilayers prepared by molecular beam epitaxy techniques. In 1989 it was shown to be a widespread phenomenon observed in sputter-deposited polycrystalline multilayers formed from almost any combination of transition metal ferromagnets and nonmagnetic metal layers. Moreover, it was discovered that the very nature (ferromagnetic vs. antiferromagnetic) of the magnetic coupling between ferromagnet layers depends periodically on the thickness of the intervening nonmagnetic films, with length scales varying over just a few atomic dimensions. This has spawned a new field of "spin engineering" of a host of new solid state storage, logic, and memory devices. Remarkably, the time from the observation of the first GMR effect to its widespread use in magnetic hard disk drives was less than ten years.



<u>Hierarchical Assembly of Magnetic Nanostructures.</u> Three levels of assembly are shown to simulate a possible future for patterned magnetic recording media. The first stage would be to imprint trenches on a substrate, followed by self-assembly of diblock copolymers within the trenches to achieve a template of finer length scale. Finally surfactant-mediated magnetic nanoparticles would selectively adsorb on the hydrophobic stripes to form individual "bits" on "tracks" (image courtesy of S. Darling, S. Bader, Argonne National Laboratory).



<u>Hierarchical Assembly of Semiconductor Nanostructures.</u> The positions of self-assembling epitaxial GeSi/Si "Quantum Dot Molecules" (QDMs) can be programmed using predefined surface topography: one QDM forms at each interstice between holes. This provides a new method to achieve controlled nanostructure assembly over multiple length scales—from individual dots (tens of nanometers) to the dot molecules (ca. 200 nm) to the macroscopic arrays defined by the surface topography (images courtesy of J. A. Floro, Sandia; J. Gray, R. Hull, University of Virginia; reprinted with permission from Nano Letters, ***4****(12), 2447. © 2004, American Chemical Society).*

Sidebar 2: Hierarchical Assembly—from Nanostructures to Macrostructures—the Core Challenge in Nanomaterials? A myriad of potential technological applications of nanomaterials rely upon the ability to define structure, chemistry, and properties over incredibly small dimensions, while simultaneously being able to engineer systems of such "nano-elements" over much greater length scales. This evolution is already inherent to the development of the microelectronics industry—and in the assembly of living systems. In particular, biological systems combine the elements of assembly, adaptation, and selection that would be highly desirable to extend to inorganic systems. The ability to engineer over multiple lengths scales, through external intervention and/or through self-assembly processes, to enable complex yet exquisitely adaptive systems, is a key nanomaterials challenge for the coming decade.

POTENTIAL ROUTES TO VIABLE NANOMANUFACTURING

To illustrate the scope of the important priority of achieving effective nanomanufacturing capability, consider the many potential applications of nanomaterials to large volume structures such as those prevalent in transportation and the civil infrastructure. The cost of most structural engineering materials—steels, plastics, aluminum alloys, etc.—are on the order of one dollar per kilogram, or as low as cents per kilogram in the case of concrete. The cost of a kilogram of high-quality carbon nanotubes or fullerenes is currently incompatible with such uses, in the range of hundreds of thousands of dollars per kilogram for highly pure single-walled carbon nanotubes. Simply put, the potential range of applications of nanomaterials is enormously compromised by the difficulties of manufacturing at competitive cost and in sufficient quantity. These challenges extend beyond volume alone. Many applications require not just large numbers of components but the ability to organize into complicated, multiscaled hierarchies (the electronic circuit being a classic example). Thus, components need not only to be fabricated in mass-production quantities, but they often need to be arranged accurately into complex patterns. Successfully overcoming such challenges is critical to realizing the potential of nanomaterials and enabling the social, economic, environmental, and technological promises of nanomaterials. Approaches currently being developed include the following:

- ***Low material volume, high precision systems:*** In some major classes of applications (such as many future architectures for electronics, telecommunications, and magnetic storage), the raw materials—silicon, silica, iron alloys—are fundamentally cheap and available in quantity. The volume of material that is engineered within a state-of-the-art microprocessor, containing over a hundred million components, is about one cubic millimeter. In these cases, the power of nanotechnology lies in the positioning of large numbers of very small objects whose functionality depends upon controlled interactions between them, and “quantity” is defined by the number of components rather than by the volume of engineered material necessary. The critical challenge is not producing sufficient material but being able to control positioning and structure of elements over large arrays. The obvious example here is the scaling of microelectronics down to the nanoscale regime. State-of-the-art microelectronic circuits are typically comprised of 10^8–10^9 individual components, each engineered with extraordinary precision to integrate with all other components in the circuit. As devices in electronics further scale down in size, the numbers of components and required engineering precision can be expected to increase. The key limitation becomes the ability to define and align structures with sufficient precision (to tens of nanometers or better), and with sufficient throughput, coupled with integration of virtually all classes of materials, over length scales spanning many orders of magnitude from atomic to macroscopic scales. This will require the development of new methods for assembly and patterning of such structures, ranging from evolution of existing lithography techniques through the development of new methods for self-assembly of complex nanostructures, including biologically inspired or mediated approaches. Such approaches should be extendible to many nanomaterials systems.
- ***Nanostructured functional coatings:*** In some applications, nanoengineered coatings can be applied to large volume structures to provide desired functionality. To cover an aircraft wing with a coating one micrometer thick would require about one hundred cubic centimeters of material, which may still be a significant quantity. Enormous scientific and engineering challenges remain to making such coatings adaptable to external responses, self-interrogating and repairing, and able to internally communicate across the structure, to mention just a few potential breakthrough capabilities envisioned for such structures. Another major challenge is the development of techniques for reliable and uniform application of such coatings to large-scale, complex shape structures comprising a wide variety of materials.

- ***Internally structured and nanocomposite systems:*** Structures with controllable internal nanostructure, such as the pore arrays in aerogels, offer the opportunity to use the enormous surface area of internal nanoscale voids to engineer nanostructured systems. Such materials have many exciting properties in their own right—such as extraordinary dielectric, optical, acoustic, and thermal properties—but can further be functionalized by controlled incorporation of active elements within the pore array. Potential applications include biological sensors and assaying, novel compound magnetic materials, and integrated optically active semiconductor nanostructures. More generally, composite materials can use relatively small fractions of a nanoscaled component to enhance properties of the matrix. In both cases, however, large-scale applications (transportation, civil infrastructure) will require relatively large volumes of the nanoscaled "filler" component, and exquisite processing control will be required to realize the desired internal structures. Preliminary applications such as sports equipment and specialized auto parts are already being commercially realized. Again, self-assembly methods may be important.
- ***Scaling of synthesis methods:*** The most important driver in many applications will remain the need for large production volume, requiring scaling of current synthesis methods by orders of magnitude in many cases. Materials such as fullerenes, carbon nanotubes, and semiconductor quantum dots and wires have properties that offer enormous potential for new applications and technologies, but they generally cannot be produced in anything like the necessary quantities for "bulk" applications such as transportation or civil infrastructure, or even for widespread use in limited quantities (for example, the use of endrohedral fullerenes as contrast agents for magnetic resonance imaging). Coupled with the need for increased volume is the need for increased control, for example in selecting the chirality (and hence electronic properties) of carbon nanotubes, requiring entirely new capabilities for *in situ* characterization and control during production. New synthesis techniques enabling production volumes are thus necessary.

THE WORKSHOP

The National Nanotechnology Initiative (NNI) Workshop on Materials by Design was convened on June 11–13, 2003, in Arlington, Virginia. The workshop was sponsored by the National Science Foundation (NSF), particularly NSF's Division of Materials Research, and the NSET Subcommittee of the National Science and Technology Council's Committee on Technology. The agenda is included as Appendix A to this report. The workshop was attended by over 100 nanotechnology experts from industry, academia, Federal agencies, and private research institutes, as listed in Appendix B.

The workshop had two overriding purposes:

- To articulate the "hard problems"—specific scientific and technological hurdles that have to be overcome to achieve broader research and development goals—related to nanoscale science and technology in materials
- To consider long-term (ten years or longer), visionary challenges for researchers in nanoscale science and technology related to materials, which could inform the development of a "grand challenge" in nanomaterials

Workshop participants were asked to both define the broad vision of this challenge and to identify a set of crucial components of the vision.

The workshop was structured around a set of visionary presentations from leaders in the nanotechnology field and two sets of breakout sessions. The purpose of the breakout sessions was to develop the rationale, vision, and material for this report.

THE REPORT

The workshop sought input from the research community on the NNI research agenda related to one of the original NNI "grand challenge" topics, "Nanostructured Materials by Design." The findings from this workshop were subsequently used in formulating the NNI Strategic Plan, released in December 2004,[1] which replaced the "grand challenges" outlined in the initial plan with "program component areas." Workshop findings helped to shape the Nanomaterials Program Component Area included in this current strategic plan, defined as

> *Research aimed at discovery of novel nanoscale and nanostructured materials and at a comprehensive understanding of the properties of nanomaterials (ranging across length scales, and including interface interactions). R&D leading to the ability to design and synthesize, in a controlled manner, nanostructured materials with targeted properties.*

Workshop findings have also been used as input to the development of programs that make up portions of the fiscal year 2006 through 2009 budgets requested for the National Science Foundation and other NNI participating agencies.[2]

Chapter 2 summarizes the emerging themes identified by the workshop participants that define the scientific challenges and opportunities in nanomaterials over the next decade and beyond, including breakthroughs in the assembly and patterning of materials, new tools in the nanomaterials construction set, breakthroughs in materials for computation and information storage, breakthroughs in virtual materials, and new properties and functionalities at the nanoscale. Chapter 3 discusses how nanomaterials could benefit society, while Chapter 4 lays out educational issues. Conclusions and recommendations are contained in Chapter 5, along with a vision for the field of nanomaterials research.

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[1] http://www.nano.gov/NNI_Strategic_Plan_2004.pdf. See also the updated NNI Strategic Plan released in December 2007, http://www.nano.gov/html/about/strategicplan.html.

[2] See http://www.nano.gov/html/res/pubs.html.

2. Exploring New Realms in Nanomaterials

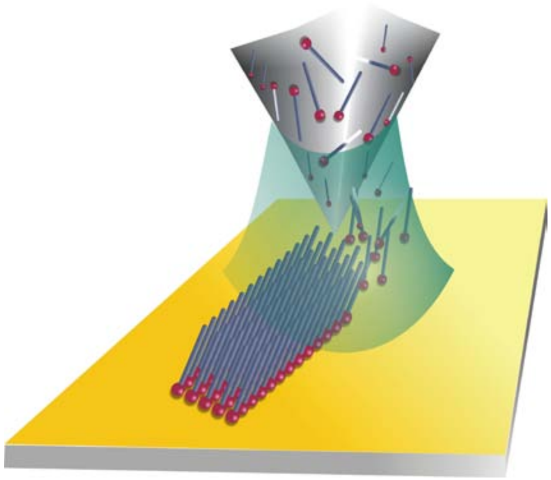
This chapter summarizes the emerging themes identified by workshop participants that define the scientific challenges and opportunities in nanomaterials over the next decade and beyond.

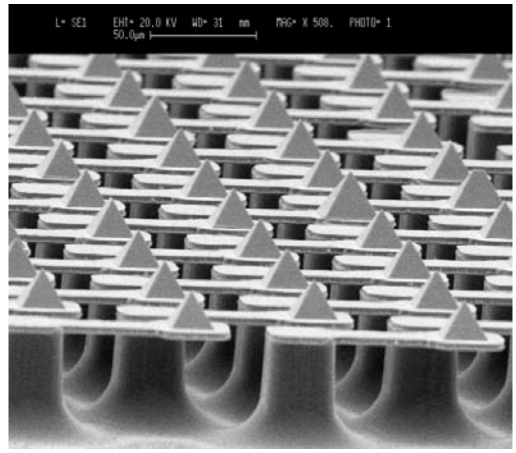
BEYOND CONVENTIONAL LITHOGRAPHY—BREAKTHROUGHS IN THE ASSEMBLY AND PATTERNING OF MATERIALS

Current technology employs two approaches to create very small structure in materials. The first is a "top-down" lithographic approach in which a bulk material is patterned in some fashion, and then some of the material is removed to leave behind very small structures whose shape and size are defined by the size of the mask and the exposure technique used to write the mask pattern onto the bulk material. These top-down techniques are limited in the size of the structures that can be created. In addition, traditional lithographic techniques operate almost exclusively on two-dimensional structures. Even smaller scale objects can be produced using self-assembly ("bottom-up") techniques, the second approach, where the combination of entropic and enthalpic energies control the shape of the structures formed. Using such techniques, it is relatively easy to produce highly ordered structures on short length scales, but it becomes extremely difficult to produce controlled, ordered structures on larger length scales.

The current limitations of both lithographic and self-assembly techniques guide one important new research direction that extends beyond lithography. This is the fabrication of highly controlled structures created by merging the two techniques in a seamless fashion. Moreover, significantly more complex structures would be produced by extending these techniques to three dimensions. This objective could be accomplished if lithographic techniques could be extended to make reliable structures at the scale of 1 nm, while self-assembly techniques could be controlled to make structures at length scales up to 100 nm, ensuring substantial overlap between the top-down and bottom-up techniques. A promising approach is to use top-down methods to direct controlled self-assembly processes within lithographically defined regions (see sidebar 2 in Chapter 1). The ultimate goal is to control material composition and structure with 1 nm resolution and extending up to macroscopic length scales. Such controlled nanomaterials would have myriad applications, including in improved catalysis, embedded healthcare systems, energy storage, and drug delivery.

One potential breakthrough research accomplishment is the inclusion of adaptive or "smart" features in the mask and in the patterned material itself. This would qualitatively change the way nanomaterials are fabricated and may be essential for producing highly complex materials with controlled structures extending from the nanoscale to macroscopic scales. In current technology, all of the information is carried in the mask, and this information is purely static in that it is written into the mask and cannot be subsequently modified. However, as lithographic techniques extend to ever smaller length scales, and as the nanoscale structures become ever more complex, new methods of encoding information should be found. The masks should become adaptive, to allow their patterns to evolve or change. In addition, methodology should be developed to allow information to be carried directly in the material being patterned. This could allow far more complex structures to be created and would also enable qualitatively new structures to be created, since a new type of information can be encoded in the patterned material. Success would make it possible to create materials that seamlessly change their structure, composition, and function on nanometer length scales and over macroscopic sizes.





Left: Schematic illustration demonstrating the concept behind dip pen lithography. Right: A portion of a 10,000-pen array used for doing massively parallel dip pen nanolithography (images courtesy of Prof. C. Mirkin, Northwestern University).

Sidebar 3: Writing at the Nanoscale. The technique of dip pen lithography is allowing researchers to build materials up from the nanoscale with extraordinary control over materials architecture. Almost any material can be used as an "ink," including DNA, proteins, and catalysts, making this a promising tool for both the inorganic and life sciences industries.

Full exploitation of all of these techniques will also require the intermingling of both "hard" and "soft" materials on the nanoscale. This will be important to access the full range of potential properties of the patterned material and the structures produced. In addition, biological applications will require the use of soft material at the interface between the fabricated structure and the intelligent nanopatterned structure. Thus, techniques must be developed to use both the traditional hard materials and soft materials concurrently in nanomaterials. Several promising advances have been made in this regard, but many challenges remain. A variety of high resolution tools are available (at moderate cost compared to state-of-the-art optical lithography techniques employed in the microelectronics industry), including dip pen nanolithography, nanoimprint lithography, electron beam lithography, and focused ion beam lithography. These methods allow patterning, processing, and selective functionalization of hard and soft matter with sub-100 nm (even sub-10 nm) resolution. Each has advantages and disadvantages in the key categories: resolution, throughput, materials flexibility, alignment registration, direct-write capabilities, and the ability to handle multiple chemical agents. Nanotechnology researchers and technologists need printing tools with the flexibility of the macroscopic tools currently available for desktop printing. The technique of dip pen nanolithography (sidebar 3) has focused on delivering this capability, employing an atomic force microscope as a nanoscopic pen to directly deliver chemical or biological inks to a surface with nanometer-scale resolution. Another recent innovation, nanoimprint lithography, offers the ability to print 10-nanometer-scale features over large areas, with feature throughput far in excess of existing technologies.

BEYOND EQUILIBRIUM MATERIALS—NEW TOOLS IN THE NANOMATERIALS CONSTRUCTION SET

An extraordinary opportunity for revolutionizing the construction of nanostructured systems is the emerging capacity for engineering hierarchical three-dimensional structures using coded molecular templates. In essence, this process uses nature's models to engineer complex materials, for example, by using DNA-like sequencing instructions or through use of biologically mediated assembly of inorganic nanostructures, such as the viral assembly described in sidebar 4. This approach could dramatically increase the ability to produce new materials, since it will enable "weaving" of materials molecule by molecule—akin to the pointillist method of painting made famous by Seurat. It offers the possibility of achieving high reproducibility on a large scale of complex materials that are individually tailored on the nanoscale. It should also be, in principle, scalable to unlimited complexity.

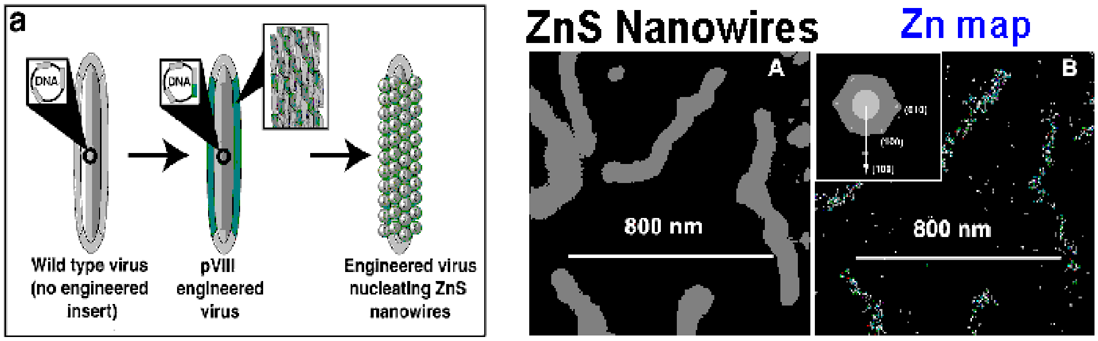
Such capabilities would have major potential technological, industrial, societal, medical, and environmental benefits. For example, new materials could be engineered that are evolvable and adaptable, comprising "smart" materials that contain embedded sensors, with the capability to respond to stimuli and communicate information. These materials could embody the ability to self-diagnose, self-heal, and morph in response to changing conditions. Such materials would be crucial for advancement of space, deep sea, and geological exploration, where components must operate under extreme conditions and where human intervention, repair, or resupply is not feasible.

Engineering diversity and chemical complexity are essential for the advancement of materials in healthcare applications. To be effective in medicine, new materials must be designed to enable seamless integration with natural tissue, where understanding of nanoscale complexity and its effect on structure and function is continuously evolving.

Engineered interfaces could be designed with molecular-level control that allows for universal integration of different materials or components. Interfacial engineering is needed that promotes molecular control of adhesion and propagation of thermal, electrical, or optical signals. This technology would enable the development of increasingly complex systems that transcend nanoscale structure into macroscale function. Specific examples of such systems would include the following:

- Advanced sensors with molecular-level sensitivity.
- Nonspecific compatibilizers allowing universal recycling of materials in an efficient and inexpensive manner.
- Synthetic materials or components for organ repair and replacement. Interfacial structure is key to control of rejection, natural tissue regeneration, and whole body function integration.
- Lubricants and coatings that perform at the nanoscale. Increased miniaturization of mechanical components, such as microelectromechanical (MEMS) devices, relies on the ability to provide lubrication at the single-molecule level. Microscale/nanoscale motors produce shear stresses orders of magnitude higher than those achieved in macroscale systems.
- Synthetic substitutes for the replacement of "perfect" natural lubricants in joints destroyed by diseases such as arthritis or by accident or injury.

Another key capability would be the engineering of multifunctional materials that satisfy intuitively conflicting conditions, allowing such materials as self-lubricating metals, "structural glasses" that are moldable, scratch- and impact-resistant, nonflammable, ultraviolet-absorbent, and strong enough to use as construction materials, and materials that can operate under extreme conditions of pressure, force, temperature, and chemical reactivity.



Sidebar 4: Harnessing Biology for Assembly of Nanomaterials. Engineered viruses (e.g., M13 bacteriophage with encapsulated combinatorially designed peptides) have been successfully used as templates for the growth of wires and other assemblies of semiconductor quantum dots from precursor solutions. This promises an entirely new route towards controlled assembly of nanoscale structures (images from Mao et al., *PNAS* 100, 6946. Reprinted with permission, © 2003, National Academy of Sciences, U.S.A.).

Many of the tools and techniques are in place to allow these advances. Over the past decade, there has been great improvement in fundamental understanding and application of nonequilibrium phenomena that produce nanoscale structures over large macroscopic areas. Examples include spinodal decomposition of multicomponent systems, self-assembled monolayers of functional molecules, complex molecular self-assembly such as that achieved with block copolymers, and interfacial segregation driven by entropic or enthalpic forces. Tools for nanoscale lithography have been greatly improved, as described above in the section *Beyond Conventional Lithography*. New methods for fabrication and control of nanocomposite materials provide enhanced strength and elastic moduli. Diagnostic tools are continually improving, bringing closer the goal of continuous analysis on length scales ranging from the nanoscale to the macroscale.

A major challenge in assembling these diverse materials is the construction of systems over the necessary hierarchical range of length scales—from the atomic to the macroscopic (see sidebar 2 in Chapter 1). Many potential technological applications of nanomaterials rely upon the ability to define structure, chemistry, and properties over the smallest dimensions while simultaneously being able to engineer systems of these nanoscale objects over much greater length scales. This evolution is already evident in the development of the microelectronics industry as well as in the assembly of living systems. The ability to apply these concepts to a far broader range of complex, yet adaptive, systems is an important nanomaterials challenge for the coming decade. For example, synthetic polymers possess neither the structural nor compositional sophistication of natural proteins. The latter combine monomer segments and specific modifications to create nanometer-sized molecules of highly specific structure and function. Synthetic polymer approaches, however, still make materials that are far less sophisticated and precise. The ability to prepare materials with specific sequences of monomers is lacking, and polymerization can be controlled only for high molecular weight materials, producing materials with characteristic distributions of molecular sizes. The combination of improved understanding of molecular assembly in biology and greatly advanced computational techniques may eventually enable synthesis of complex polymeric materials with very precise structures and functional properties.

BEYOND MATERIALS FOR BINARY LOGIC—BREAKTHROUGHS IN MATERIALS FOR COMPUTATION AND INFORMATION STORAGE

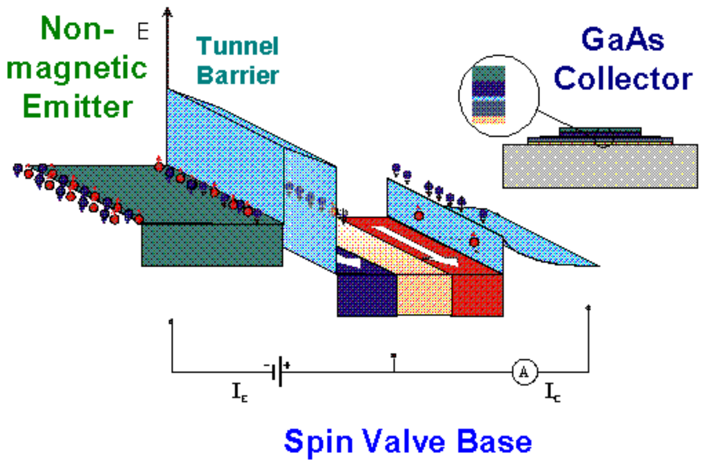
One of the most important aspects of replacing conventional electronic devices with those fabricated at the nanoscale level is that new phenomena arise because the size of the objects are on the same order as the atomic or molecular interaction distances that give rise to properties. As materials approach a size regime where classical behavior is no longer operative, quantum effects become important. This opens up a realm of possibilities for discovering new physical phenomena and for enabling new technologies based on quantum devices, most notably quantum computing. In terms of information technology, the vision is to use nanoscale objects (whether atom or molecule-based components) to build integrated, multifunctional, multidimensional devices. The opportunities are extraordinary for major advances in new information technology technologies based on new nanomaterials as well as new integrated, hybrid systems based on nanomaterials.

One enormous future opportunity in electronically functional materials is to be able to use directed self-assembly to make multifunctional, multidimensional materials systems from integrated organic, inorganic, and biological components. The combined use of intermolecular interactions such as van der Waals, hydrogen, electrostatic, and covalent bonding allows for a diverse number of different materials to be combined into one system, as discussed above in the section *Beyond Equilibrium Materials*. Examples include molecular electronic materials and nanowire/nanotube materials. Such components can be envisaged in a broad spectrum of connection, sensing, and input/output applications.

Another major opportunity emerging in nanomaterials is to use the spin of an electron, its manipulation, and its measurement to produce a new class of integrated device structures for use in the storage, logic, communication, and sensor industries (see sidebar 5). These structures would fall in the class of “beyond binary logic” because of the complexity of information that might be stored, addressed, manipulated, and read out. The ability to combine magnetic materials with semiconducting/metallic, molecular structures to produce spin transistors, spin or magnetic tunneling devices, spin filters, and spin readout devices must be developed first. Excellent interfaces between these materials need to be developed. The quantum mechanical coupling of two or more spins will also have applications for quantum computing, as discussed in Chapter 3.

For the future implementation of electronically functional nanomaterials, it will be necessary to identify and develop new magnetic, electronic, and photonic materials that can be integrated into more complex hybrid nanostructures containing much more functionality than currently possible. The progress in carbon nanotube research provides basis for the belief that more work on inorganic fullerenes could produce even more functionality and diversity that could be easily integrated into complex nanomaterials.

Almost all of the applications of nanomaterials for information technology require learning how to rapidly and reliably address the information embedded at the nanoscale. Success will require development of materials and systems with error and defect control or tolerance. This is especially true for structures that attempt to use quantum information because of the probabilistic nature of quantum mechanics and quantum information. This is well known in quantum computation architectures, and it will also be true for most quantum devices.



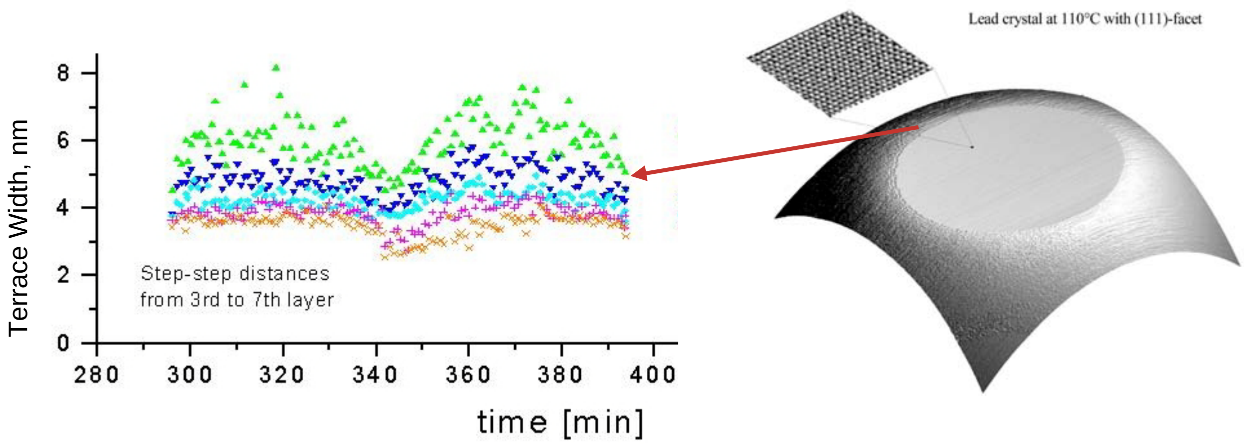
(image courtesy of Stuart Parkin, IBM)

Sidebar 5: Harnessing the Spin of Electrons. If we could harness the spin of the electron as well as its charge, new functionalities would emerge, spurring radical advances in computer and electronic development. For example, in present-day computers the file storage system is based on magnetic hard disks. In the future it is possible that random access memory (RAM) could be based on magnetic nanomaterials that would be *nonvolatile* (i.e., information is not lost when the power is removed, whereas conventional semiconductor RAM is volatile), ushering in a new era of instant boot-up computers. Such magnetic RAM would also need no power drain to refresh the RAM as in today's devices, so it could be addressed and written with lower power consumption. (Power dissipation presents a major obstacle to further miniaturization of high-end microelectronic chips.) Magnetic RAM will become increasingly commercially available over the next few years.

Another longer-term goal is the development of magnetic logic elements based on spin transistors. These would be inherently reprogrammable, such that we can imagine a magnetic central processor unit that adapts itself to the task at hand instantaneously in order to enhance computer performance on the fly. This would serve as an auxiliary strategy, in addition to massively parallel processors, to reach the goal of petaflop performance levels. A hard problem in magnetic nanomaterials related to the development of spin transistors is to realize nearly 100% spin-polarized sources where the spin polarization is preserved across diverse interfaces. Current candidate materials tend to be complex magnetic oxides whose stoichiometry and structure are difficult to control, especially at interfaces. Thus once again, progress requires a concerted effort to master materials at the nanoscale.

Another emerging possibility is to use biologically inspired routes to design new multifunctional nanomaterials and assemblies. While it may be possible to eventually employ or mimic living systems in nanotechnology, there is little doubt that the immediate future of nanotechnology will benefit from the study of how biological molecules sense their surroundings and how they manufacture complex materials, as discussed above in the section *Beyond Equilibrium Materials*. One of the most important lessons that scientists and engineers can learn from nature is that complex biological materials can perform a variety of complex functions at the nanoscale level. They have exquisite control over recognition "addressability," they behave as switches, and they perform catalysis with high specificity.

An overarching hard problem in realizing these new possibilities is developing a more complete understanding of how precisely these new nanoscaled systems are required to be—or can be—assembled. New methods for massive fault tolerance may have to be designed, to encompass, for example, errors in self-assembly processes. And, at the most fundamental level, researchers need to understand just how perfectly the laws of nature will enable such systems (see sidebar 6). Finally, how can the massive inherent information rates be manipulated, read, and stored sufficiently rapidly and with sufficiently low error rates? Inevitably, these challenges will require further departures from serial processing concepts and a minimization or elimination of mechanical processes (for example, the replacement of conventional hard drive storage technology by solid state magnetic or other nonvolatile memories). Ultimately, simple extrapolation or miniaturization of existing technologies will realize only a small fraction of the full potential of the new phenomena available through nanomaterials engineering.



Example of structural fluctuations in the nanoscale features of a micrometer-scale lead crystallite as it approaches its equilibrium shape. The terraces bounding the edge of the crystallite fluctuate with increasing amplitude until just before the nucleation of a new shrinking layer occurs at ~340 minutes (figures courtesy of K. Thürmer, Sandia National Laboratories).

Sidebar 6: Fluctuations at the Nanoscale: Good, Bad, or Interesting? Nature does not allow us to build structures with arbitrary precision. The thermodynamic rule of thumb that the magnitude of thermal fluctuations in a system scales as the inverse square root of the number of particles is the basis for some of the most exciting fundamental issues in nanoscience. When one is interested in controlling materials phenomena of individual nanoscale structures, the size of the fluctuations can easily become comparable to the system size. Theoretical approaches to dealing with the potentially interesting new phenomena include the concepts of the “first passage problem,” entropy production during fluctuations, ratchet motors, and issues of work in irreversible systems.

In solid state systems, structural fluctuations will occur most readily (and most observably) at surfaces, as illustrated in the figure above. Structural features fluctuate due to atomic motion if the thermal barriers are comparable to the available free energy, but the atomic fluctuations are correlated via the restoring forces holding the structures together. As a result, structural fluctuation time scales can be much slower than individual atomic hop rates, and amplitudes of fluctuation can be much larger than a single atomic displacement. Given real-time measurements of structural fluctuations from direct imaging techniques such as scanning tunneling microscopy and low energy electron microscopy, quantitative analyses of distribution functions and correlation functions have begun to provide tests and challenges for theory.

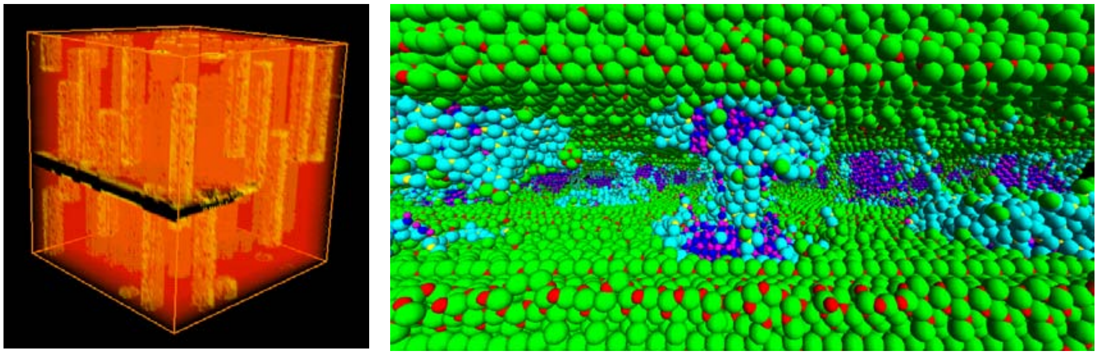
The exciting implications of these fundamental questions will occur in a broad range of potential applications for nanoscale materials, including information storage, noise, electrical transport and switching, self-assembly into patterned structures, chemical reactivity, and sensing. In each of these applications, fluctuation phenomena can generate nanoscale behaviors that are not simply scaled-down versions of the macroscopic analogs. Harnessing or controlling these new behaviors is one of the great challenges in the near future of nanoscience.

BREAKTHROUGHS IN VIRTUAL MATERIALS

Exponentially increasing capabilities in the field of computation enable the exploration and design of virtual (i.e., in computer space) nanoscale materials with desired structure, properties, and functionalities in advance of their actual fabrication. A confluence of ideas and expertise from multiple disciplines has set the stage for enormous advances in this field. Success will require new technologies and methods for the collaborative construction and execution of complex, multicomponent, computationally demanding numerical simulations for virtual materials. Such approaches will need to bridge enormous ranges of time and length scales and provide new methods for accurate simulation of processes that are currently computationally inaccessible. Progress in high-performance distributed systems can produce required new technologies, motivated by the challenge of producing entirely new arrays of nanomaterials, sensors, and devices, as well as aiding the discovery of new phenomena at the nanoscale. Impacts could include prediction of the structure and performance of nanomaterials from fundamental principles, the rational design of materials without extensive experimentation expenditures, and the development of crosscutting simulation technologies across all potential applications of nanotechnology (see sidebar 7).

Functional nanomaterials span length scales from interatomic distances (0.1 nm) to cellular dimensions (1–10 μm) and beyond. The challenge in accurately designing virtual materials is to describe electronic processes over length scales of 5–10 nm, atomistic processes over submicrometer dimensions, and macroscopic materials processes beyond the submicrometer length scale. This requires melding of a 10^5-atom quantum mechanical computation, e.g., in the framework of the density functional theory; a 10^9-atom molecular dynamics simulation; and mesoscopic and continuum models (see sidebar 8). A 10^5-atom density functional theory simulation is two orders of magnitude larger than allowed by the current state of the art of computational power, and therefore, algorithms scaling optimally with the number of computer processors and number of atoms (N) are essential.

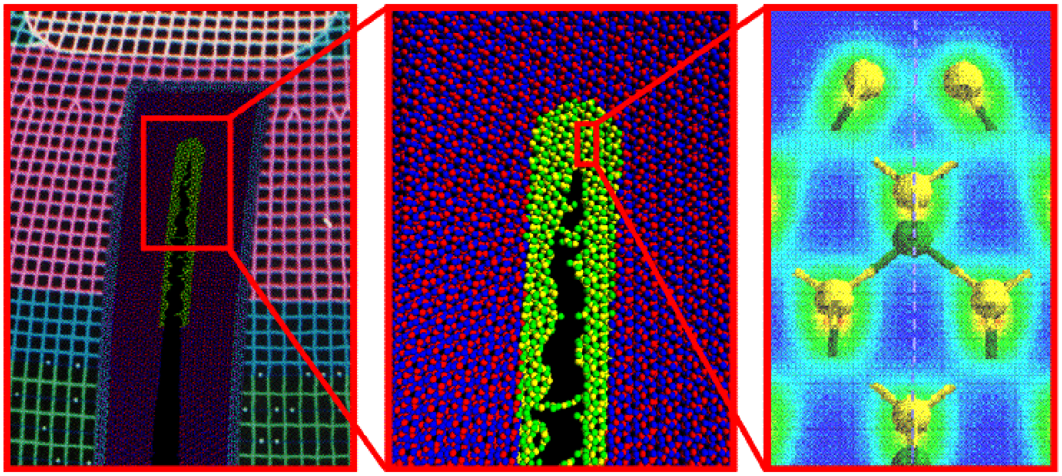
Key barriers to addressing these particular challenges include (1) design of approaches based on cost and error models to dynamically meld all of the above techniques; (2) deployment of distributed resources to enable two orders-of-magnitude larger density functional theory and molecular dynamics calculations within an integrated system simulation; and (3) reduction of the complexity of density functional theory simulations to order N through discovery of new algorithms. Comparable development of methods that extend or bridge to longer time scales is also critical, including the ability to accurately treat rare events. Entirely new methods that enable accurate calculation of electronic excitations are also highly desirable.



Left panel: Simulation of fractured silicon nitride (red) ceramic reinforced with silica-coated silicon carbide fibers (yellow). Right panel: Close-up of the fractured composite system. Small spheres represent silicon atoms and large spheres represent nitrogen (green), carbon (magenta), and oxygen (cyan) atoms (figures courtesy of R. K. Kalia, A. Nakano, and P. Vashishta, University of Southern California).

Sidebar 7: Modeling of Ceramic Fiber Composites. Physical properties of composite materials often exhibit synergistic enhancement. For example, the fracture toughness of a fiber composite can be substantially larger than a linear combination of the toughness values of the constituent materials. This enhanced toughness has been attributed to the frictional work associated with pulling out of fibers, which suggests that tough composites can be designed by combining strong fibers with weak fiber-matrix interfaces. Recently, molecular dynamics simulations have been performed to investigate the atomistic toughening mechanisms in Si_3N_4 ceramic matrix (bulk modulus 285 GPa) reinforced with SiC fibers (bulk modulus 220 GPa) coated with amorphous silica (bulk modulus 36 GPa). 1.5 billion atom simulations were performed on a 1,024 processor parallel computer. Fiber reinforcement is found to increase the fracture toughness by a factor of two. The atomic-stress distribution shows an enhancement of shear stresses at the interfaces. The enhanced toughness results from frictional work during the pullout of the fibers. Immersive visualization of these simulations reveals a rich diversity of atomistic processes, including fiber rupture and emission of molecular fragments, which must be taken into account in the design of tough ceramic composites.

While it is clear that the unprecedented complexity of nanomaterials makes numerical simulation a critical pathway to scientific progress, discovery of new phenomena, and the design of novel sensors and hybrid devices, extensive investment and development will be necessary to realize the full potential of virtual nanomaterials. Recent advances in simulation technology position researchers to address the necessary multidomain simulation challenges. However, these challenges cannot be addressed with today's high-performance computing technology and software, due to enormous computational requirements (even on 100 teraflop platforms), the complexity of the simulation structure, the dynamic nature of the simulation space, and the need to explore many alternative scenarios. One likely answer to these challenges lies in exploiting emerging grid computing concepts to manage dynamic simulation structure and in harnessing orders-of-magnitude more resources for simulation workloads than those available to researchers on any terascale system.



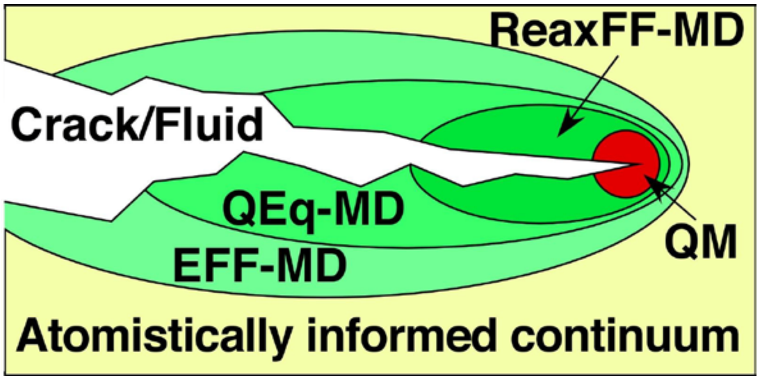
Finite Element (FE) **Molecular Dynamics (MD)** **Quantum Molecular (QM) Dynamics**

Schematic of hybrid multiscale finite element/molecular dynamics/quantum mechanical simulation of fracture. Continuum FE simulation invokes MD simulation near the crack tip and fractured surfaces to describe atomistic processes, which in turn invokes QM simulation at the crack tip to handle bond breakage/formation and chemical reactions involving environmental molecules (images courtesy of P. Vashishta, University of Southern California).

Sidebar 8: Geographically Distributed Multiscale Simulations on a Grid. "Metacomputing"—on a grid of geographically distributed teraflop-to-petaflop computers and immersive/interactive virtual reality environments connected via high-speed networks—will potentially revolutionize and democratize virtual nanomaterials design by enabling hybrid simulations that integrate the expertise of multiple scientists distributed globally. Key to the success of this approach are hierarchical multiscale simulations in which accurate calculations (e.g., 10^3- to 10^4-atom quantum mechanical) are invoked within coarser simulations (e.g., 10^7 to 10^{10} atoms using atomistic molecular dynamics, or from 0.1 μm to millimeters using finite-element-based continuum mechanics) only where or when high-fidelity modeling is required.

To achieve the goal of synthesis and fabrication of virtual nanomaterials it is imperative to take advantage of the advances in computing technologies from teraflop to petaflop (hardware, software, algorithms, and simulation methodology) to:

- Perform realistic simulations of nanomaterials, nano-bio interfaces, sensors, and devices
- Develop new methods for accurate predictions of electronic excitations in a nanoscaled system
- Demonstrate the feasibility of simulating virtual materials and processes not yet attempted (see sidebar 9)
- Incorporate simulation and parallel computing in physical and biological sciences and engineering education



Sidebar 9: Hierarchical Multiscale Simulations of Stress Corrosion Cracking. Corrosion is an enormously complex technological and economic problem with an annual cost of about 3% of the U.S. gross domestic product. The performances and lifetimes of materials widely used in defense and industrial applications are often severely limited by corrosion of these systems in environments containing oxygen and water, particularly in marine environments. The basic requirements for the operation of structural systems exposed to corroding conditions under stress loads are safety and reliability; these are endangered by the uncertainties regarding stress corrosion cracking (SCC). To prevent SCC and to predict the lifetime beyond which SCC may cause failure requires that we understand the atomistic mechanisms underlying SCC, that is, the conditions influencing initiation of SCC and the dynamics and growth rates. In multiscale simulations of SCC, quantum mechanical methods need to be employed around the crack tip, where atomic bonds break and highly nonequilibrium processes prevail. This region requires quantum mechanical (QM in figure above) computations of about 10^4 atoms. Quantum-mechanically informed reactive force fields in molecular dynamics (ReaxFF-MD in figure above) can extend the simulation of the reaction region around the crack tip to 10^6 atoms. With coupling between reactive force field and charge equilibration (QEq in figure above) schemes, it is feasible to scale up the system size to 10^8 atoms. Coupling of the charge-equilibration scheme to an effective force field (EFF in figure above) molecular dynamics approach with accelerated dynamics can further reduce the computational complexity and allow SCC simulations of up to 10^{10} atoms approaching microscopic time scales. Finally, an atomistically informed mesoscale continuum approach can extend the hierarchical multiscale computations to the macroscopic level.

Development of virtual nanomaterials over the next decade would thus incorporate the following key elements:

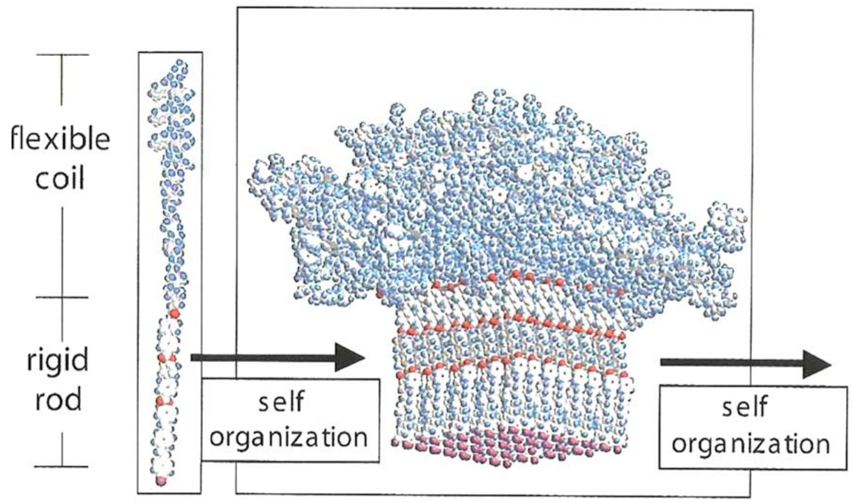
- Improved methods for first-principles modeling of growth, self-assembly, and interactions between nanoscale objects
- New methods for accurate predictions of electronic excitations in a nanoscaled system
- Methods for seamless multiscale modeling of complex nanosystems (e.g., inorganic/biological interfaces) using methodological advances such as integrated methods in a single program and parameter passing
- Algorithm development for computational nanotechnology
  - multiscale hierarchical modeling
  - treatment of rare events and long time scales (by continuum as well as atomistic methods)
  - development of order *N* first-principles methods
- Development of methods for accurate prediction of quantum transport in nanosystems
- Modeling of bio-inspired inorganic materials

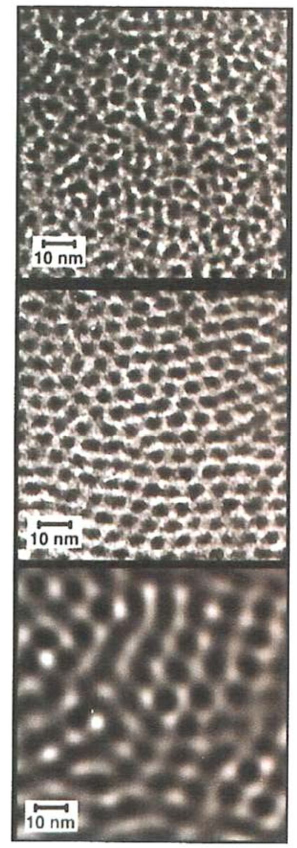
- Ability to model cooperative processes across coupled energy domains (e.g., living/non-living domains)
- Simulating and elucidating the constitutive relations and rules that govern the biological/inorganic interface (e.g., self-organization, self-replication, repair)
- More complete understanding of the effects of noise and entropy
- Discovery and implementation of entirely new computational algorithms, methods, and theory for atomic, molecular, and nanoscale simulation

NEW PROPERTIES AND FUNCTIONALITIES AT THE NANOSCALE

Remarkable progress has been made in pioneering research in nanomaterials. While the great majority of the materials researchers work with are created by deliberate design, there are very significant examples of accidental or serendipitous discoveries (such as fullerenes and nanotubes) that continue to be developed and exploited. It is now possible to form almost all classes of materials (metal, ceramic, polymer, glass, semiconductor) into nanoscaled structures of a wide variety of types:

- *Nanoparticles and Isolated Macromolecules*, used as precursors for bulk forms, catalysts, and in a variety of sensor applications. These often have novel structures and phases, induced by surface energy effects, and can exhibit unusual physical, chemical, and mechanical properties. Ongoing challenges include the synthesis, process yield, stabilization, and characterization of the materials.
- *Bulk Nanostructured Materials*, in which the profuse internal interfaces generate novel properties. Materials of this type are typically used in structural applications and provide the potential for extreme strength, hardness, and ductility. Challenges include scaling up to tonnage production, microstructural stability, characterization, and various fundamental problems related to understanding the deformation and failure mechanisms.
- *Thin Films, Nanowires, Quantum Dots, and Surface Phases,* which exploit quantum confinement effects to enable novel computing technologies and optoelectronic applications. These materials exploit techniques such as epitaxy, topotaxy, and (unguided or guided) self-assembly, to create topologies that are able to store, transmit, and read information in novel forms, such as single electrons, electron spin, or magnetic effects, as discussed earlier in this chapter under the section *Beyond Materials for Binary Logic*. Researchers working in this field must overcome stability problems at very fine scales and cope with problems of long-range coherence in array structures.
- *Composites and Heterogeneous Structures*, which combine the properties of differing nanoscale materials and often produce new properties deriving from the high density of interfaces. This class of materials is very broad, encompassing nanocomposites (in which two or more distinct materials are both present in nanoscale dimensions); nano/conventional composites (in which a nanoscaled material is used to enhance the properties of a conventional one); nanoporous materials (in which one phase is a vacuum or a gas); and microelectronics (where gate oxides, diffusion barriers, and dielectrics are all nanoscaled components within the integrated circuit structure). Control and placement of the individual components are the major challenges in creating materials of this type.





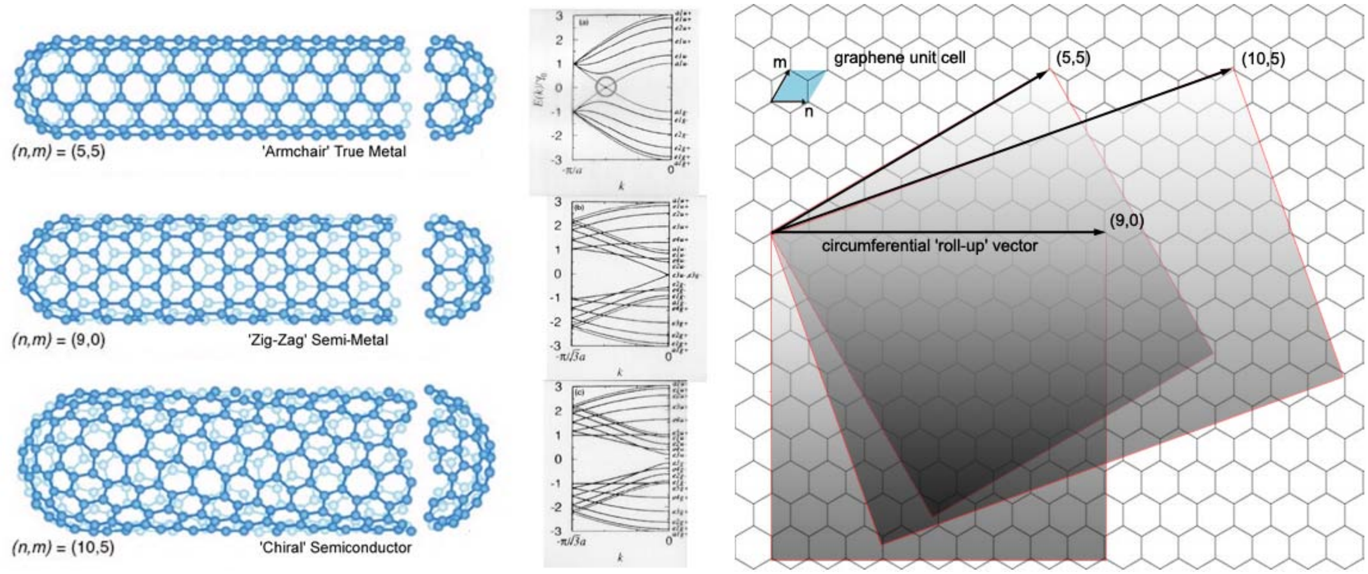
Shown above are supramolecular structures that have both a stiff and flexible character. Due to this dichotomy, these molecules self-organize into mushroom-like objects. The electron microscope images (right) show that a collection of mushroom-like objects can undergo further self-organization into a hexagonal pattern (right-middle) or stripe pattern (right-bottom), depending on the experimental conditions (images courtesy of Samuel Stupp, Northwestern University).

Sidebar 10: Bridging the Scales of Length and Time. Nanoscale materials frequently involve self-organization over many length scales into a variety of patterns. First-principles predictions of such patterns require a multiscale computational approach that can span the enormous range of length scales evident in the figure above. The challenge in developing such a method is that different computational approaches are usually employed to address phenomena that occur on different length scales. For example, as discussed in other sidebars in this section, quantum mechanical calculations are employed to predict the properties of individual molecules, whereas continuum-based methods are used on the larger length scales over which the patterns form (Tew et al., *J. Am. Chem. Soc.* **121**(42), 9852).

The rapidly developing ability to manipulate materials at the nanoscale has enabled some exciting discoveries in basic science, such as the anomalous transmission of light through nanoscaled holes. Phenomena such as this are likely to fuel the development of novel nanoscaled devices and create new demands for materials processing and control of properties.

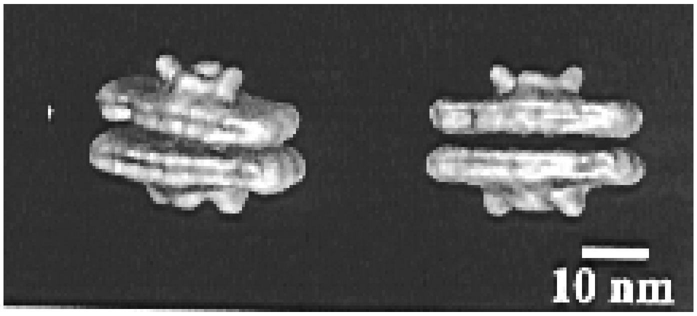
There are a number of emerging themes and opportunities for the next decade:

- New breakthroughs in synthesis methods
  - Computational design of nanoscale materials, elucidation of their properties, and integration
  - Controlled templating of quantum dots with controlled size, density, and geometrical relationships
  - Control and characterization of chemistries and properties of nanoscale building blocks
  - Directed self-assembly, manufacturing, and integration, including dynamic approaches
  - Single-walled carbon nanotubes—scale-up of selective (n, m) growth (see sidebar 11)
  - Control and characterization of chemical, physical, and biological properties of nanoscale entities
  - Designing, manufacturing, and addressing materials and systems from macroscopic to nanoscopic scales, in multiple dimensions
  - Integrating biologically produced components into synthetic systems, especially in sensor applications
  - Realization of necessary levels of reproducibility and uniformity at the nanoscale
- Exploitation of new phenomena
  - Controlling photonic and electronic behavior at multiple length scales; making use of novel phenomena that emerge at the nanoscale
  - Creation of programmable, adaptive, or responsive materials, especially at surfaces
- New devices and applications
  - Addressability of materials systems at nanoscale resolution. Although it is possible, in many cases, to build exquisitely fine structures in which information can be stored at tiny locations, that information must be accessible reliably and repeatably. Conventional wire array structures for this purpose become relatively large and very power-hungry components of overall devices based upon nanostructures, so novel approaches to this problem are required, perhaps based upon the ways in which biological systems access, transmit, and use information.
  - Nanomaterials for sensitive sensing and control of vehicle emissions. This application is expected to be a commercial reality within a few years.
  - Multifunctional, stable materials with broad sensing capabilities, which will be useful in many applications, including biomedical monitoring, environmental monitoring, and various security applications.
  - Bio-inspired nanomaterials with selective multifunctionality.
  - Creating and interrogating nanoscale sensors capable of collective behavior.

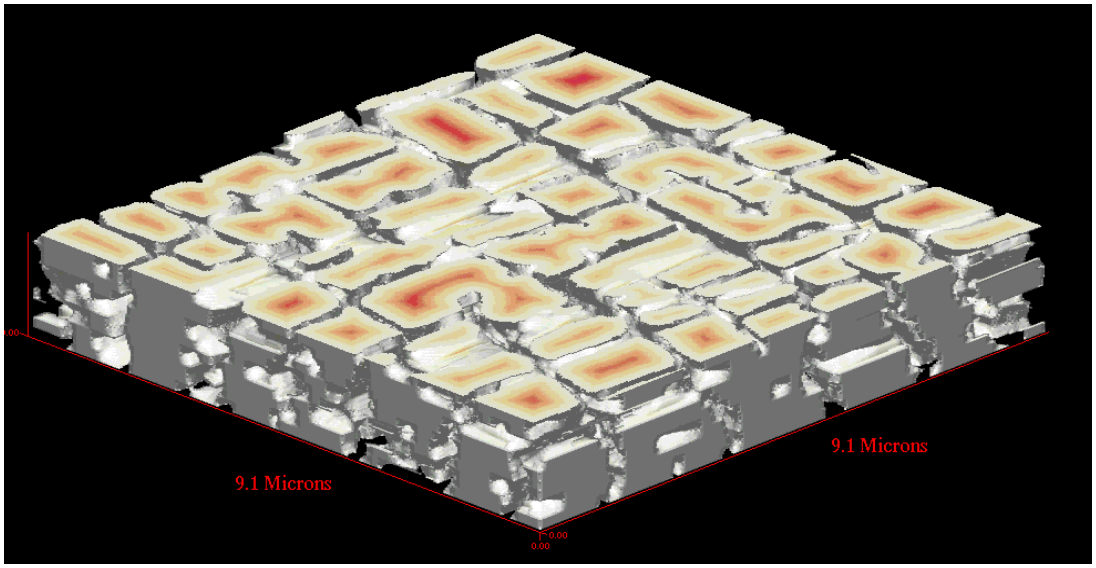


Sidebar 11: Nanotube Engineering: Chirality—It Matters How You Spin Them. Single-wall carbon nanotubes (SWNTs) are vastly elongated fullerene molecules. Produced via catalyzed carbon polymerization, they can be most easily described as tubes obtained by "rolling-up" a rectangular strip of graphene. All such carbon nanotubes have exceptionally high tensile strength, modulus, and thermal conductivity—in each case, the highest known. The "roll-up" vector can range from 0º to 30º relative to a basis vector of graphene's unit cell. Many different tube structures are therefore possible, and almost 100 are known to exist.

The axis along which one cuts and rolls the graphene has a profound effect on the tube's final electronic structure and optical properties. The special case where n=m, the "armchair" nanotube, is particularly intriguing. These are one-dimensional true metals with ballistic electron transport under certain conditions. Single nanotubes have been shown to conduct over 25 µA—a current density above 10^9 A cm^{-2}. When (n-m)/3 is an integer, the nanotube is a semimetal with electrical conductivity similar to that of graphite. All other types of nanotubes are direct band gap semiconductors with carrier mobilities (up to 10^5 cm^2/s) that substantially exceed silicon. Their band gaps vary inversely with tube diameter, ranging from 0.4 to 1.6 eV. Physically stable SWNTs range in diameter between 0.7 nm and about 3.0 nm. Typical synthetic methods produce SWNTs about one micrometer in length, although centimeter-long tubes have been observed. All current synthetic methods produce a complex mixture of nanotube types, and no bulk separation methods now exist. Type separations and type-specific nanotube production are critical goals (images courtesy of A. Cox and H. Schmidt).



The three-dimensional structure of a plant photo system super complex is reconstructed with sub-nanometer resolution using transmission electron microscopy (image adapted from Nield et al.; reprinted with permission from Nat. Struct. Biol. ***7****, 44. © 2000, Nature Publishing Group).*



Focused ion beam tomography is used to reconstruct the internal cellular temperature of a high temperature Ni-based super alloy with a spatial resolution of order 10 nanometers (image courtesy of A. Kubis, D. Dunn. R. Hull, UVa, and D. Bachmann, GE).

Sidebar 12: Reconstructing the Nanoworld—Emerging Tomographic Techniques. Major breakthroughs in science often are driven by major advances in instrumentation. One of the requirements of success to attain the potential of nanomaterials is to be able to three-dimensionally characterize new functional materials in order to optimize their growth and performance. Examples of the questions that need to be addressed are, What is the identity of each atom in the structure (composition)? Where are the atoms (structure)? How are they bonded (spectroscopy)? If they are magnetic, in what direction are their spins oriented? The ability to elucidate three-dimensional structure, chemistry, and properties from the microscale to the atomic scale—in essence, a "nano-GPS"—is a key challenge for the field, and one that may be attainable within the next decade, with advances in aberration-corrected electron microscopes, new forms of scanning probes, X-ray nanoprobes, focused ion beam tomography, and other techniques.

3. How Advances in Nanomaterials Could Change Society

NANOMATERIALS FOR FUTURE ENERGY TECHNOLOGIES

It is anticipated that nanomaterials will have a profound impact on broad aspects of energy technologies. For example, within the next decade, computational studies of nanomaterials will be of increasing benefit to the development of new materials for energy technologies. Such advances will require the development of robust, seamless, multiscale modeling methods and scalable, first-principles, quantum mechanical methods. Experimental synthesis of nanomaterials that are multifunctional will also be a major driver of innovations that improve energy efficiency and reduce the costs of new energy technologies (e.g., fuel cells and solar cells), and will benefit from the insights and guidance provided by the synergy with computational studies.

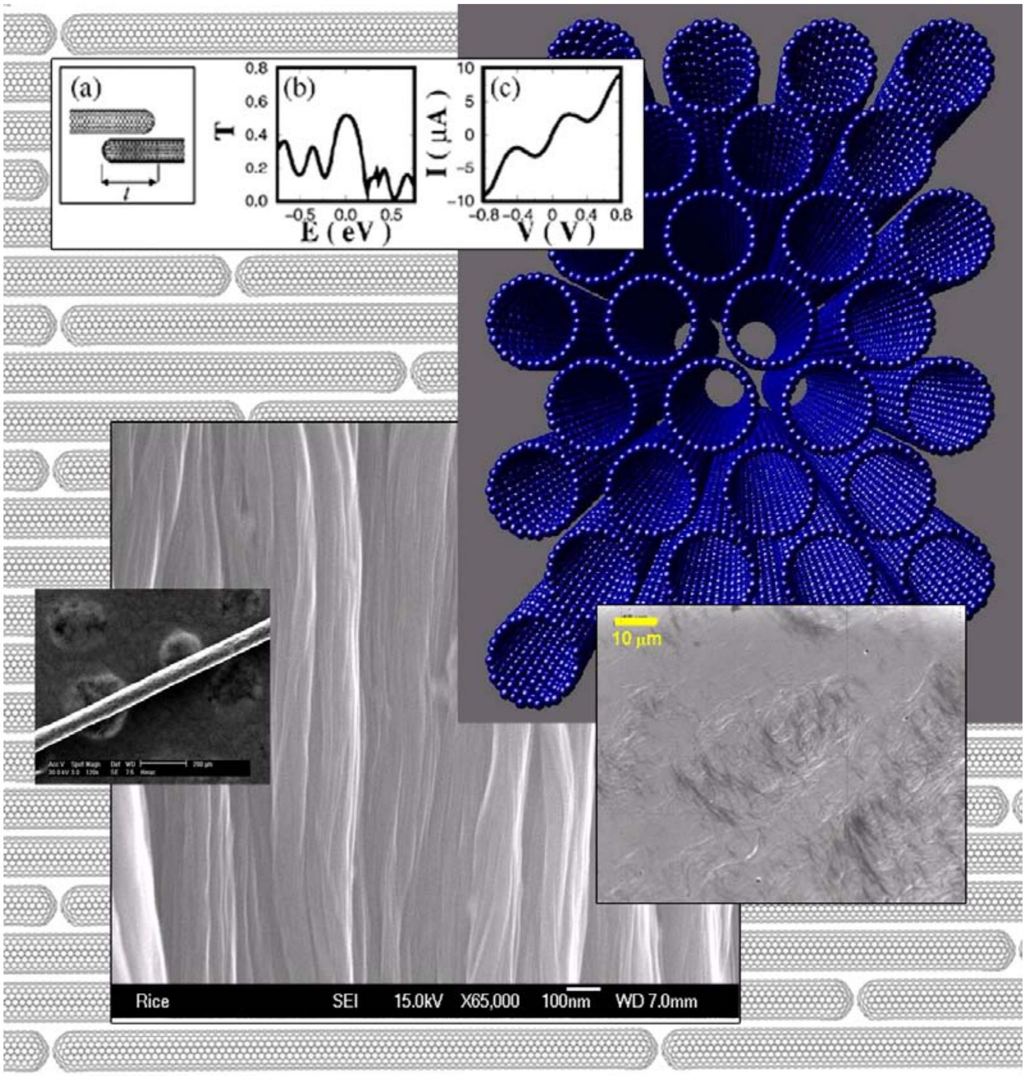
One example of such a material would be a hierarchically assembled membrane structure for use in catalysis, fuel cells, environmental sensors, and water purification systems. Another potential example is the use of single-wall carbon nanotubes that could provide high electrical and thermal conductivity, enhanced strength for power lines, and high surface area supports for new catalysts. A final example is a nanomagnet that can be used in a variety of sensing applications. A hard problem is to master control of synthesis (be it of nanotubes, nanowires, nanomagnets, lightweight materials, or self-repairing and self-cleaning materials) in a manner that transforms nanofabrication from an art into a science that enables technology. The synergy between experiment and computational studies will advance this goal.

Nanomaterials offer the opportunity to reconfigure chemical processes in order to protect the environment while providing energy and economic savings. Nanomaterials offer the hope to replace nonrenewable resources and rare source materials in diverse applications. An example is to replace platinum metal that is now used as a catalyst in a broad range of chemical applications. In addition, nanomaterials are critical to enabling the use of renewable energy (e.g., storage, transport, photovoltaics, photocatalytic reduction of CO_2 and direct production of H_2 from H_2O).

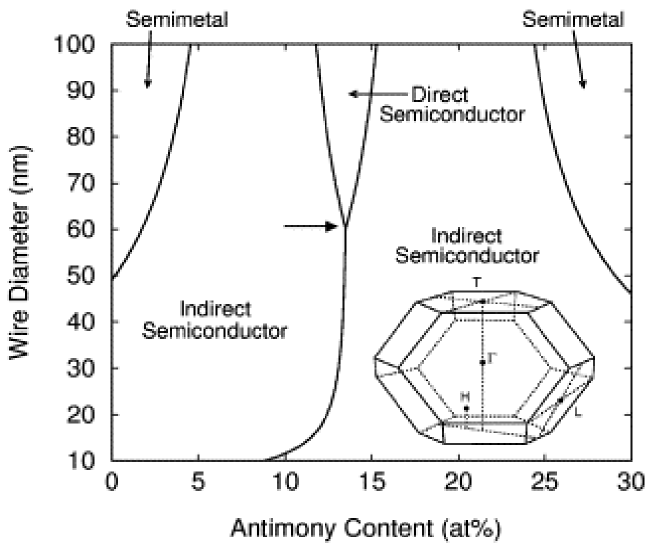
Nanomaterials can enable sensors to perform process monitoring, waste reduction, and real-time analysis to ensure energy efficiency in industrial manufacturing applications. For example, magnetic sensors are presently found in magnetic recording applications, but their use could be extended to monitor environmental variables such as temperature, strain, magnetoresistive, and optical inputs. Optimization of these responses could lead to sensors and other devices fabricated as micro- and nanoelectromechanical systems (MEMS and NEMS) based on functional magnetic heterostructures.

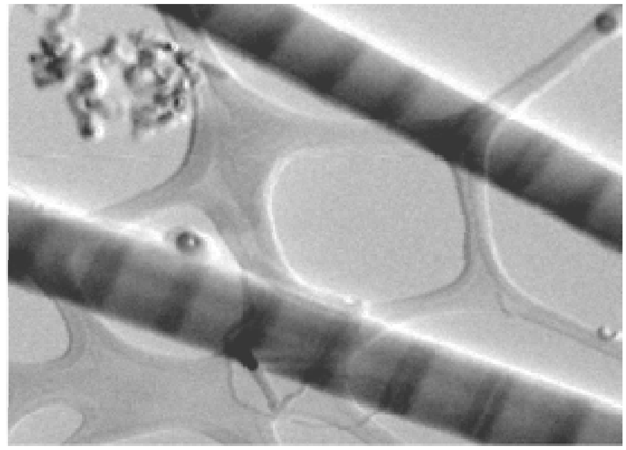
Nanomaterials have strategic importance in a range of areas that affect national security, from the replacement of fossil fuels to the development of sensors for homeland security and defense applications (e.g., the Army’s soldier nanotechnologies initiative, and the strategic goal of energy self-reliance).

As described earlier in this report, an overriding hard problem is to control the size, distribution, placement, orientation, coherency, and addressability of nanoscale objects. But this challenge needs to be overcome in order to realize the new functionalities that could benefit the nation’s pressing energy issues. In the computational arena, solving these control problems will require new developments in the seamless integration of multiscale approaches, in the temporal tracking of rare events, and in monitoring entropic considerations as well as energetic barriers.



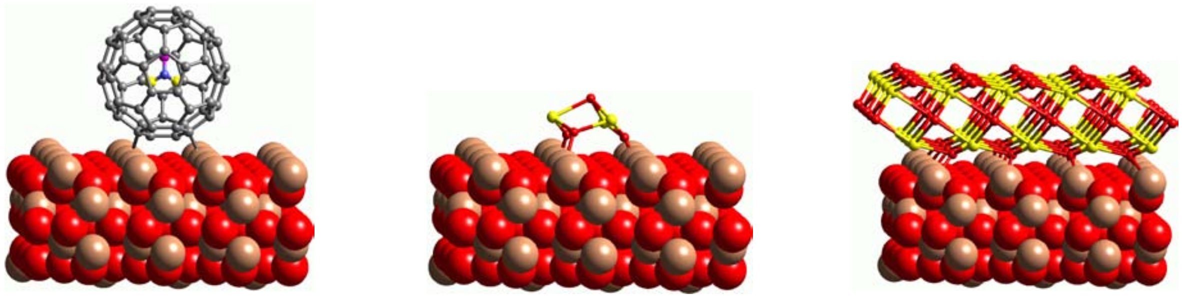
Sidebar 13: A Potential Revolution in Power Transmission. Armchair single-wall carbon nanotubes with structural indices n=m, as described in sidebar 11, are highly electrically conductive. They act like “light pipes for electrons,” conducting electrical charges as coherent, quantized wave packets. Such nanotubes can be “spun” from a quasi-liquid crystalline state in super-acids to form continuous fibers, in much the same way that Kevlar™ fibers are commonly produced. In such fibers, many billions of tubes are in side-to-side and end-to-end contact. Theoretical calculations have shown that conduction electrons can transfer from one armchair tube to any adjacent armchair tube by an efficient quantum tunneling process. If means could be developed to produce SWNTs such that all the tubes are of the n=m armchair type, fibers spun from these tubes would be expected to have extremely high electrical conductivity at room temperature—perhaps substantially better than copper. Since the density of these fibers is only one-sixth that of copper and they have very low thermal expansion, they could be excellent replacements for electrical power transmission lines throughout the energy grid (images courtesy of Smalley Laboratory, Rice University, and Computing and Computational Science Directorate, Oak Ridge National Laboratory).





Left: Variation in electronic structure of Bi-Sb nanowires as functions of composition and wire diameter (image from Lin et al., Proceedings of the 21st International Conference on Thermoelectronics, *253; reprinted with permission, © 2002, IEEE). Right: Superlattice Ge/Si nanowire (image adapted from Li et al.,* Appl. Phys. Lett. ***83****, 3186; reprinted with permission, © 2003, American Institute of Physics).*

Sidebar 14: New Thermoelectric Materials. Nanostructured systems offer the possibility of greatly enhanced thermoelectric energy conversion efficiency. Reducing the dimensionality of materials to ultra-small diameter (tens of nanometers or less) enables the band structure of the bulk material to be tuned, as for the calculations of Bi-Sb wires shown above. Further, manipulation of band structure enables the ratio of electrical to thermal conductance to be maximized, particularly in segmented or superlattice wires, where scattering of thermal conductors (phonons) at the segment interfaces reduces the thermal conductivity. Such low dimensional engineering provides opportunities for greatly improved thermoelectric conversion. A century of research in bulk materials has limited the "thermoelectric figure of merit," ZT, to a maximum value of about 1. Measured values of ZT have improved to values of 2 in low-dimensional structures, and calculations suggest values as high as 6 may be accessible in superlattice wires. This could lead to greatly improved fuel economy in numerous applications, including automobiles. It is estimated that almost half of the energy developed by the internal combustion engine is wasted as heat through the exhaust system. Greater thermoelectric efficiency could economically harness and recycle this energy and reduce fuel consumption by as much as 20%, with enormous benefit to the economy and national interests.



$La_2CeN@C_{80}$ on Al_2O_3 | **La_3O_4 cluster on Al_2O_3** | **La_2O_3 surface on Al_2O_3**

Schematic of novel molecular and nanometer lanthana catalytic materials for potential application in the activation and functionalization for a range of hydrocarbon intermediates. Left: La_2CeN encapsulated endohedral fullerene cages supported on alumina. Middle: Supported molecular La_xO_y complexes. Right: Nanometer La_2O_3 thin films supported on alumina (figures courtesy of M. Neurock, University of Virginia, and H. Dorn, Virginia Tech).

Sidebar 15: New Nanocatalytic Materials. Increasing the rate and selectivity of chemical catalysis via nanostructured material design will have a major impact on decreasing energy consumption worldwide and is key to progress and development within many industries.

New nanomaterials that can be used to selectively catalyze chemical reactions have a tremendous potential for energy savings from the perspective of lowering or, in some cases, completely obviating the need for separation costs. This spans all areas of the chemical process industry, in particular the areas of fuels and fine chemicals (pharmaceuticals). Examples in the fuels industry include conversion of methane to methanol for methane transport and the use of new catalysts to convert light alkanes into heavier ones. This ultimate feat of chemical selectivity is being accomplished with catalysts that are being synthesized based on new nanomaterials.

The translation of paradigms from biological catalysts to the design of synthetic analogs offers a viable route for the design of new nanostructured materials for catalysis. Biological catalysts such as enzymes are examples of catalysts that have mastered many of the challenges of nanostructured materials design by evolution over eons. Enzymes incorporate nanostructures into exquisitely functional catalytic devices, including catalysis of methane-to-methanol transformations as well as catalysts that selectively form pure chiral products for many classes of chemical reactions. An open challenge is the synthesis of new nanostructured catalysts that incorporate paradigms of biological catalysts into synthetic systems that can function under industrially optimal conditions.

The synthesis of nanostructured materials for catalysis will impact many other technologies, such as alternative methods for generating power. These include areas such as fuel cells and other enablers of the hydrogen economy. Examples include nanomaterials for selective combustion and the synthesis of selective membranes and adsorbents with nanoscale structure. These advances will require new strategies for synthesizing and understanding the assembly of nanomaterials using inorganic, organic, and hybrid organic-inorganic building blocks.

NANOMATERIALS FOR FUTURE INFORMATION TECHNOLOGIES

At the nanoscale level, new phenomena arise as quantum effects become important. This opens up a realm of possibilities for enabling new technologies based on quantum devices, most notably quantum computing and engineering with electron spins. The opportunities are tremendous for major advances in new information technologies based on new nanomaterials, as well as for new integrated hybrid systems based on nanomaterials.

There are four broad impact areas for nanomaterials in the area of information technology, namely *storage*, *logic*, *communications*, and *sensors*. In all of these areas, the biggest challenge is no longer simply the design of conventional devices based on nanomaterials and the recording of information, but the ability to increase the dimensionality and functionality of the system and to be able to read the information rapidly and reliably. One of the biggest challenges in the future growth of information technology will be the degree to which it is necessary to control and/or tolerate errors (defects) in the stored information. In this regard, self-correcting materials will play a prominent role.

Although it is difficult to compete with silicon technology in current microelectronic paradigms, researchers must look to the future of new devices based on nanomaterials that have the possibility of allowing for much faster communication due to the advantages of multifunctional components. They must also address the inevitable limits of the scaling of conventional electronic circuits based upon continued shrinking of the dimensions of metal-oxide-semiconductor field effect transistors (MOSFETs) (see sidebar 16). The limitations of power in conventional electronic devices can also, in principle, be solved by the use of quantum devices whose operation is not governed by classical principles. The goal of combining “top-down” with “bottom-up” techniques will take nanotechnology beyond the confines of the current state-of-the-art devices.

There are numerous hard problems that will need to be overcome for successful nanoscale device fabrication to be achieved in the next ten years. These hurdles all relate to the desire to build integrated, multifunctional, multidimensional devices that surpass the current performance standards of the information technology industry. Correspondingly, nanomaterials provide broad new opportunities for providing solutions to these hard problems.

As discussed in Chapter 2, mastering the self-assembly of organic, inorganic, and biological materials is likely to provide a key set of solutions. One promising area for self-assembly is the development of new methods for interconnecting or “wiring” the components of the system or circuit. Two excellent possibilities for connectors are organic molecular wires and single-wall carbon nanotubes. Organic molecular wires have the advantages of ease of large-scale preparation and the fact that they can be chemically functionalized, but it is obvious that the low power dissipation, strength, and diameter of single-wall carbon nanotubes render them excellent choices for molecular electronics applications as well. Success in solving this problem is also intimately tied to advances in nanolithography that are being developed.

As discussed in Chapter 2 and sidebar 5, manipulation of electron spins is already providing the basis for new classes of electronic and magnetic devices. Extension of these concepts to the realization of solid state quantum computers is an exciting possibility. To realize this goal, it will be necessary to learn how to quantum mechanically entangle two or more spins, or the wave functions of atomic or subatomic particles more generally, to make use of the complexity of information that can be imprinted or stored in the combined quantum state. In particular, it is hoped that spin and charge separation can be achieved in order to develop new transport mechanisms where the total power consumption to perform new functions can be reduced without loss of information content. In quantum systems, both the amplitude and phase of the wave function contain information that might be harnessed to enable more powerful storage and complexity for quantum information devices.

In such quantum systems, the problem of measuring and controlling decoherence time is emerging as one of the hard problems. It is known that quantum coherent systems can be very sensitive to the environment and the details of the size, shape, and composition of the structure. It has already been identified that proximity effects are important to the operation and control of nanodevices. In complex multifunctional devices, nearby devices or materials can alter the environment seen by a particular device and alter its function and most likely the quantum coherence time. Many of the nanomaterial devices that will attempt to use quantum information for specific functions will require that all operations such as storage, manipulation, and readout must be done on time scales that are short compared to the decoherence time. Understanding how to engineer the desired coherence time (short or long) remains a critical area for further research.

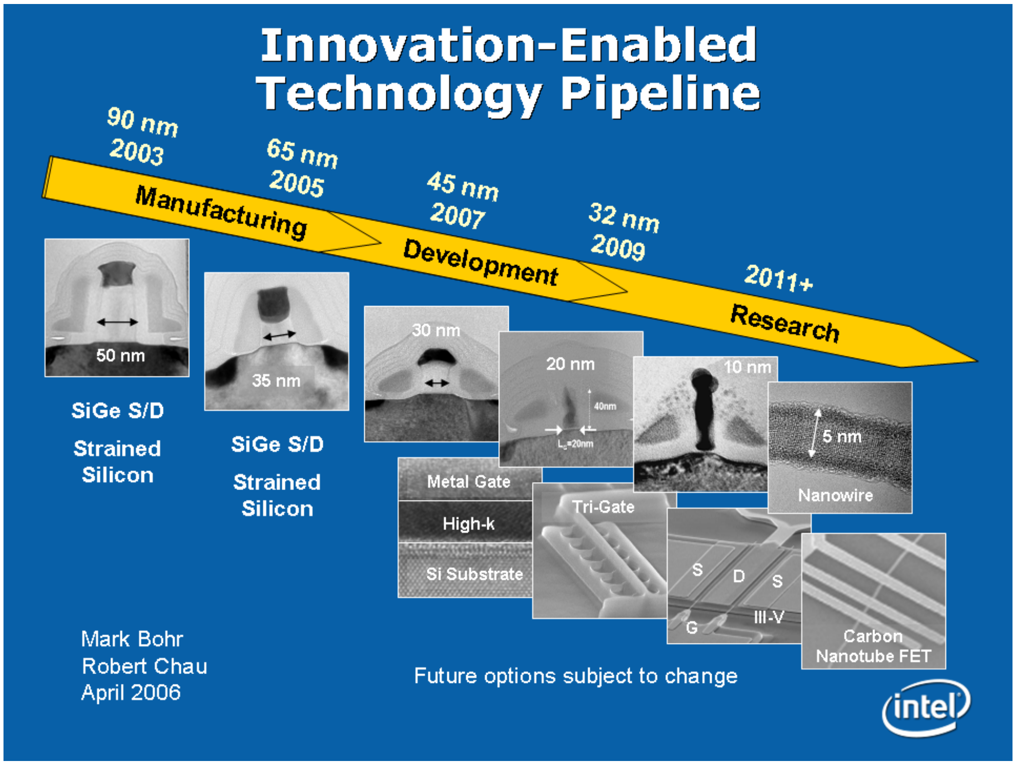
To realize these broad visions, researchers must learn how to address information embedded at the nanoscale rapidly and reliably. Success requires development of materials with error and defect control or tolerance. This is especially true for structures that attempt to use quantum information because of the probabilistic nature of quantum mechanics and quantum information. This is well known in quantum computation architectures, but it will also be true for other quantum devices.

NANOMATERIALS FOR FUTURE HEALTHCARE TECHNOLOGIES

Nanomaterials could enable effective, minimally invasive, personalized healthcare in the coming years. Advances are possible that span the three critical areas of prevention, diagnosis, and therapy. Workshop participants envision that in the future, nanomaterials and nanotechnology will contribute to radical improvements in the ability to repair human vision, treat paralysis, and locally diagnose and treat cancers.

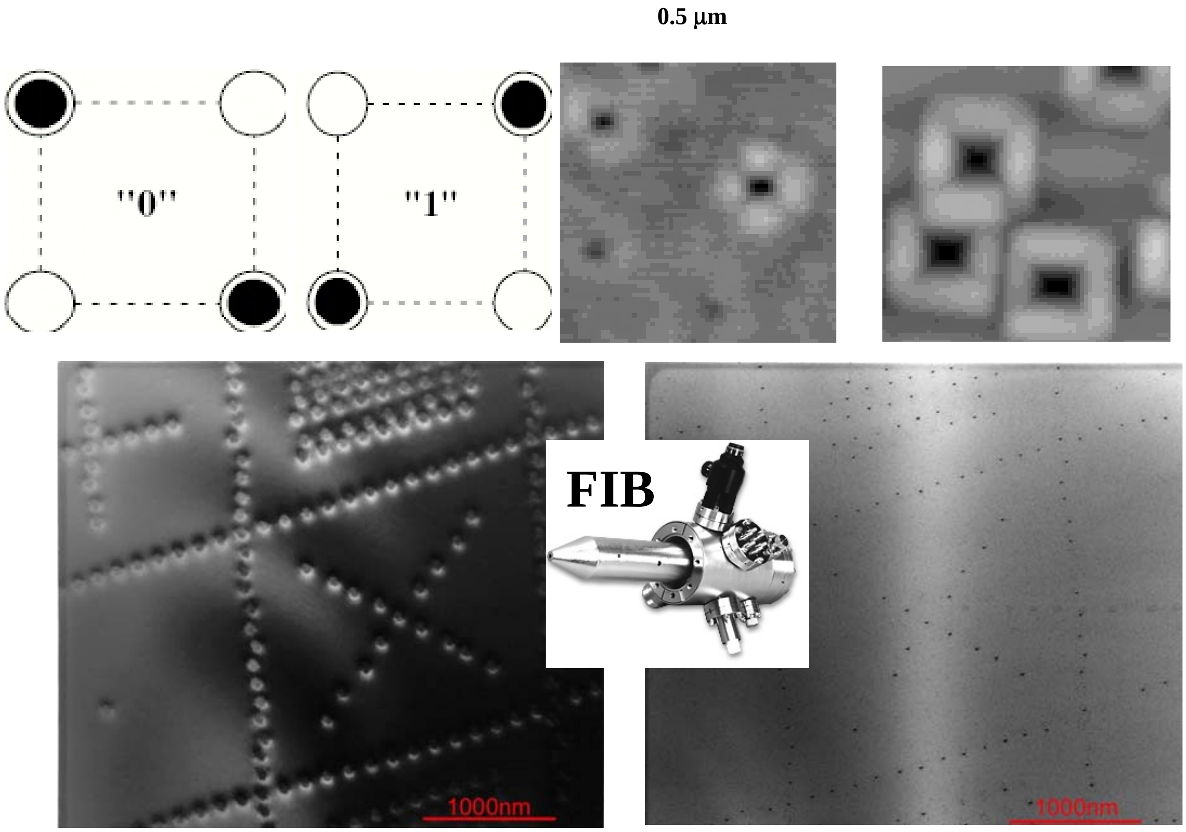
In the area of disease prevention, it is envisioned that vaccines, now delivered using 40-year-old technology, will be delivered by means of intelligent-release algorithms and devices. Genomic monitoring of susceptibility to diseases, immune responses, and a wide range of environmental factors may become possible. Environmental remediation could be effected by novel and specifically active nanomaterial-based systems and devices. There is potential for routine availability of nonfouling surfaces, capable of repelling a wide range of disease-producing agents from specific pathogens to nonspecific dirt.

In the area of medical therapy, a set of dramatic advances and new capabilities is expected to be enabled by nanomaterials and nanotechnology in the coming years. New and more effective and selective drugs will be created. Gene and cell therapy could allow for the prevention, remediation, and cure of a wide range of health problems. The engineering of hard and soft tissue, and perhaps even regeneration of such tissue, for repair and replacement of human body parts may become routinely available. This engineering capability, enabled by new artificial nanomaterials that are inspired by nature's own nanomaterials, could be extended to include joints, circulatory system components, and organs of increasing complexity. New surgical tools and devices that are more effective and less invasive than any currently available will result from the future creation of a wide range of multifunctional nanomaterial systems. These would also allow for the creation of new implant materials with biocompatibility for long-term viability in biological environments.



Sidebar 16: The Incredible Shrinking Transistor. The explosive growth in computational power over the past two decades has been fueled by continued scaling of the individual components in a microelectronic circuit. While advances in conventional or alternative designs for MOSFET transistors are enabling some of the node boxes above to be eventually filled in, new paradigms for electronic devices need to be urgently explored for the future. Candidates include molecular electronics, single-electron devices, spintronic devices, and nanotube/nanowire-based devices (image courtesy of Mark Bohr and Robert Chau of Intel).

An area of particular promise is diagnostics, where nanotechnology-enabled sensor development can be expected to provide major breakthroughs in healthcare in the next decade. In medical diagnostics, there are two principal ways of detecting and diagnosing diseases, those that target protein markers and those that target DNA markers. The majority of such diagnostics are not done at the point of care because of significant limitations in existing detection technologies. Recent advances in using nanoscale materials as probes suggest routes to next-generation detection technology and versatile point-of-care diagnosis (i.e., in the hospital, the doctor's office, the battlefield, water processing facilities, or the patient's home). Nanotechnology may one day make it possible for a doctor to completely diagnose a patient using a 5 ml blood, urine, or saliva sample during an ordinary office visit. Doctors who work in developing countries could readily take these kinds of analysis systems right to villagers to rapidly obtain accurate information regarding their health. Such point-of-care analysis is critical where the spread of diseases like HIV is threatening to wipe out entire communities. Key challenges associated with nanomaterials-based detection systems include (1) sample acquisition and handling, (2) sample processing and delivery to a sensor, (3) detection and quantification without external target amplification, (4) interfacing of nanomaterials with macroscopic and microscopic device hardware, and (5) selectivity and discrimination among multiple targets. Near- and long-term research projects must focus on providing technologies that address each of these categories.



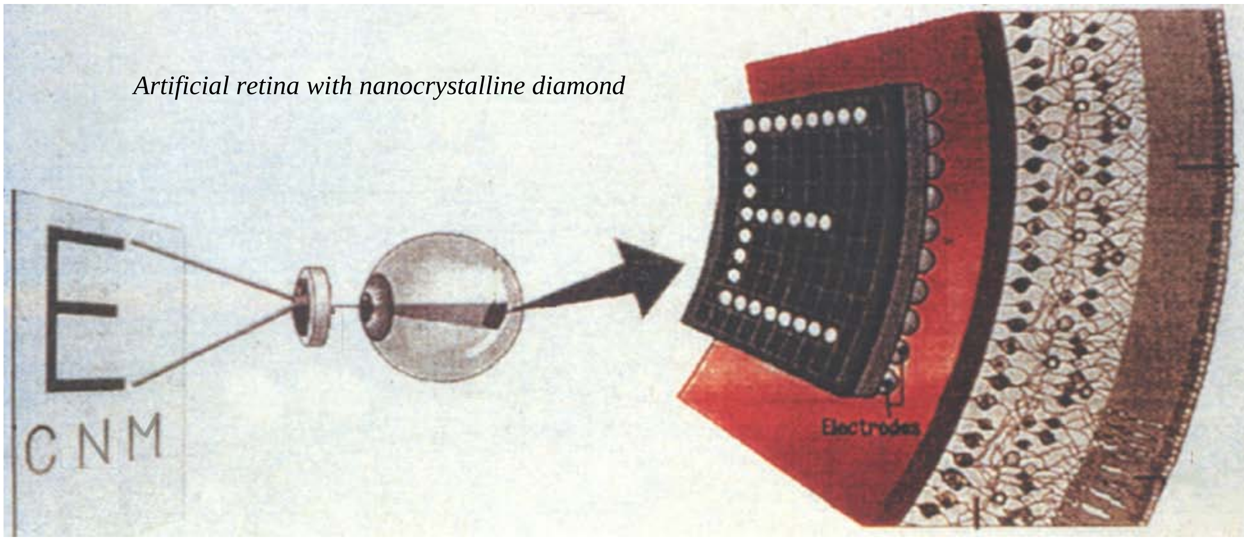
Realization of many novel electronic architectures will require the ability to accurately position individual nanoscale elements within large arrays. Top left: The concept of quantum cellular automata relies upon bistable charge distributions in a four-fold cell, arising from Coulomb repulsion. Top right: Self-assembling quadruplet quantum dot "molecules" have recently been observed under kinetically limited conditions in the Ge_xSi_{1-x}/Si system (image adapted from Gray et al., Appl. Phys. Lett. ***81****(13), 2445; reprinted with permission, © 2002, American Institute of Physics). Bottom:* In situ *focused ion beam patterning of Si(100) surfaces (left) allows patterned nucleation of Ge quantum dots by chemical vapor deposition (right) (image adapted from Kammler et al.,* Appl. Phys. Lett. ***82****(7), 1093; reprinted with permission, © 2003, American Institute of Physics).*

Sidebar 17: Playing Nano-Dominos with Electrons—Materials for Quantum Cellular Automata. One very exciting potential nanoelectronic circuit architecture is quantum cellular automata (QCA), where electrons or holes in a quadruplet of quantum dots align into bistable states through Coulomb repulsion. These create binary configurations—replicating the logic states "0" and "1"—and QCA cells can then be assembled into logic gates and circuits. The primary advantages of such structures compared to conventional MOSFET circuits is that QCAs potentially offer orders of magnitude higher packing densities and lower power-delay products, and interconnection schemes can be much more flexible. However, severe technological challenges remain to practical implementation of such structures. Operation at anything other than cryogenic temperatures requires control of quantum dot placement and size with precisions approaching ten nanometers. Proof-of-principle has been demonstrated in metal/metal oxide systems at temperatures below one degree Kelvin. Realization of this concept using either self-assembly of "quantum dot molecules" or directed assembly (employing focused ion beam seeding of quantum dot nucleation sites) in epitaxial semiconductor systems, or extension to molecular materials, offers the possibility of more practical technologies operating at much higher temperatures.

Being able to build sensors based upon nanostructures is more than just an opportunity to miniaturize sensor devices. Indeed, small structures (1–100 nm) often have unique chemical and physical properties that can be exploited in the development of novel signal transduction schemes. Examples include quantum dots, which exhibit size-dependent emission properties and very narrow emission bands. These can be used in a variety of multiplexing schemes that have the potential to be superior to those based upon molecular fluorophores. For example, on a particle-to-particle basis, gold nanoparticles are more intensely colored than the best organic dye molecules by many orders of magnitude, making them strong candidates for colorimetric sensor probes. A wide variety of metal nanoparticle probes can exhibit unusual catalytic properties that can be exploited in signal amplification schemes. Clusters of nanostructures can be used to generate field enhancement, also leading to new possibilities for signal amplification based upon physical phenomena such as surface-enhanced Raman spectroscopy. Nanotubes and nanowires have all sorts of interesting physical properties that can be deliberately made to change upon a surface-binding event, forming the basis for new signal transduction schemes.

Nanotechnology also offers many opportunities to develop miniaturized, low-power-consumption, ultra-sensitive, and ultra-selective detection systems for a wide range of medical and other applications. For example, when one considers the possibilities of building receptor arrays based upon features that are tens of nanometers in size, rather than hundreds of micrometers as in current technologies, the potential of this technology is impressive. As illustrated in sidebar 19, with modern nanolithographic and random bead array capabilities, it is becoming possible to place millions of individual sensor receptors within the space of a couple of hundred micrometers. To put this in perspective, one could use the area occupied by a single feature in a conventional gene chip based upon conventional microtechnology and replace it with an entire gene chip or proteomic array with thousands of features. This can translate into advantages in sample processing, required sample size, sensitivity (number of molecules required for a detection event), ability to incorporate massive redundancy, and even sensor readout.

Strategies must be developed for collecting, extracting, and concentrating analytes from biological media (blood, saliva, or urine) for subsequent detection and analysis. The existing method of building detection systems is to synthesize or isolate a compound with known recognition properties for a particular target (e.g., an oligonucleotide, antibody), and then to interface it with a probe or device that transduces a signal upon analyte binding. One way to take advantage of nanotechnology and, in particular, the ability to build surface architectures on the molecular length scale, is to learn how to build receptors from *de novo* principles. This objective can be achieved by constructing arrays of molecule-based features on a surface that recognize a larger target through complementarity based upon feature size, composition, and spatial arrangement. To this end, combinatorial nanotechnology approaches become very important. While it is very difficult to design the perfect receptor for a biostructure of interest (e.g., a virus particle), by having some knowledge of the basic structure of the target, a series of educated guesses can be made about a complementary pattern that might recognize that agent. Such structures could be screened to evaluate which is the optimum receptor. Lithographic/printing procedures with sub-100 nm capabilities are key enablers in making this approach viable, building upon techniques discussed under *Beyond Conventional Lithography* in Chapter 2 and in sidebar 3, for example. New methods for nanoscale grafting, nanoscale screening, and related methodologies will also need to be developed.

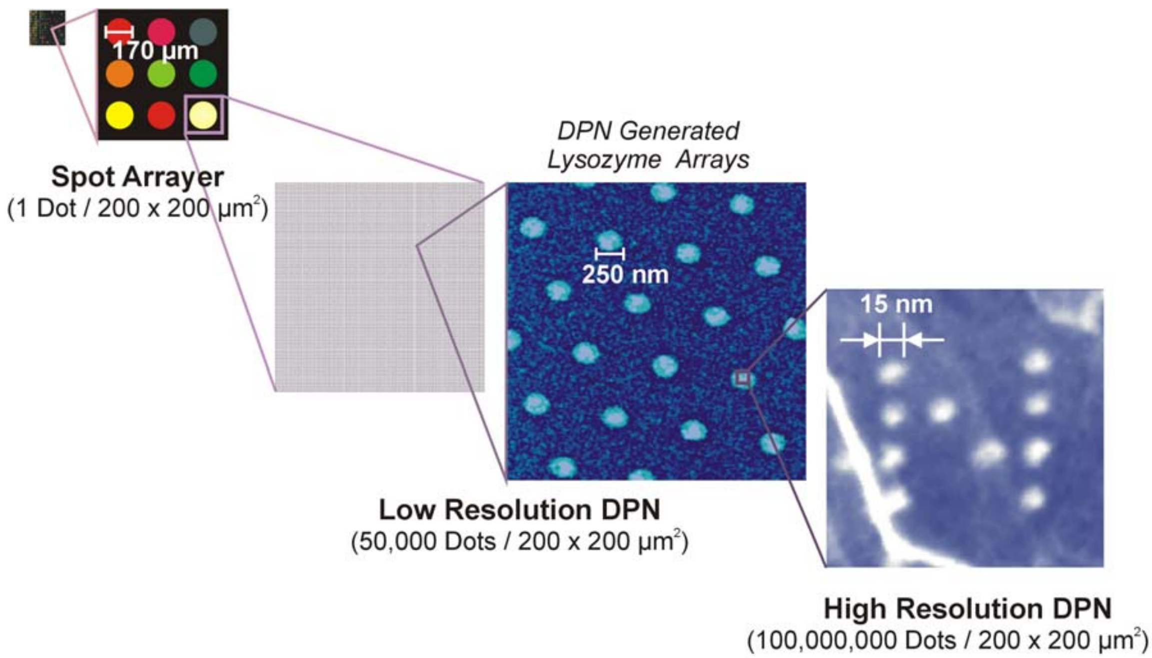


Sidebar 18: Helping the Blind to See: Nanomaterials for Artificial Retinas. Nanocrystalline diamond is biocompatible and has mechanical and tribological properties suitable to serve as a protective coating for artificial retinal implants. Nanocrystalline diamond also can be doped and patterned to form optical arrays for bioengineering projects such as that to create artificial retinas (image courtesy of M. Humayun, University of Southern California, and J. Carlisle, Argonne National Laboratory).

To realize these broad visions, several generic hard problems must be solved by the interdisciplinary nanomaterials research community:

- Interfacing and transducing biomolecular and biological systems information to the physical world
- Creating nanoscale materials and controlling their structure and properties in biological environments
- Creating nanoscale devices for use in biological environments

Solving these major problems will require that the nanoscience and nanotechnology research community address the particularly important and overriding issues of biocompatibility, interfacing heterogeneous (e.g., biological/artificial) materials, targeting specific locations for nanosensors and nanotherapeutics with sufficiently high resolution, amplification in both directions, and the creation or use of *in situ* energy sources. In parallel with understanding and harnessing the enormous potential benefits of nanotechnology for healthcare, it is critical that the potential effects of nanometer-sized particles upon living systems should be understood in the greatest possible detail. Recent research has suggested that nanoparticles are capable of nonspecific penetration into cells, so that even inert metals such as gold that are approved by the FDA for medical applications may conceivably become bioactive when present as nanoparticles that accumulate in the cells. To allay any potential risks or concerns, these issues should be thoroughly addressed to understand and control in advance any possible deleterious biological effects or other environmental issues.



Sidebar 19: Development of Ultra-Miniaturized Medical Detection and Diagnostic Systems. The possibility of unprecedented array density through nanopatterning techniques such as dip pen nanolithography (DPN) affords advantages in terms of required sample size, screening methods, and receptor design. The area occupied by a single feature in a conventional gene chip based upon conventional microtechnology can be replaced with an entire gene chip or proteomic array with thousands of features (image courtesy of C. Mirkin, Northwestern University).

NANOMATERIALS FOR FUTURE INFRASTRUCTURE AND TRANSPORTATION TECHNOLOGIES

Civil infrastructure and transportation constitute some of the largest aggregate industries in the nation. Both industries are very materials-intensive but are not necessarily perceived as "high technology." This perception is particularly true in the field of civil infrastructure (roads, bridges, railways, tunnels, buildings, waste treatment, utilities), which to a large extent relies on traditional, and inexpensive materials such as steel, concrete, and asphalt. Transportation modes (trains, planes, automobiles, and ships) incorporate advanced technologies in their methods of propulsion and communication, but they also typically rely primarily upon traditional structural materials.

Some of the most important needs from a materials point of view include safety, security, energy efficiency, maintainability, sustainability, recyclability, environmental compatibility, favorable strength/weight ratio, and low cost. Commonly used materials include metals and alloys, concrete, asphalt, glass, ceramics, polymers, rubber, composites, wood, and fuels, as well as materials for thermal insulation, sensors, and coatings.

Nanoscience research is presently underway on many of these materials, particularly where there is a perceived or hoped-for benefit in high-technology industries such as information technology, healthcare, or energy with relatively low-volume materials needs. However, little or no research is aimed at exploring the possible impact nanotechnology may have in industries with extremely high-volume materials requirements such as construction. But that is not to say that such opportunities do not exist. Two notable examples follow.

Example 1: Nanoengineered Concrete

Concrete is not by itself a high strength structural material, and it is usually strengthened by the incorporation of steel reinforcing bars (rebar). The layout of rebar on the construction site is labor-intensive and expensive. The bonding of concrete to the steel surface is affected by steel corrosion prior to installation. In recent years, fibers have been included in concrete to either replace or supplement conventional rebar, but the mechanical properties have not improved to the point where steel reinforcement can be eliminated in the most demanding applications. Nanofibers based on carbon or boron nitride nanotubes are among the strongest materials known. Their surfaces can be functionalized to form strong chemical bonds with their environment. It is possible that the mechanical properties of concrete could be substantially improved with the use of such functionalized nanofibers, which can be mixed into the concrete prior to pouring. The homogeneous dispersion of nanofibers throughout the material will result in more uniform properties and reduced susceptibility to local weak spots, wear, and damage.

Example 2: Infrastructure Monitoring

At present, the structural integrity of most bridges, buildings, and other large structures is not continuously and actively monitored. While the placement of sensors is technologically possible, high costs limit their widespread use. Nanotechnology offers an avenue to dramatically change this by inexpensive integration of nanoscale sensor elements capable of monitoring a wide range of materials characteristics as well as environmental parameters, energy harvesting elements for signal processing, and wireless communications channels that allow sensors to be routinely embedded in locations and environments that are otherwise inaccessible. Novel manufacturing and packaging methods are likely to make multifunctional sensors cheap, enabling their ubiquitous deployment. Pervasive sensors may lead to improvements in infrastructure safety and security, reduced cost of maintenance, and improved energy efficiency, among other benefits.

Realization of such opportunities requires addressing the following hard problems:

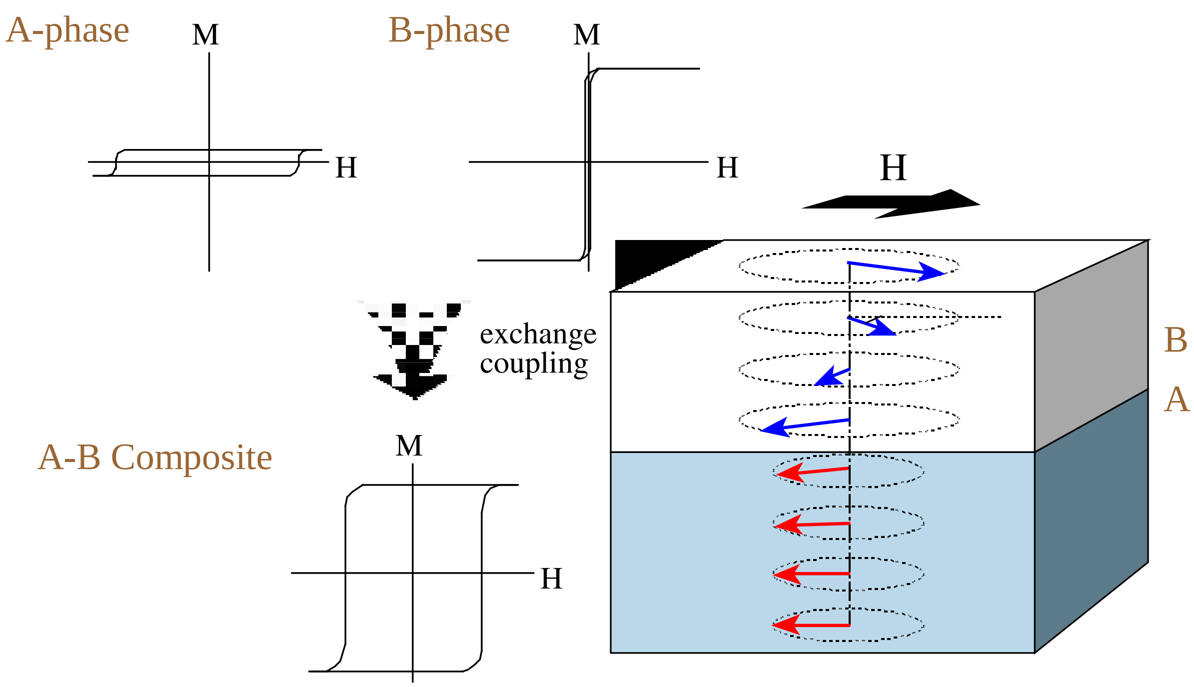
- Functionalization and optimization of heterogeneous interfaces between a range of disparate materials systems: metals, polymers, ceramics, and glasses
- Engineering and control of mechanical properties, on length scales from nanometers to hundreds of meters, in extreme operating conditions (temperature, pressure, corrosive environments, high radiation, electromagnetic fields, etc.)
- Development of design and engineering tools to integrate and place nanotechnology components optimally in complex materials and systems
- Analysis and monitoring of nanoscale properties in macroscale objects
- Nanotechnology device manufacturing at extremely large volumes

There are also substantial gaps in the national research infrastructure with respect to this area of science and technology. The apparently low-technology nature of the civil infrastructure field leads to perception of a lack of glamour and a relative lack of interest within academia. The scientific community is poorly connected to this very large industry, and information flow across disciplinary boundaries is problematic. Thus, while the basic science underlying the use of nanotechnology in areas such as information technology, energy, healthcare, and civil infrastructure and transportation shows many commonalities, a deliberate focus on applying nanoscience to civilian infrastructure and transportation will be needed in order to realize some of the possibilities discussed above.

Meeting this objective will require a deliberate choice and commitment on the part of the national funding agencies, coupled to a change in culture and perception of academic institutions and industries.

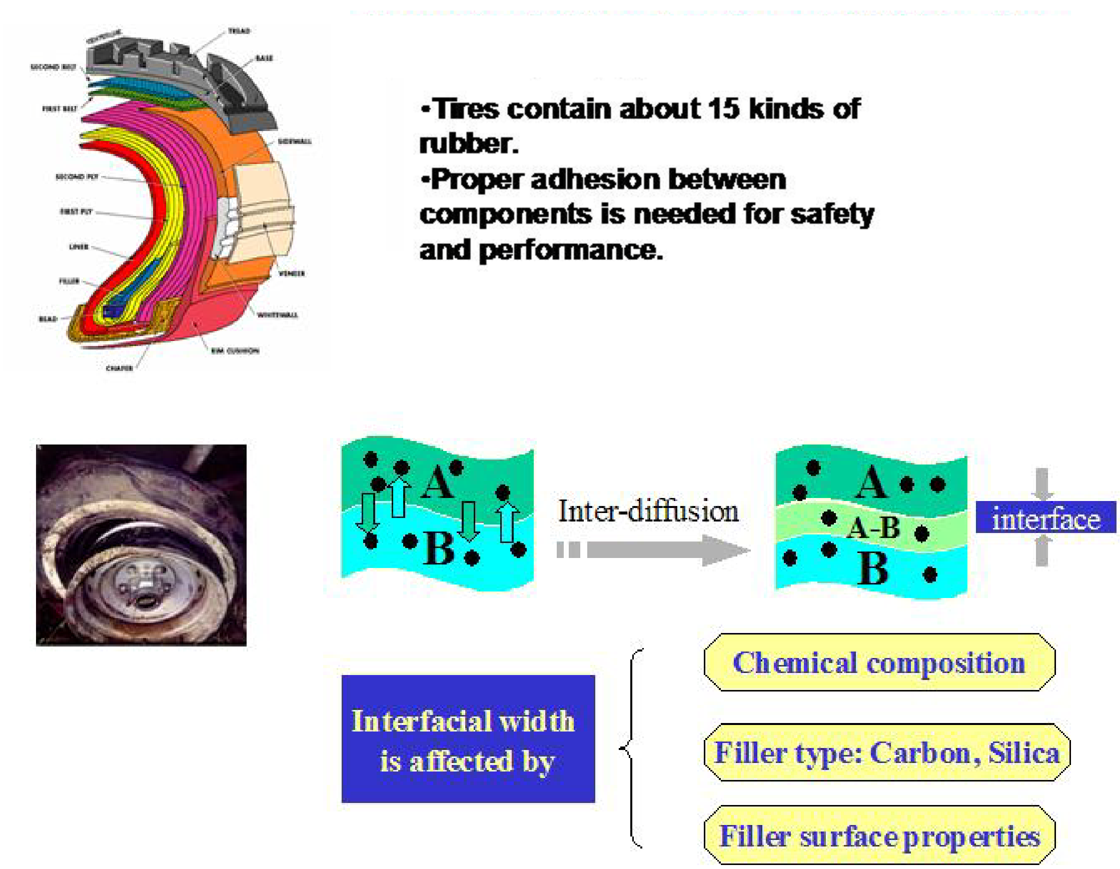
Notwithstanding the above challenges, the workshop participants could envision several major breakthroughs in this field in the next decade and beyond. The workshop participants recommend establishing, within five years, a national focus on nanoscience and nanotechnology research related to civil infrastructure and transportation. Novel materials development could then proceed immediately and have significant impact over the next decade. Examples of materials systems that are likely to have a major impact within the decade include ceramic/metal interfaces, metal/polymer composites, catalysts, and coatings.

On the timeframe of a decade and longer, workshop participants believe that nanocomposites will become pervasive in the fields of civilian infrastructure and technology, as will the use of embedded sensors that enable continuous monitoring, adjustment, and repair. Novel technologies to manufacture multifunctional and graded materials for structural components could radically change present design, building, and construction methods; reduce cost of construction and maintenance; and provide improved and more reliable performance and longer lifetime for civil infrastructure.



Exchange-Spring Principle for Nanocomposite Permanent Magnets: As long as the length scale does not exceed a magnetic domain wall thickness, the composite behaves likes a single new composite material. When it does exceed this critical length scale, a twist can develop, as shown, in response to a reverse external magnetic field (image courtesy of Samuel Bader, Argonne National Laboratory; reprinted with permission from Rev. Mod. Phys. ***78****, 1, © 2006, American Physical Society).*

Sidebar 20: New Nanocomposite Permanent Magnets. Advances in hard permanent magnets have potential impact on energy efficiency in a broad range of applications. New permanent magnets with maximum energy product values (BH_{max}, a measure of magnetic strength) that are twice those exhibited by present-day ultra-strong permanent magnets, such as NdFeB or SmCo, hold great potential to increase the efficiency of electric motors, actuators, and transformers. Miniaturization of magnetic components will reduce weight, which will result in energy savings in automotive and air transportation sectors. New hard permanent magnets will also usher in new electric motor designs with fewer moving parts that will yield devices of simpler architecture with higher reliability and with greater ease and efficiency of manufacture. However, new bulk permanent magnet compounds are difficult to discover because they embody properties that tend to be mutually exclusive (such as a high coercivity as well as a high magnetization per unit volume). What nanotechnology provides is a prescribed way to create composites of two known materials, each of which possesses one of the two necessary complementary properties. The composite then behaves as a single material. Commercializing such nanocomposites could have enormously beneficial consequences. There are a number of promising synthetic routes being investigated, including surfactant-mediated chemical self-assembly, that could be promising for different applications.



Sidebar 21: Nanoscale Engineering of Rubber Tires. Nanoscale fillers are important to many industries since they can be used to engineer the properties of materials such as hardness, heat resistance, and electrical conductivity at the molecular level. In the past decade different techniques that can probe molecular structure have been used to map polymer chain dynamics with nanoscale precision. Results from the various methods have demonstrated that surfaces can have a profound effect on dynamics. Depending on the interactions, the viscosity, glass transition, and melting point are all affected within the first few nanometers of the interface. Nanocomposites are effectively the three-dimensional analogues where nanoscopic phenomena become manifested on a macroscopic scale. An example of such molecular-level engineering is provided by an ExxonMobil collaboration with the NSF Garcia Materials Research Science and Engineering Center at the State University of New York at Stony Brook, which used the high penetrating power of neutron reflectivity to characterize the interfaces between different elastomers commonly used in rubber tires. These researchers reported that the interfacial width between layers of partially miscible polyolefin rubbers (brominated isobutylene methylstyrene and butadiene) decreased from 100 nm to 2 nm with the addition of only 2.5% commercial carbon black. This was interpreted as being the three-dimensional analogue of previously observed behavior for thin polymer films adjacent to an attractive substrate, where the dynamics of the polymer chains can be reduced within a “sphere of influence” that can extend several hundred nanometers from the interface. Since direct contact is not required, the amount of filler needed to affect the viscosity can be much smaller than expected. The narrow interfaces can have a profound effect on interfacial adhesion between the different components that in turn affects the overall performance and safety of the product. This work led to joint work with the Sid Richardson Carbon Company, a leading manufacturer of carbon black, to produce an experimental version that was molecularly engineered to minimize the polymer surface interactions. Neutron reflectivity and adhesion testing showed that these new nanoparticles restored the adhesive properties without compromising either the electrical or mechanical reinforcement inherent in the carbon black particles (figure courtesy of Miriam Rafailovich, SUNY Stony Brook).

4. EDUCATIONAL ISSUES

As this report has illustrated, nanoscience makes possible the creation of fundamentally new materials to address critical modern issues. However, the educational infrastructure must be built that will support the multidisciplinary, highly innovative, and technical R&D work that remains to be done. Elementary, high school, undergraduate, and graduate science curricula must incorporate training for students of all ages in nanosciences and in appreciating their importance to solving the pressing economic, environmental, and social problems. One goal is to train the next generation of researchers in a new, multidisciplinary environment that will foster the cross-pollination of ideas in order to further innovation. An equally important goal is to help the general public become more knowledgeable about technology issues so that informed decisions can be made. Societal and economic impact offers the greatest motivations to invest in nanomaterials for a broad range of future technologies. This is because nanoscience offers the possibility to create new functional materials to address the critical issues that face modern society. These new materials can be designed computationally and experimentally utilizing the principles that underlie nanoscience of (a) geometric confinement, (b) physical proximity and (c) chemical self-organization. No longer is there a need to rely on serendipity to discover new routes to technological breakthroughs.

Promoting such understanding will require initiatives ranging from integration of nanoscience and nanotechnology topics into the K-12 curriculum to development of university-level core courses in order to provide interdisciplinary training for students at high school, undergraduate, and graduate levels. An extensive, committed effort must also be made to disseminate information to the public.

Cross-cutting educational issues were raised among several breakout groups in this workshop:

- How can nanoscience be used to educate and inspire society to be technologically literate?
- How can medical professionals be encouraged to avail themselves of the latest advances in nanotechnology?
- How can educational institutions be encouraged to value and reward interdisciplinarity?
- How can high-risk, high-cost research be performed that will primarily benefit societies, or portions of societies, that cannot afford it?

In working toward these goals, it is important to begin and maintain dialogues with all relevant stakeholders—the scientific and educational communities, the general public, and government office holders—with respect to the existing and potential societal impact of nanomaterials. While workshop participants believe these to be overwhelmingly positive in potential, it is important to keep an open mind about the societal ramifications of nanomaterials developments and breakthroughs.

Equally, potentially adverse environmental and health implications need to be aggressively researched and discussed openly, so that issues and solutions are identified well in advance of any possible negative impacts. For example, some research suggests that nanoparticles are capable of nonspecific penetration into cells. As the importance of nanotechnology continues to increase, significant resources and effort should be devoted towards increasing fundamental understanding of the interaction between nanoscale materials and living systems. By acting responsibly and in concert as a community, public concerns and health and environmental issues can be thoroughly researched and addressed in advance of potential hazards.

Scientists need to recognize that the research community has not to date been sufficiently effective at conveying its message to the lay person. A concerted effort should be made, hand in hand with experts who specialize in the mass dissemination of information, to develop a clear message for delivery through a broad range of media. Further, this delivery should not only be through specialized publications or programming that targets those already interested in science and technology, but also as much as possible through mainstream or "prime time" channels.

Impacts of new nanomaterials technologies upon everyday lives are already pervasive. These range from the breakthroughs in telecommunications that allow crystal clear voice communication around the world at a fraction of its cost two decades ago, to the electronic automation of countless record-keeping and administrative functions—with the myriad personal privacy issues this raises—and to new paradigms for entire fields of human commerce, activity, and leisure. Consider, for example, the revolution in the music industry brought about by the MP3 player, which relies upon ultra-high-capacity hard drives enabled by the breakthrough giant magnetoresistive technology described in sidebar 1 (p. 3). This development has changed the way in which an entire generation acquires, listens to, and uses music and voice recordings. It has also spawned major growth in other related industries not directly dependent upon nanotechnology, such as those devoted to developing encryption and licensing tools, as well as to defining new territory in the legal and intellectual property fields, and to developing new "on-the-fly" educational paradigms. Similar upheavals can be expected in many other fields as nanomaterials enable new technologies. For example, in the field of medical diagnostics, what would happen to the entire cost structure of the medical profession and public health infrastructure if many more diagnostic capabilities were available over the counter, at minimal cost, and able to be administered in the home? While workshop participants are firmly of the opinion that new technologies bring new opportunities for broad benefit, it is important that all concerned stakeholders work together to understand the broad societal implications of these new technologies.

The nanotechnology community should capitalize upon the fact that nanotechnology has captured the imagination of the general public and has helped revive interest in science and engineering. As described in the previous paragraph, nanotechnology has produced not only tangible results in consumer products but also in new scientific instrumentation such as scanning probe microscopes that have become commonplace in research laboratories around the world. These instruments are relatively easy to master and have produced spectacular images of atomic and molecular arrangements that have further fueled public imagination. Workshop participants therefore believe that there is a unique opportunity at this point to use nanotechnology as a vehicle for attracting young people back into science and engineering careers. This is critical because, despite exciting advances in sciences and an increase in public information through the media, there has been a steady erosion over the past three decades in the number of U.S. students choosing to enter science careers.

Workshop participants therefore strongly recommend that the research community capitalize on the renewed interest in science and engineering brought about by nanotechnology to try to recruit students into these fields as early as possible in their educational careers. Furthermore, the nanoscience and nanotechnology research community should also aim outreach efforts towards teachers and members of the community, since their support is crucial to the success of science education of citizens, beginning at an early age. For example, several programs associated with large centers funded by the National Science Foundation have proven successful and should be encouraged. Of note are programs that have allowed undergraduate students and high school teachers to participate in center research programs. These centers have also extended their outreach to high schools and younger children through a range of activities such as mentoring, partnering with science museums, and sponsoring summer camps (see sidebar 22).

Sidebar 22: Nanomaterials in High Schools. The winners of the 2001 Siemens-Westinghouse competition, high school students Ryan Patterson, Shira Billet, and Dora Sosnowik, meet with President George Bush (center) and the CEO of the Siemens' Foundation, Albert Hoser (right). Shira and Dora designed a viscometer for nanometer-thick polymer films. Ryan built a system for speech recognition for the deaf. Shira and Dora were mentored by researchers in the Garcia Materials Research Science and Engineering Center, funded by the National Science Foundation at the State University of New York Stony Brook campus, and came from a small private girls' school with no science research program. Even though neither had originally considered science as a career option, both are now enrolled in prominent research institutions and pursuing technology-oriented majors.

5. Conclusions and Recommendations

As this report documents, there is potential in the coming decades for massive impact of nanomaterials upon technology, industry, healthcare, the environment, the national economy, education, and society. The workshop participants summarized the most important mission for the next decade of research in nanomaterials as development of effective "nanofoundries." By this is meant developing the knowledge, methods, and instruments for fabrication of nanoscaled materials that enable economically viable applications with broad benefit to industry, technology, the economy, the environment, health, and society.

Workshop participants developed a "twelve-point plan" for realizing this mission:

1. Support high risk, high payoff projects, emphasizing discovery of new nanomaterials and properties and invention of new techniques and instruments for nanoscale fabrication, measurement, and synthesis
2. Emphasize research that addresses understanding and exploiting interfacial properties between dissimilar media such as interfaces between organic and inorganic materials, nanoscale fillers and matrices, and heterogeneous biomaterials
3. Develop new techniques for synthesizing and refining nanomaterials in large quantities
4. Invent, develop, optimize, and control new methods for self-assembly of materials based on both biological and nonbiological methods
5. Develop methods for realization of controlled hierarchical structures with multiple length scales down to the nanoscale
6. Emphasize materials, methods, and instruments for harnessing subatomic properties such as electron spin and quantum interactions, with potential for revolutionary advances in electronic logic, data storage, and computation
7. Improve instruments and techniques for structuring and patterning materials at increasing levels of precision
8. Develop techniques to measure the structure, properties, and chemistry of materials with full three-dimensional addressing at the atomic scale (in essence, a "nano-GPS")
9. Develop computational methods, algorithms, and systems—both classical and quantum—to enable realistic simulation of processes over all relevant length and time scales
10. Emphasize the interface between nanomaterials and biological systems to enable widespread improvements in human health. In parallel, the potential toxic effects of "nano-sized" particles on living systems and the environment should be fully investigated.
11. Focus on fundamental understanding of fault tolerance, that is, the degree of perfection necessary in nanoscaled systems to attain desired functionality, and the degree of perfection allowed in such systems by the fundamental laws of nature
12. Develop internal sensing methods for use in assembling or operating systems to optimize synthesis, evolution, and adaptation

In addition to the twelve points listed above, the workshop generated eight broad-based, cross-cutting recommendations to enable nanotechnology to achieve the advances described above:

1. Increase efforts to understand the potential effects of “nano-sized” particles upon living systems in the greatest possible detail and thoroughly address in advance any possible toxic effects or other environmental issues
2. Create a vigorous educational program addressing the nature and potential impact of nanomaterials, encompassing all segments of society and all levels of the educational spectrum
3. Expand research in the field of structural materials to provide the foundations for new breakthroughs at the nanoscale in this important field
4. Develop a national focus on nanoscience and nanotechnology research related to civil infrastructure and transportation
5. Expand programs designed to support the operation of medium-sized specialized instruments for nanoscale science and engineering, and to develop more affordable instruments
6. Recruit students into nanomaterials-related fields as early as possible in their educational careers
7. Reach out to the general public, legislators, and community agencies—conveying the benefits, while also carefully considering ethical, environmental, and societal dimensions of nanoscience and nanotechnology
8. Strengthen the interactions between industry, academia, and government laboratories

APPENDIX A. WORKSHOP AGENDA

NNI Grand Challenge Workshop on Nanomaterials

11–13 June 2003

National Science Foundation
4201 Wilson Blvd.
Arlington, VA 22230

Wednesday, 11 June 2003

7:00 a.m.	Breakfast meeting for Session Chairs, Room 370
7:30 a.m.	Continental breakfast for participants, Room 375 Registration desk, Room 375 Staff: Patricia Anthony (NNCO)
8:00 a.m.	**Opening Plenary Session, Room 375**
8:00 – 8:15 a.m.	*Introductory Remarks: Charge for the Workshop* Robert Hull (Univ. of Virginia)
8:15 – 8:30 a.m.	*Overview of the National Nanotechnology Initiative (NNI)* Sharon Hays (OSTP)
8:30 – 8:50 a.m.	*The Promise and Challenges of Nanotechnology* David Swain (Boeing)
8:50 – 9:00 a.m.	Discussion
9:00 – 9:20 a.m.	*Nanoimprint Lithography—An Engine of Low-Cost and High Throughput Nanomanufacturing* Stephen Chou (Princeton)
9:20 – 9:30 a.m.	Discussion
9:30 – 9:50 a.m.	*Perspectives: Beyond Equilibrium Materials—Nature's Routes Grow and Assemble Materials* Angela Belcher (MIT)
9:50 – 10:00 a.m.	Discussion
10:00 – 10:30 a.m.	Coffee break, Room 375
10:30 – 10:50 a.m.	*Perspectives: Beyond Classical (Binary Logic) Materials* Paul Alivisatos (Berkeley)
10:50 – 11:00 a.m.	Discussion
11:00 – 11:20 a.m.	*Computational Materials Science at the Nanoscale: Challenges and Opportunities* Peter Voorhees (Northwestern)

11:20 – 11:30 a.m.	Discussion
11:30 – 11:50 a.m.	*Perspectives: What's New at the Nanoscale—The Brave New World of Buckytubes* Richard Smalley (Rice)
11:50 a.m. – 12:00	Discussion
12:00 noon	Lunch

1:00 – 1:15 p.m. Charge to the Breakout Groups, Room 375
Robert Hull

1:15 – 4:00 p.m. First Breakout Sessions

The goals for each of the first breakout sessions are to explore advances in—and the potential of—key research areas, in order to help define a new grand challenge for nanomaterials for the next decade. We anticipate that there may be considerable overlap in the topics identified by each of the first breakout groups as potential components of the new nanomaterials grand challenge. These will be consolidated in the subsequent plenary session and refined in the second group of breakout sessions. Co-chairs of the breakout sessions will be responsible for summarizing the conclusions of each breakout group and presenting them to the plenary session. Some writing will need be done in each session for possible use in preparing the final report of the workshop.

Session 1: Beyond Conventional Lithography, Room 340
Session Chairs: David Weitz (Harvard), Ruud Tromp (IBM)
Staff: W. Lance Haworth (NSF)

- *Discussion topics to begin this session may include, for example, structure building, self-organization, directed assembly and self-assembly, the "quantum quill," …*

Session 2: Beyond Equilibrium Materials, Room 365
Session Chairs: James Heath (UCLA), Miriam Rafailovich (Stony Brook)
Staff: LaVerne Hess (NSF)

- *Discussion topics to begin this session may include, for example, evolving living/non-living systems, hybrids, hard and soft materials, adaptive materials, the integration of dissimilar materials …*

Session 3: Beyond Classical (Binary Logic) Materials, Room 370
Session Chairs: Kim Dunbar (Texas A&M), Richard Webb (Maryland)
Staff: Hugh Van Horn (NSF)

- *Discussion topics to begin this session may include, for example, multistate quantum entanglement, tunneling, quantum transport, molecular materials, controlled spin coherence lifetimes, quantum mechanical signatures designed into useful materials …*

Session 4: Virtual Materials, Room 380
Session Chairs: Samuel Bader (Argonne), Priya Vashishta (USC)
Staff: Geoff Holdridge (NNCO)

- *Discussion topics to begin this session may include, for example, multiscale simulations, classical/quantum hybrid simulations, rules governing self-organization…*

Session 5: What's New at the Nanoscale?, Room 390
Session Chairs: Alexander King (Purdue), Richard Siegel (RPI)
Staff: Stephen Gould (NNCO)

- *Discussion topics to begin this session may include, for example, new, novel, or tailorable properties at nanodimensions, emergent behavior, thermodynamics, structure, new paradigms for new materials …*

4:00 p.m. **Second Plenary Session, Room 375**

This plenary session will hear reports from the first set of breakout sessions and begin the process of collective identification of potential flagship components of the nanomaterials grand challenge.

4:00 – 4:10 p.m.	Report from Breakout Session 1
4:10 – 4:20 p.m.	Discussion
4:20 – 4:30 p.m.	Report from Breakout Session 2
4:30 – 4:40 p.m.	Discussion
4:40 – 4:50 p.m.	Report from Breakout Session 3
4:50 – 5:00 p.m.	Discussion
5:00 – 5:10 p.m.	Report from Breakout Session 4
5:10 – 5:20 p.m.	Discussion
5:20 – 5:30 p.m.	Report from Breakout Session 5
5:30 – 5:40 p.m.	Discussion

5:40 – 6:00 p.m. **Discussion: Preliminary Identification of the Nanomaterials Grand Challenge and its Flagship Components**

6:00 p.m. Adjourn for day

6:00 – 6:15 p.m. Meeting of Workshop Steering Committee, Room 375

6:30 – 7:30 p.m. Reception, Hilton Hotel, "Gallery III"

Participants are free to make their own dinner arrangements. A list of nearby restaurants is provided in the packet of registration materials.

8:00 p.m. Dinner for Workshop Steering Committee at Bistro Bistro

<u>Thursday, 12 June 2003</u>

8:30 a.m. Continental breakfast, Room 375

9:00 a.m. Second Plenary Session (Continued), Room 375

This session will continue the discussion of the nanomaterials grand challenge and identify new groupings for discussion of the flagship components of this grand challenge by defining an entirely new set of 3–5 breakout sessions.

10:00 – 10.30 a.m. Coffee break, Room 375

Workshop Steering Committee meeting, Room 375

During this meeting, the Workshop Steering Committee will complete the selection of topics for the second set of breakout sessions and reassign participants to these sessions.

10:30 – 11.00 a.m. Topics and Chairs for Second Breakout Sessions;
Assignment of Participants to Sessions;
Charge for Second Breakout Sessions
Robert Hull

11:00 a.m. – 12:00 noon Second Breakout Sessions

These sessions will discuss and refine each of the newly identified potential flagship components of the nanomaterials grand challenge.

Some writing will be done in each session for use in preparing the final report of the workshop.

Session A, Room 340
Session B, Room 365
Session C, Room 370
Session D, Room 380—*if needed*
Session E, Room 390—*if needed*

12:00 noon Lunch

1:00 – 3:00 p.m. Second Breakout Sessions Continue

3:00 p.m. Coffee Break, Room 375

3:30 p.m. Concluding Plenary Session, Room 375

The concluding plenary session will begin with reports from the second breakout sessions and refine the flagship components of the nanomaterials grand challenge through further discussion.

3:30 – 3:45 p.m.	Report from Breakout Session A
3:45 – 4:00 p.m.	Discussion
4:00 – 4:15 p.m.	Report from Breakout Session B
4:15 – 4:30 p.m.	Discussion
4:30 – 4:45 p.m.	Report from Breakout Session C
4:45 – 5:00 p.m.	Discussion
5:00 – 6:00 p.m.	Reports and Discussion from Breakout Sessions D and E—*if needed.*

6:00 – 6:30 p.m.	**Discussion of the Nanomaterials Grand Challenge**

The concluding discussion will refine the definition of the over-arching nanomaterials grand challenge.

6:30 p.m.	Adjourn for day
6:30 – 6:45 p.m.	Meeting of Workshop Steering Committee, Room 375
	Participants are free to make their own dinner arrangements.

<u>Friday, 13 June 2003</u>

8:30 a.m.	Continental breakfast, Room 375
9:00 a.m.	**Plenary Session for Writing Subgroups, Room 375** **General Discussion and Assignment of Writing Tasks** **(for workshop committee and volunteers)**
	Discussion of format of the report and assignment of individual writing subgroups.
9:30 – 12.00	Writing report
12:00 noon	Working lunch
1:00 p.m.	Writing groups reconvene
3:00 p.m.	Draft report completed, workshop adjourns.

Appendix B. List of Workshop Participants and Report Contributors*

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APPENDIX C. LIST OF ABBREVIATIONS

AAAS	American Association for the Advancement of Science
AFOSR	Air Force Office of Scientific Research
AFRL	Air Force Research Laboratory
DOE	Department of Energy
DOT	Department of Transportation
DPN	Dip pen nanolithography
EPA	Environmental Protection Agency
FDA	Food and Drug Administration
FE	Finite element
GMR	Giant magnetoresistance
GPS	Global positioning system
MD	Molecular dynamics
MEMS	Microelectromechanical
MOSFET	Metal-oxide-semiconductor field effect transistor
NEMS	Nanoelectromechanical
NIST	National Institute of Standards and Technology
NNCO	National Nanotechnology Coordination Office
NNI	National Nanotechnology Initiative
NSET	Nanoscale Science, Engineering, and Technology Subcommittee of the National Science and Technology Council
NSF	National Science Foundation
OSTP	Office of Science and Technology Policy (Executive Office of the President)
QCA	Quantum cellular automata
QDM	Quantum dot molecule
QM	Quantum mechanical
RAM	Random access memory
SCC	Stress corrosion cracking
SWNT	Single-wall carbon nanotube
USDA	(U.S.) Department of Agriculture
U.K.	United Kingdom
UV	Ultraviolet
WTEC	World Technology Evaluation Center

National Science and Technology Council

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