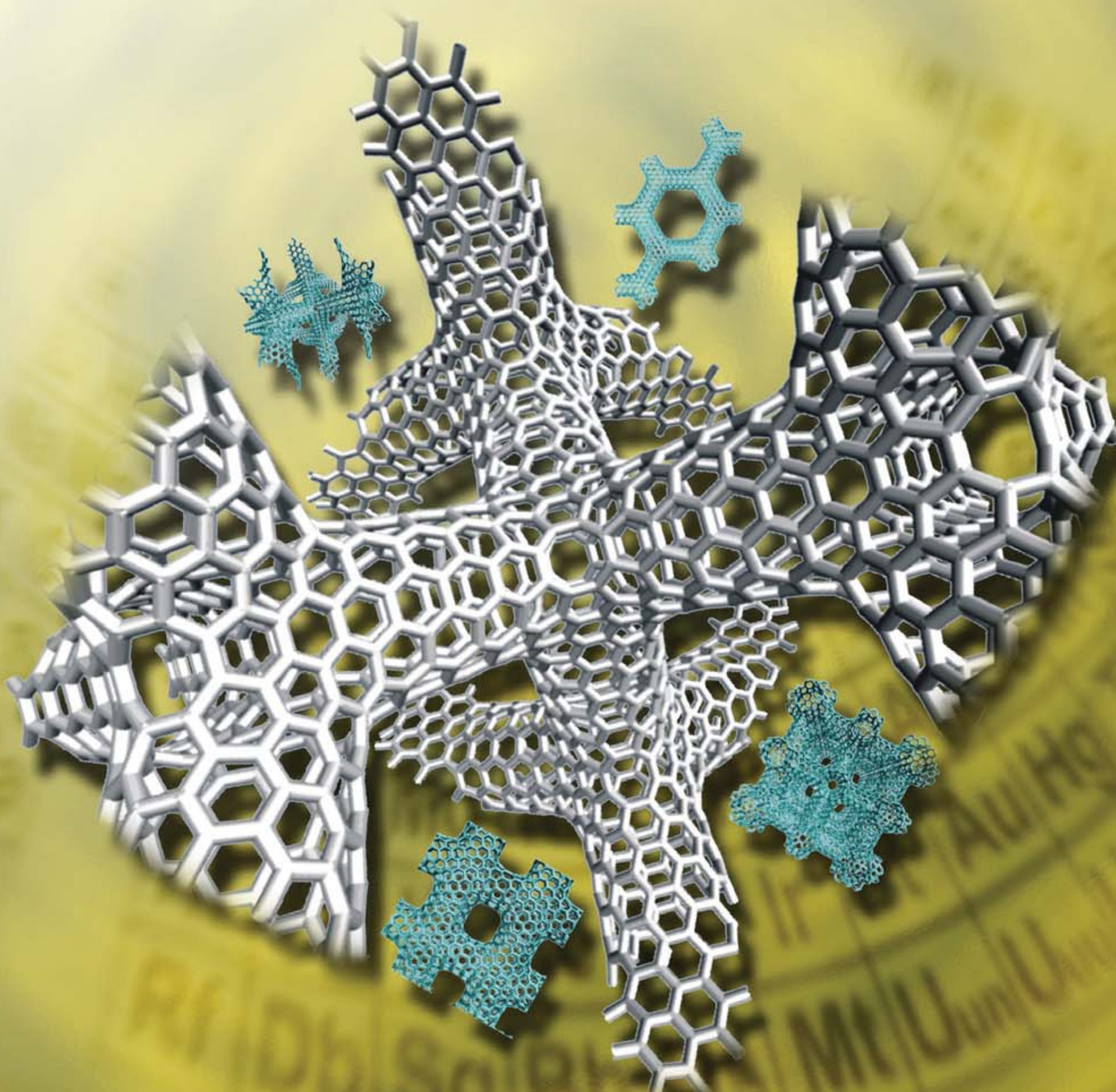
RESEARCH DIRECTIONS II

Long-Term Research & Development Opportunities in Nanotechnology

Report of the National Nanotechnology Initiative Workshop



About the Nanoscale Science, Engineering, and Technology Subcommittee

The Nanoscale Science, Engineering, and Technology Subcommittee (NSET) is the interagency body responsible for coordination of the National Nanotechnology Initiative. It is a subcommittee of the National Science and Technology Council's Committee on Technology. The National Science and Technology Council is the principal means within the Executive Branch to coordinate science and technology policy across the diverse entities that make up the Federal research and development enterprise. The National Nanotechnology Coordination Office (NNCO) provides technical and administrative support to the NSET Subcommittee and assists the subcommittee in preparing planning, budget, and assessment documents for the National Nanotechnology Initiative. More information is available at http://www.nano.gov.

About this Report

This document is the report of a workshop held in September 2004. It was the final event in a series of topical workshops sponsored by the NSET Subcommittee. These workshops were part of the NSET Subcommittee's long-range planning efforts for the National Nanotechnology Initiative, the multiagency Federal nanotechnology R&D program. The recommendations of the Research Directions II workshop provided guidance to the NSET Subcommittee in development of the 2004 and 2007 strategic plans for the National Nanotechnology Initiative.

Cover

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Front cover, central image: Molecular models of two- and three-dimensional carbon networks created from one-dimensional nanoscale building blocks. Calculations predict unique and unusual electrical and mechanical properties that depend on the hierarchical system architecture. For example, electrical charges travel along specific paths through the branching point of these multiterminal systems. This observation suggests the possibility of using these networks to form complex nanoelectronic circuits. (From J. M. Romo-Herrera, M. Terrones, H. Terrones, S. Dag, V. Meunier, "Covalent 2D and 3D Networks from 1D Nanostructures: Designing New Materials," *Nano Letters*, **7**, 570-576 (2007). Copyright 2007, American Chemical Society; used by permission. Image provide by Vincent Meunier, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory.)

Back cover, central image: A topograph, recorded using an atomic-force microscope, of a device used to separate electrons according to their spin, which could be used in next-generation "spintronic" devices. Spatial separation of electrons is achieved in this device using cyclotron motion in the presence of a weak magnetic field. (From L. P. Rokhinson, V. Larkina, Y. B. Lyanda-Geller, L. N. Pfeiffer, K. W. West, "Spin Separation in Cyclotron Motion," *Physical Review Letters*, **93**, 146601 (2004). Copyright 2004, American Physical Society; used by permission. Image provided by Leonid P. Rokhinson, Department of Physics, Purdue University.)

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RESEARCH DIRECTIONS II

LONG-TERM RESEARCH & DEVELOPMENT OPPORTUNITIES IN NANOTECHNOLOGY

Report of the National Nanotechnology Initiative Workshop

National Academy of Sciences, Washington, DC
September 8–10, 2004

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National Science and Technology Council
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Acknowledgements

The Nanoscale Science, Engineering, and Technology Subcommittee extends its thanks to the organizers, presenters, and participants of this workshop. Particular thanks go to the workshop chair, Dr. Altaf Carim, for his leadership in organizing this workshop, in cooperation with Dr. Celia Merzbacher and Dr. Clayton Teague. Thanks also to the report editors, Prof. James Baker, Dr. Robert Hwang, and Dr. Judith Stein, for their time and effort spent in shaping this document; and to the session chairs, named on the chapter title pages, for leading the breakout sessions and authoring the corresponding chapters of this report. The workshop presentations and session discussions provided the basis of this report; without the valuable input of all who participated, this report would not have been possible.

Thanks are due to the NNCO staff members, who made sure that the meeting logistics were handled properly and efficiently, and to all those who provided editorial support and review of the draft prior to publication of the report. Thanks also to Dr. Roger van Zee, who as Executive Editor prepared this report as part of his Department of Commerce Science and Technology Fellowship year work assignment.

Finally, thanks go to the National Academy of Sciences for providing a venue for the workshop, and to the member agencies of the Nanoscale Science, Engineering, and Technology Subcommittee and their representatives for joint sponsorship of the workshop.

PREFACE

This report is the outcome of the Research Directions II Workshop held in September 2004. The Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the National Science and Technology Council's Committee on Technology sponsored this workshop, the final event in a series of topical workshops it sponsored in 2002 and 2004. These workshops were part of the NSET Subcommittee's long-range planning efforts for the National Nanotechnology Initiative (NNI), the multiagency Federal nanotechnology R&D program. The recommendations of the Research Directions II workshop provided guidance to the NSET Subcommittee in development of the 2004 and 2007 National Nanotechnology Initiative strategic plans, much as the 1999 Nanotechnology Research Directions Workshop guided the development of the original NNI Implementation Plan. The NNI is driven by long-term goals based on broad community input, in part received through workshops such as this one. The NNI aims to coordinate Federal activities that accelerate the discovery, development, and deployment of new technologies that exploit the unique biological, chemical, and physical properties at the nanometer length scale, as a means to address national needs, enhance our nation's economy, and improve the quality of life.

In each of the topical workshops, experts from academia, government, and industry examined a particular aspect of nanotechnology in detail. They 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 R&D regarding long-term goals and hard problems.

The Research Directions II Workshop participants were asked to take a high-level view of nanotechnology research and development, to identify the broad scientific and technical challenges that should be targeted, and to examine the NNI from a programmatic perspective. This report is intended to give a broad exposition of the thinking behind the strategic plan and to serve as a guide in its implementation.

The workshop proceeded in three phases. It began with a series of plenary lectures in which subject matter experts shared their insights and discussed the status of specific nanotechnology research areas. Parallel breakout sessions followed in five broad technology categories. The aim of these sessions was to distill and integrate the workshop presentations, to identify research targets, and to spell out indicators of progress for those targets. Last was another series of five breakout sessions. The aim of these was to identify opportunities, mechanisms, and strategies to accelerate and enhance realization of the specific nanotechnology goals identified in the first breakout sessions, in the context of responsible, proactive planning. This report delineates the findings and recommendations of the participants in the breakout sessions.

On behalf of the NSET Subcommittee, we thank Prof. J. R. Baker, Jr., Dr. R. Q. Hwang, Dr. J. Stein, and Dr. R. D. van Zee, the report editors, and all the chapter authors, speakers, session chairs, and participants for their contributions to the workshop and to this report. Their generous sharing of time and expertise made the workshop a success and should make this report a valuable reference.

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EXECUTIVE SUMMARY

Novel properties emerge in biological, chemical, and physical systems at dimensions of between approximately 1 nanometer and 100 nanometers. These properties can differ in fundamental ways from the properties of individual atoms and molecules and the properties of bulk materials. Exploring and understanding these nanoscale phenomena are at the forefront of scientific and engineering research. Drawing upon nanometer-scale science and engineering, nanotechnology involves the ability to manipulate, measure, and model physical, chemical, and biological systems at nanometer dimensions, in order to exploit nanoscale phenomena.

The National Nanotechnology Initiative (NNI) is the multiagency program established in fiscal year 2001 to coordinate Federal nanotechnology R&D. The NNI expedites the discovery, development, and deployment of nanoscale science and technology to serve the public good, through a program of coordinated research and development aligned with the missions of the participating agencies. It provides a vision of the long-term opportunities and benefits of nanotechnology: a future in which the ability to understand and control matter at the nanoscale leads to a revolution in technology and industry that benefits society.

The NNI is driven by long-term goals based on broad community input. This input is received, in part, through workshops. The NNI Research Directions II Workshop was convened to obtain input concerning the broad scientific and technical challenges facing the nanotechnology research and development community and to recommend strategies for addressing these opportunities. The participants were asked to take a high-level view of nanotechnology research and development and to identify the scientific and technical challenges that should be targeted. They also examined the NNI from a programmatic perspective. Representatives from industrial labs, research universities, and government agencies were invited, in order to have a full spectrum of perspectives. Scientific, societal, and technology innovation issues were considered.

RESEARCH AND DEVELOPMENT DIRECTIONS IN NANOTECHNOLOGY

In a set of parallel breakout sessions, workshop participants considered five broad areas of nanotechnology research and development (R&D). They were asked to consider scientific opportunities, potential impacts, and required resources. They were charged with identifying specific research targets and metrics of progress towards those targets. Summarized below are the findings, recommendations, and conclusions of these technical breakout sessions.

Nanomaterials by Design, Electronics/Photonics/Magnetics, CBRE

New nanostructured materials with specific designed-in properties and functions have the potential to impact many areas of nanoscience and nanotechnology. They are the bedrock of advances in structural applications; energy and the environment; nanomedicine; information processing; and chemical, biological, radiological, and explosive (CBRE) detection. The group taking part in this session recommended that R&D emphasis be placed on design and discovery of new nanomaterials; hierarchical self-assembly; materials for sensing applications; and new information processing and storage technologies.

Energy and the Environment

Nanotechnology research has tremendous potential for strengthening energy security and for protecting and improving the environment. The group taking part in this session recommended targeting R&D on technologies for the transformation, storage, and transmission of energy; developing tools to better understand the environmental impacts of nanotechnology; designing materials to reduce waste and improve the efficiency of manufacturing processes; and understanding and controlling the creation, transport, fate, and health effects of nanomaterials in the environment and in the workplace.

Nanomedicine, Nanobiotechnology, Agriculture, and Food Systems

Opportunities abound for integrating biology and nanotechnology. The group taking part in this session recommended developing nanotechnology tools capable of studying cell function within tissue environments; developing nanoparticles that target specified cells and tissues in humans, probe the local environment, act as contrast markers, deliver therapeutics, and sense cellular responses; developing hybrids of biological and physical systems; and developing a safety framework for medical, agricultural, and food products that incorporate nanotechnology. The important science questions relate to the creation of nanostructured materials that operate in biological systems and to the ability to measure phenomena at the nanoscale in living systems. Computation capacity and software development are needed to organize information and facilitate modeling of nanoscale biological processes.

Nanomanufacturing, Nanomachines, and Nanosystems

The ultimate success of nanotechnology R&D will depend upon the successful transition of advances in the nanosciences from the laboratory bench to the marketplace. Methods to fabricate nanosystems are at the heart of any commercial realization of nanotechnology. Opportunity areas include investment in tool development, manufacturing protocols for multifunctional and adaptive materials, fundamental research on mesoscale mathematics and physics, and ultimately integration of nanomaterials into macroscale devices. The participants in this session recommended that R&D efforts focus on factors that affect manufacturability (e.g., cost effectiveness, production rate); on standardization of functional interfaces between length and time scales; on translation of nanoscale functionalities to macroscale systems; and on multiscale modeling and characterization.

Instrumentation, Metrology, Advanced Environments, and Simulation

Issues regarding instrumentation, metrology, advanced environments (e.g., buildings), and simulation are crosscutting, inasmuch as they affect all aspects of nanotechnology. The participants in this breakout session concluded that a lack of progress in these areas would seriously hamper the discovery and innovation process. This group recommended developing robust high-speed instruments, models, and standards to enable measurement of material properties such as size and structure with < 0.01 nm accuracy in normal laboratory environments; developing devices and instruments for three-dimensional, automated, real-time measurement and control of manufacturing processes with subatomic precision; developing multiscale models that model material properties and nanomanufacturing; and building facilities that meet the exacting requirements of nanocharacterization research and manufacturing.

SPEEDING RESPONSIBLE DISCOVERY AND INNOVATION IN NANOTECHNOLOGY

In a second set of breakout sessions, workshop participants were asked to consider how the Federal research and development effort could be organized and focused to most efficiently achieve its goals. The objectives of these breakout sessions were to identify strategies and tactics to expedite discoveries in nanoscale science and engineering and to responsibly translate these discoveries into tangible products. The findings and recommendations coming out of in these breakout sessions are summarized below.

Fundamental Scientific Issues

Recent years have witnessed an explosion of new scientific discoveries and inventions in nanoscale science and engineering. Yet many fundamental problems remain to be addressed. The group taking part in this session recommended focusing on understanding single and collective effects and design of integrated systems; studying the mechanisms of self-assembly; and investigating the interfaces between hard and soft materials and appropriate engineering approaches to making and controlling those interfaces. The group also identified two important, if general, goals: developing new nanotechnology-derived materials and developing instrumentation for studying nanoscale materials and phenomena. Concurrently, the group noted, it will be important to focus on fundamental research in manufacturing to be able to effectively commercialize new nanosystems.

Application Opportunities and Technology Transfer

To derive maximum benefit from nanotechnology R&D, there must be a focus on applications and commercially viable products. The group taking part in this session observed that new collaboration paradigms are needed between industrial, academic, and government labs, and also between the private sector and government agencies. Developing commercially viable nanotechnology-enabled products will rely on the development of an accessible nanotechnology infrastructure, including instrumentation, metrology, advanced buildings, simulation technologies, and nanomanufacturing prototyping facilities. The group members concluded that commercialization would be accelerated by implementing better information sharing and technology transfer mechanisms, goal-oriented peer review, regular goal setting, industry involvement in setting directions and priorities, and streamlined and uniform intellectual property transfer processes.

Infrastructure Needs

Building the infrastructure to meet the goals of the NNI is an important aspect of U.S. investment strategy. To maximize the benefit of the existing infrastructure and to provide strategic input into further investment, participants recommended that the agencies of the NNI catalog the existing resources. High-throughput instruments to monitor and assess nanomaterials in the workplace and in the environment should be a priority. Computational resources should be dedicated to highest-priority research problems. NNI agencies should work with regional, state, and industrial sectors to develop a structure for highly leveraged, distributed approaches to infrastructure development.

Societal Implications

The societal implications of nanotechnology are important and involve many stakeholders. The participants in this session felt that it is imperative to pursue multidisciplinary research, education, and outreach programs focused on the full spectrum of society's interactions with nanotechnology (social, ethical, economic, commercial, workforce, etc.). The group recommended that emphasis be placed on preserving and nurturing public trust in nanotechnology, and on understanding environmental and human exposures to potentially hazardous new materials. The group also emphasized that coordinating a multidisciplinary approach will better enable programs that communicate with and educate the public.

Funding Strategy, Interdisciplinary Opportunities, Grand Challenges, and Interactions with Other Stakeholders

In order to ensure the most rapid commercialization of nanotechnology and maintain the economic competitiveness of the United States, the group taking part in this session recommended that fundamental research remain a significant part of the NNI investment over the next two decades. Session participants recommended that funding for applied research be shifted towards R&D centers with more industry participation. Some aspects of nanotechnology have become sufficiently mature and the potential benefits are sufficiently great that it is now possible for relevant government agencies to team together to pose a small set of very specific challenges to the research and engineering communities. For maximum effectiveness, the group recommended establishing a nanotechnology alliance for sharing information, best practices, and roadmaps across all sectors. Workforce development would be accelerated by creating a clearinghouse to match graduate students with internships in industry.

1. Introduction

BACKGROUND

Novel properties emerge in biological, chemical, and physical systems, at dimensions of between approximately 1 nanometer and 100 nanometers. These properties can differ in fundamental ways from the properties of individual atoms and molecules and those of bulk materials. Drawing upon nanometer-scale science and engineering, nanotechnology involves the ability to manipulate, measure, and model physical, chemical, and biological systems at nanometer dimensions, in order to exploit nanoscale phenomena.

Nanotechnology holds great potential and stands to impact a broad range of fields. It offers, for example, the promise of new information processing systems, new disease therapies, and new ways to collect and store energy. In the near term, nanotechnology will improve existing devices and systems. In the long term, nanotechnology will lead to an array of entirely new materials and products with new functionality and properties.

The National Nanotechnology Initiative (NNI) is the multiagency program established in fiscal year 2001 to coordinate Federal nanotechnology R&D. The NNI expedites the discovery, development, and deployment of nanoscale science and technology to serve the public good, through a program of coordinated research and development aligned with the missions of the participating agencies. Serving as a central locus for communication, cooperation, and collaboration for all participating Federal agencies, the NNI brings together the expertise needed to guide and support the advancement of this broad and complex field. The NNI creates a framework for a comprehensive nanotechnology R&D program by establishing shared goals, priorities, and strategies, providing avenues for each individual agency to leverage the resources of all participating agencies. While the NNI as a program does not fund research, it informs and influences the Federal budget and planning processes through its member agencies. Moreover, it provides a common vision of the long-term opportunities and benefits of nanotechnology: a future in which the ability to understand and control matter at the nanoscale leads to a revolution in technology and industry that benefits society.

Between 2002 and 2004, the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the National Science and Technology Council's Committee on Technology sponsored a series of topical workshops. These workshops were part of the NSET Subcommittee's long-range planning efforts for the NNI. The NNI is driven by long-term goals based on broad community input received, in part, through such workshops. Each topical workshop examined a particular aspect of nanotechnology in detail. The workshop participants were asked to develop long-term (ten years or longer) visionary goals and to identify scientific and technological barriers that once overcome would enable advances toward those goals. The reports resulting from this series of workshops inform the scientific and engineering community, as well as the Federal agencies that implement the NNI. The reports also provide direction to researchers and program managers in specific areas of nanotechnology regarding long-term goals and hard problems.

The NNI Research Directions II Workshop was the final workshop of the 2002-2004 series. The participants were asked to take a wide-angle view of nanotechnology research and development, to identify the broad scientific and technical challenges that should be targeted, and to examine the NNI from a programmatic perspective. Representatives from industrial labs, research universities, and government agencies were invited, in order to have a broad range of perspectives. The recommendations of this workshop provided guidance to the NSET Subcommittee in development of the 2004 and 2007 National Nanotechnology Initiative strategic plans, much as the first Nanotechnology Research Directions Workshop, held in 1999, guided the development of the original NNI Implementation Plan.

THE WORKSHOP

Experts from academia, industry, and government laboratories and agencies assembled at the National Academy of Sciences in Washington, DC to take part in the National Nanotechnology Initiative Research Directions II Workshop. As noted, the goals of the workshop were to obtain input from the scientific community on planning NNI research directions and to inform development of the NNI strategic plan mandated by the 21st Century Nanotechnology Research and Development Act (Public Law 108-153).

The workshop began with a set of plenary lectures. Following the background lectures, parallel breakout sessions convened in which structured focus groups examined five broad technology areas. These technology areas were:

- Nanomaterials by design, electronics/photonics/magnetics, CBRE
- Energy and the environment
- Nanomedicine, nanobiotechnology, agriculture, and food systems
- Nanomanufacturing, nanomachines, and nanosystems
- Instrumentation, metrology, advanced buildings, and simulation

In each breakout session, the participants were asked to select major areas of research opportunity. The participants were also charged with identifying specific research targets and suitable indicators of progress towards those targets.

In a second set of breakout sessions, participants considered strategies and tactics for achieving the research goals and targets set out in the first set of breakout sessions. These breakout sessions considered the following:

- Fundamental scientific issues
- Application opportunities and technology transfer
- Infrastructure needs
- Societal implications
- Funding strategy, interdisciplinary opportunities, grand challenges, and interactions with other stakeholders

In each of this second set of breakout sessions, the participants were asked to identify and prioritize the opportunities and needs, to suggest mechanisms to address these opportunities and needs, and the recommend strategies by which NNI investments might be leveraged against the investments of other stakeholders.

THE REPORT

The remainder of this report summarizes the findings and recommendations developed in the breakout sessions described above. Chapters 2-6 present the research targets and indicators of progress developed in the technology-oriented sessions. Chapters 7-11 present the strategies and mechanisms recommended for realizing the proposed research targets. Appendix A gives the workshop agenda. Appendix B lists the workshop participants. Appendix C is a list of abbreviations used in the report. Appendix D lists the NNI-sponsored workshops held between 2001 and 2004.

Because the subjects covered in the technical and strategic breakout sessions are broad and complementary, common themes appear in some chapters. These apparent redundancies reflect the crosscutting nature of the field and of this report's recommendations.

2. Nanomaterials by Design, Electronics/Photonics/Magnetics, CBRE

Session Chair: R. S. Williams

INTRODUCTION

New nanomaterials have the potential to impact all areas of nanoscience and nanotechnology. Development of materials with highly structured designs and functions originating in their properties at the nanoscale will be fundamental to advances in structural applications; energy and the environment; nanomedicine; and chemical, biological, radiological, and explosive (CBRE) detection. Future information processing technologies will also rely heavily on new nanomaterials.

RESEARCH TARGETS

The participants in this session recommended that emphasis be placed on the following technology challenges and research targets:

- Design and discovery of new nanomaterials
- Hierarchical self-assembly
- Future information processing technology
- Addressable terabit storage
- Ubiquitous biosensing and chemically responsive materials

Discovery and Design of New Nanomaterials

Fabrication of any new materials requires understanding, measuring, and ultimately controlling matter on many scales of length and time. The frontier of new materials design is at the nanometer length scale. The nanoscale is between the atomic scale phenomena that drive condensed matter physics and synthetic chemistry, and the microscopic and macroscopic scales where structure/property/function relationships have constituted the central paradigm of traditional materials science. Researchers are keenly aware of significant missing links in their abilities to design new nanoengineered materials; acutely needed are fundamental investigations of phenomena that emerge on the nanoscale, and new tools and techniques that will allow researchers to visualize, characterize, model, and simulate materials with nanometer resolution.

Targeted efforts to accelerate the pace of new materials discovery and to enhance our ability to design properties and functions into materials should lead to breakthroughs in a variety of fields. In the area of energy applications, materials R&D should lead to development of thermoelectric materials, energy-harvesting materials and devices, and membranes and electrodes for fuel cells. Nanotechnology also holds promise for new materials that can sustain high doses of radiation without degradation or that lead to a new generation of radiation detectors (for example, gamma spectrometers that outperform germanium-based detectors). New nanotechnology-inspired polymers, alloys, and composite materials could improve the civil infrastructure by making longer-lasting roadway surfaces, better buildings and bridges, and stronger but lighter trains, planes, and automobiles. Materials with enhanced performance in the biological environment are essential to improved medical devices, prosthetics, and drug delivery. Finally, understanding and control of the wet/dry interface will allow development materials that are biocompatible and with enhanced corrosion resistance in natural environments.

Some central themes are evident in efforts to discover or design new nanomaterials. Foremost among these is emergent properties: R&D must be done to correlate collective properties of nanomaterials with nanoscale theory, modeling, and simulation of materials properties. A second central theme is R&D for molecular- and biological-recognition materials and systems. Techniques modeled on biological processes (for example, using bioscaffolds to synthesize absolutely monodisperse materials) will have widespread application. A third central theme in the area of nanomaterials R&D is surface engineering—of coatings, interfaces, and membranes. A fourth central R&D theme is the development of multifunctional materials as the basis of future applications such as smart textiles.

Information technology will also benefit from multifunctional materials. New systems architectures for information processing could alleviate "the interconnect problem" by integrating presently dominant charge-based electronics with spintronics and photonics.

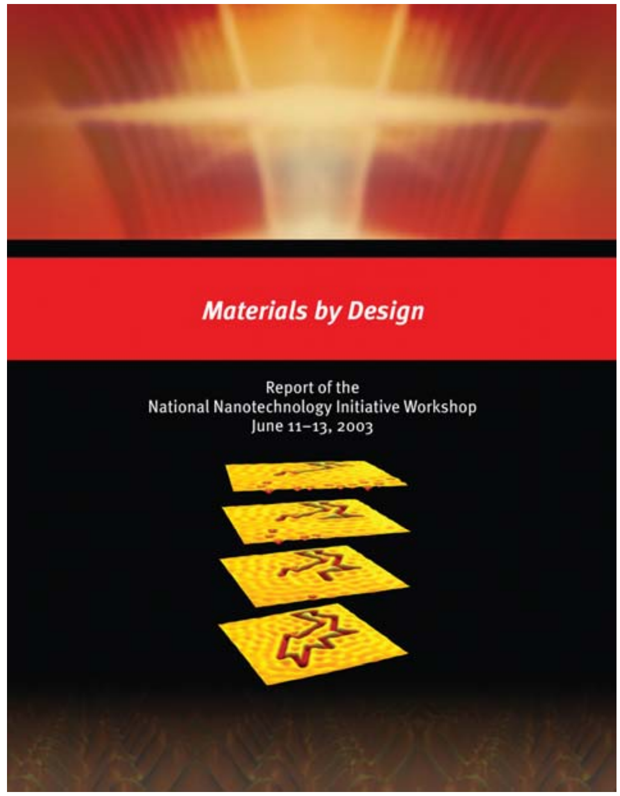


Figure 2.1. The Nanomaterials workshop explored the use of nanoscale phenomena to design materials with specific physical and chemical properties. Report available at http://www.nano.gov/html/res/pubs.html.

Smart textiles are fabrics that combine the ability to clothe a body with additional tailored functions such as monitoring of physiological functions, embedded processing and communications, controlled permeability to regulate humidity, optical properties that can change in response to light, and germicidal properties. Fabrics are already emerging that meet two or three of these needs simultaneously; the vision is to provide them all. Such fabrics would have clear applications for military personnel, emergency first responders, and persons with special medical needs, as well as for potential spin-off products for the general population.

Indicators of progress in discovery and design of new materials will include:

- New photovoltaic cells based on nanomaterials
- Incorporation of nanomaterials into aircraft
- Successful modeling and simulation of nanomaterial properties

Hierarchical Self-Assembly

The chemical industry considers self-assembly to be one of the most promising means for cost-effective manufacturing of hierarchically structured nanomaterials for commercial applications. Electronics and photonics technology developers also see a critical need for developing techniques and tools to self-assemble systems starting from the atomic scale as successors to current technologies based upon assembling, manipulating, and integrating bulk materials. Tools and techniques such as epitaxy, optical lithography, polishing, and substrate bonding, while currently used for fabricating, assembling, and integrating electronic and optical devices in high volumes, are simply not capable of organizing nanoscale materials into useful device configurations with reasonable throughput. If the electronics and photonics industries are to take advantage of nanoscale structures and properties in new device technologies, the devices must self-assemble on multiple levels.

Biological systems assemble themselves hierarchically. Nature creates life from atoms and molecules, which evolve into living systems by self-assembling into complex forms. Each molecular component performs its assigned function in full coordination with the other components. Biological assembly processes will remain a rich source of ideas for researchers seeking to emulate nature's ability to create complex self-assembling systems. Techniques like biased self-directing self-assembly and templated self-assembly should be fully developed through experiment, simulation, modeling, and theorizing. Appropriate targets should be identified, such as the creation of man-made polymers that are truly monodisperse, as proteins are.

Currently there is a lack of sufficient understanding of how materials self-assemble. There is a critical need for focused research to develop a fundamental understanding of the chemistry of self-assembly processes across multiple length scales and volume scales. Specific issues to be addressed include the kinetics of self-assembly processes, the effects of external stimuli (e.g., electric or magnetic fields) on self-assembly, and formation of composite materials and hierarchical structures with complex functionality through self-assembly. An accelerated research program addressing these issues will yield the necessary knowledge to design and develop materials with tailored properties for self-assembly in desired device configurations.

Indicators of progress in hierarchical self-assembly R&D will include:

- Improved understanding of the kinetics and thermodynamics of self-assembly for prototypical systems
- Industrial application of self-assembly-driven fabrication

Future Information Processing Technology

Even while extending complementary metal oxide semiconductor (CMOS) electronics technology to its ultimate limit, the semiconductor industry must simultaneously invent new information-processing technologies to go beyond that boundary. In order to achieve another ten-fold improvement in information processing capabilities over the next fifteen years, manufacturers of CMOS will rely heavily on nanoprocessing and nanomaterials. Future exponential increases in information processing performance will require fundamentally new technologies based on nanoscale properties.

New technologies for performing logical functions are in an embryonic state. The *International Technology Roadmap for Semiconductors* (ITRS) "Emerging Research Devices" section (http://www.itrs.net/) notes that none of the currently proposed post-CMOS technologies—including spin logic, phase logic, quantum cellular automata, molecular devices, crossbar devices, and cross-net devices—appear poised to solve all problems inhibiting large-scale commercialization. A major research effort is necessary to identify, develop, and commercialize a new nanotechnology-based paradigm for information processing.

This effort must include several features. One of the most important is discovery and exploitation of a "post-CMOS switch" or of any element capable of representing bits of information for processing and storage. Another is the exploration of new "state variables" that may represent bits of information and means for addressing and accessing a high density of devices that utilize these new state variables. The state variable might be the spin state of an atomic nucleus or the polarization state of a photon. For any high-density computational architecture, the design must encompass fault- and defect-tolerant systems. For this to be achieved, the thermodynamic limits to the formation of defect-free logic and memory elements must be identified, understood, and compensated for. Fault tolerance may be achieved through self-test, self-repair, and self-healing mechanisms. Last, it will be important to develop new architectures that reduce power density in both space and time and employ heterogeneous integration of nanowires, nanotubes, or organic molecular components with existing materials and architectures.

One goal of the program for information processing beyond CMOS will be to increase the information throughput per joule of dissipated energy to one thousand times that anticipated for CMOS technology at the end of the ITRS roadmap. Another goal will be integrating the selected post-CMOS technology with CMOS, which would remain a supporting platform technology. This implies that commercialization of these technologies will involve both the existing manufacturing industry and new start-up companies.

Indicators of progress in future information processing technology will include:

- Discovery of a reliable post-CMOS switch
- Information transfer per unit energy dissipation significantly less than CMOS

Addressable Terabit Storage

Information has the unusual property of being both an end in itself and a commodity that enables economic development across all areas of business and society. To continue the pace of advances in information technology into the middle part of the twenty-first century, new technologies must be developed for information storage as well as for information processing. Present storage technology already relies on nanotechnology and must continue to do so in order to develop materials and methods that will keep magnetic storage density on its exponential growth curve until fundamental limits are reached.

Simultaneously, scientists and engineers must search for the ultimate successor to magnetic storage. The target for the successor technology should be nonvolatile storage with three orders of magnitude improvement in density that maintains historical trends in decreasing access time and storage costs. As real-time business and entertainment applications grow, there will be an increasing public appetite for higher transmission bandwidth and information storage capacity. Military and security applications also depend on the same capabilities.

Environmental considerations must be a part of every aspect of new storage technology development, including the selection of materials and lifecycle design for devices.

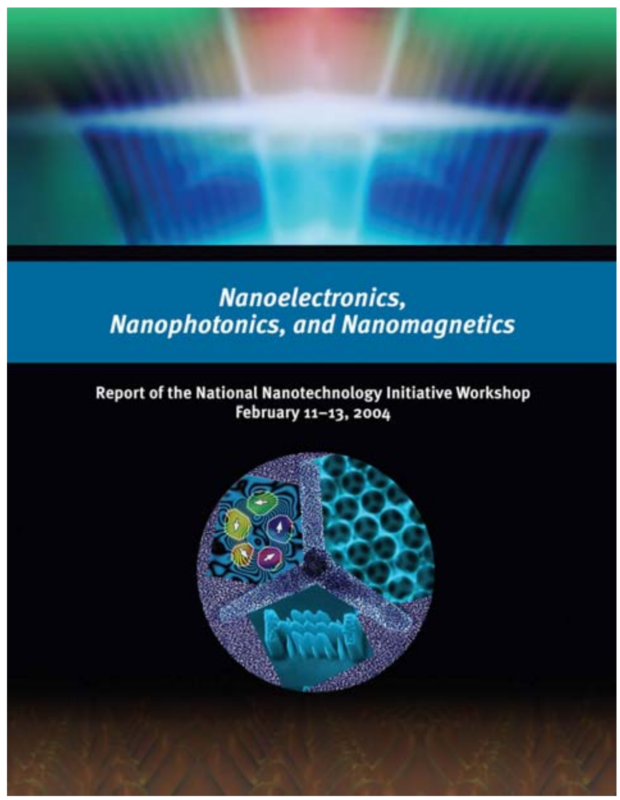


Figure 2.2. The Nanoelectronics, Nanophotonics, and Nanomagnetics workshop explored how to use nanoscale phenomena to create information technology systems with unprecedented capabilities. Report available at http://www.nano.gov/html/res/pubs.html.

Ubiquitous Biosensing and Chemically Responsive Materials

The primary targets of this research area are molecular-recognition materials with the specificity and affinity of antibodies but with extended stability both in the environment and in the body. This single type of innovation is essential to meeting the cancer challenge and enhancing our homeland security through sensing of chemicals, radiological materials, and explosives. It would also improve food security, increase agricultural production, and enable new methods of environmental remediation.

Nanotechnology can easily provide single-molecule sensitivity, but the major technical challenges in sensing systems today are selectivity and specificity rather than sensitivity. Nanotechnology offers answers to these challenges too. First, it provides materials with the highest possible surface area, allowing the use of compact preconcentrators for integrated biosensors. Second, it allows the design of materials and transducers at the biological length scale, which is central to biosensing; the ultimate prospect here is synthetic antibodies. Finally, nanotechnology provides maximal surface-area-to-volume ratio for the final transduction event in biosensing.

Achieving the specificity and selectivity of antibodies with the robustness and stability of inorganic systems underpins many of the key stated goals of researchers in the area of nanobiotechnology.

Indicators of progress in ubiquitous biosensing and chemically responsive materials will include:

- Tags and labels moving like antibodies within the body (“Ab mimetics”)
- Minimal-dose targeted drug delivery
- Biological surveillance of the food and water supplies using single-molecule detection of biological species
- Real-time monitoring to track changes in the environment on an ongoing basis, including detection of chemical, biological, radiological, and explosive materials
- Environmental remediation using nanostructured chemical binding agents with high specificity and extremely high specific surface area

3. ENERGY AND THE ENVIRONMENT

Session Chair: R. J. Hamers

INTRODUCTION

Nanotechnology research has tremendous potential for strengthening our energy security and protecting and improving our environment. General target areas for research include the use of nanotechnology to achieve the long-term goals of clean water, clean air, and clean earth; improving the transformation, transmission, and storage of energy; and assessing and managing the possible risks and benefits associated with nanotechnology. Specific long-term research targets should be geared primarily toward understanding nanomaterials in the environment and in the workplace, using nanotechnology to better understand the environment, and using nanoscale materials to reduce waste and improve energy efficiency.

RESEARCH TARGETS

The participants in this session recommended that emphasis be placed on the following technology challenges and research targets:

- Nanoscale materials with specific physical and chemical properties by design
- Nanoscale materials for energy storage, conversion, and transmission
- Nanoscale catalytic materials
- High-density, wireless, multianalyte sensor arrays
- Proactive risk assessment and risk management associated with nanotechnology

Nanoscale Materials with Specific Physical and Chemical Properties by Design

Rules that correlate chemical composition and nanostructure morphology have not been developed for nanometer-scale materials, so it is not yet possible, in general, to design nanoscale materials and nanoscale composites with specific properties. Because existing computational models are not well adapted to the nanoscale regime, materials development is largely empirical. Research is underway now addressing these challenges; the potential payoff from this work is significant. Future increases in the complexity of nanoscale materials and the integration of biological systems with nanotechnology will make it possible to synthesize complex nanomaterials that integrate many specific types of functionality. This challenging area would integrate the theory, modeling, and simulation of nanoscale interfaces of variable composition and structure to predict chemical reaction pathways, electromagnetic properties and energy transport, mechanical properties, and methods of efficient assembly.

Research in this area could lead to major advances in several fields mentioned elsewhere, including energy production, conversion, and transmission; structural materials for aircraft and other applications; hydrogen storage; and environmental remediation.

Indicators of progress in design of nanoscale materials with specific physical and chemical properties will include:

- Engineered nanoscale materials that decrease energy use of aircraft or other transportation modes
- Engineered nanoscale materials applied to environmental cleanup of contaminated sites

Nanoscale Materials for Energy Storage, Conversion, and Transmission

Use of nanoscale materials could provide a number of potential improvements in energy management. For example, new materials could provide scalable methods to use sunlight to split water for hydrogen production. Other materials could harvest solar energy with an efficiency exceeding twenty percent at a fraction of the production cost of existing, inorganic solar cells. Other applications include highly efficient solid-state lighting, low-loss power transmission lines with gigawatt capacities, and a new generation of batteries, thermoelectric conversion devices, and capacitors.

These new materials and devices would have a number of economic and environmental benefits. Ultimately, they could reduce dependence on fossil fuels, reduce the environmental impact associated with energy use, and reduce the cost associated with industrial manufacturing, thereby increasing economic competitiveness.

Indicators of progress in the use of nanoscale materials in energy applications include:

- High-efficiency solid-state lighting technologies based on nanomaterials
- Nanomaterials that harvest solar energy with efficiencies greater than twenty percent

Nanoscale Catalytic Materials

It has long been known that catalytic processes often involve complex physical and chemical phenomena operating on nanometer length scales. But until recently it has not been possible to control the structure and composition of matter on these length scales. For example, gold nanocrystals are able to catalyze the oxidation of carbon monoxide to carbon dioxide at room temperature (hundreds of degrees lower than conventional catalysts), which demonstrates the dramatic improvements that can be achieved using nanoscale catalytic materials. Acquiring an ability to fabricate catalytic materials with identical properties would be expected to further improve the selectivity of catalytic processes and reduce waste, while the ability to fabricate more complex catalytic systems with multiple reactive sites (even, for example, integrating biological materials with inorganic materials) would facilitate more complex catalytic processes. One high-priority target area of research should be the nanoscale design of highly selective catalytic materials able to reduce waste and improve the efficiency of manufacturing processes.

This research will include several elements. The goal will be bottom-up design and fabrication of catalysts to achieve specific reaction products with high efficiency. First-principles understanding and design of catalytic reactive sites will be a necessary foundation for this activity. When the relevant processes are understood, multiscale modeling and simulation of complex physical and chemical processes will make it possible to predict catalytic activity of specific particle types.

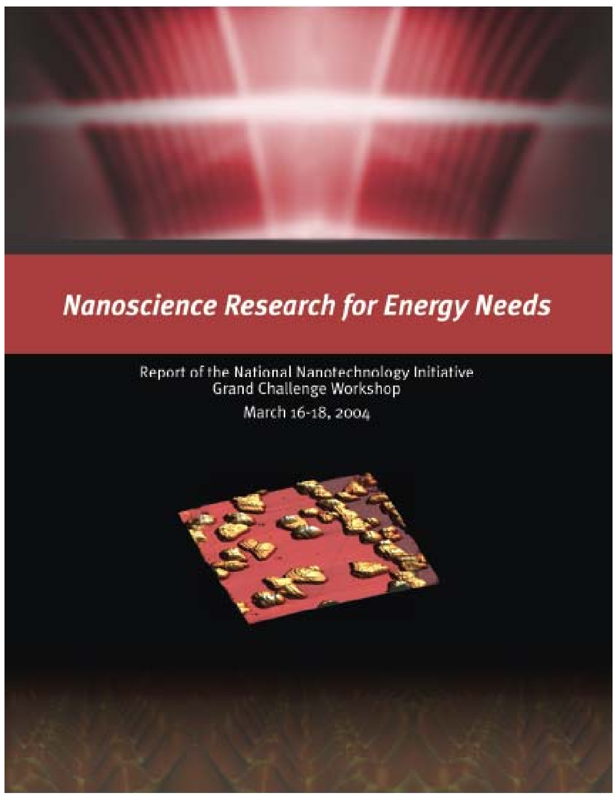


Figure 3.1. The Nanoscience Research for Energy Needs workshop explored the use of nanoscale materials and phenomena to improve the transmission, transformation, and storage of energy. Report available at http://www.nano.gov/html/res/pubs.html.

R&D for nanoscale catalytic materials could have a number of positive effects on society and the environment. For example, energy costs associated with manufacturing processes could be reduced, as could waste. The use of noble metals in automobile catalytic converters could be further reduced. Additionally, new, highly selective catalysis methods could produce new materials and products and lower the production cost of existing products.

Other opportunities related to the environment in which new nanostructured materials (membranes, filters, and catalysts) can have a huge impact include remediation of contaminated sites, reduced use of hazardous chemical feedstocks, and capture and treatment of environmental pollutants.

Indicators of progress in the use of nanometer-scale engineered materials for catalysis will include:

- Measurements of the efficiency of specific catalytic processes involving engineered nanoscale materials
- The integration of engineered nanoscale materials into industrial catalytic processes

High-Density, Wireless, Multianalyte Sensor Arrays

One of the major limitations in our current understanding of the environment stems from the fact that the environment is a dynamic system with a wide diversity of chemical and biological species that vary in time and space in a complex manner. Existing sensors are typically targeted toward only one analyte at a time and do not have the stability needed for continuous monitoring. The ability to fabricate individual nanoscale sensor elements has been demonstrated. Because biomolecular recognition is inherently imperfect, robust identification of biological species is best achieved by looking for patterns of binding to multiple receptor elements using a process similar to that used by a nose. Current-generation microprocessor chips have ten million active transistor elements per square centimeter. It should be possible to create sensor arrays with similar densities of sensor elements, able to provide real-time detection of up to ten million chemical and/or biological species.

Such sensing systems would provide the ability to identify point sources of pollution rapidly and give the detailed information needed to model the environment. They could be used to monitor the safety of food, the presence of hazardous agents in airports and subways, and a variety of human health indicators.

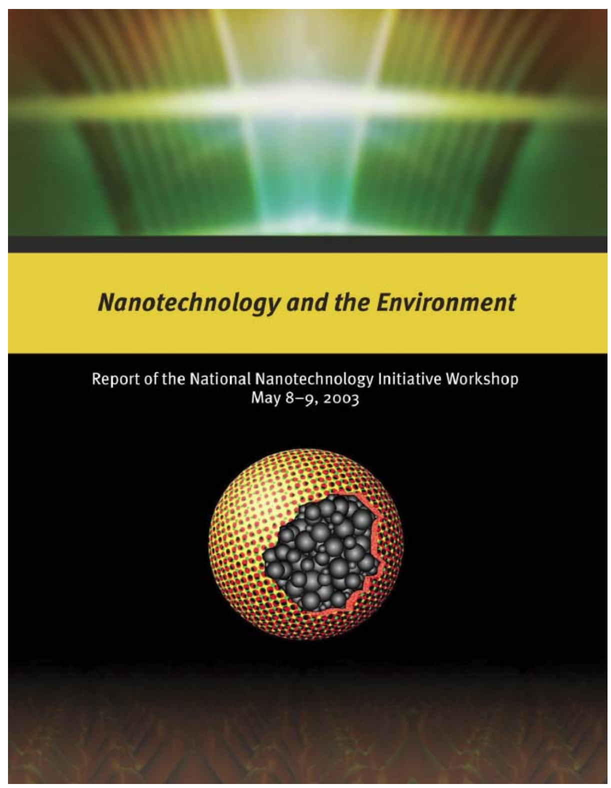


Figure 3.2. The Nanotechnology and the Environment workshop explored environmental implications and applications of nanotechnology. Report available at http://www.nano.gov/html/res/pubs.html.

Indicators of progress in developing high-density, wireless sensor arrays will include:

- Development of nanosensor materials able to withstand long-term environmental exposure
- Increases in the number and density of sensor elements
- Demonstrated ability to detect multiple chemical and/or biological species

Proactive Risk Assessment and Risk Management Associated with Nanotechnology

Harvesting the full benefits of novel technologies and revolutionary materials at the nanoscale depends vitally on ensuring the health and safety of workers and consumers and on understanding and mitigating potential environmental impacts. A lack of studies and hard data hinders research efforts in this area, specifically in assessment of the safety and environmental fate of consumer products and manufacturing by-products. Better understanding is needed of the hazardous properties, if any, of these materials, as well as exposure measurements and routes. Data are required concerning the effectiveness of protective equipment, engineering control methods, and safe work practices to ensure that nanomaterials are handled safely and workers are protected. Study is needed to better understand the fate, transport, and transformation of representative nanomaterials. The appropriate government agencies need to develop new capabilities to conduct these studies.

These issues have to be addressed and communicated to stakeholders to enable commercialization of nanotechnology. They cannot be handled solely by businesses; there is also a role for the government. Some participants expressed the view that the level of funding for risk assessment and risk management needs to be significantly increased.

4. NANOMEDICINE, NANOBIOTECHNOLOGY, AGRICULTURE, AND FOOD SYSTEMS

Session Chair: B. A. Baird

INTRODUCTION

Opportunities abound for integrating biology and nanotechnology. For example, many of the new tools and instruments used in the study of physical and chemical phenomena at the nanometer scale also can be used to investigate complicated systems at fundamental biomolecular length scales. These tools also offer the potential for intervening at molecular levels for medical treatments and agricultural improvements. Among these are biological materials and devices that can be altered and hybridized with inorganic materials for new applications. More generally, the wisdom and inspiration gained from the study of biological structures and functions will have many applications to nanotechnology.

With these opportunities come the corresponding challenges of obtaining a detailed understanding of biology and how to effectively interface dry to wet, inorganic to organic, and designed, fabricated systems to complicated living systems. It is essential that a broad disciplinary range of engineers, physical scientists, and life scientists be engaged in developing the technology. The benefits of nanotechnology to medicine and agriculture and the creation of new classes of materials and devices will only be possible if the knowledge and technology can be transferred easily between disciplines. In addition, the nanotechnology community as a whole must consider the broad range of potential societal implications of these technologies early on and continuously in the development process.

RESEARCH TARGETS

The participants in this session recommended that emphasis be placed on the following technology challenges and research targets:

- Analysis of molecular and subcellular events at the nanometer scale
- Smart nanoparticles
- Hybridization of biological and physical systems
- Safety assessment

Analysis of Molecular and Subcellular Events at the Nanometer Scale

Analysis of molecular and subcellular events in living systems is the central research target in this topical area, and this target enables the others. Specific probes, nanofabricated surfaces, and advanced microscopies allow single molecules and supramolecular assemblies to be observed in the context of a living cell and ultimately within humans, livestock, or plants. One example would be observing proteins fold—or to aberrantly misfold—in neuronal cells. Understanding the folding or misfolding process would be useful in designing effective inhibitors of amyloid fibers that form in Alzheimer's disease, bovine spongiform encephalopathy, and other neurodegenerative processes. Another example would be examining receptor-mediated signal transduction and other cellular events under controlled conditions. For instance, with controlled initiation of signaling events (chemical, mechanical, electrical), one could observe the spatially and temporally regulated cellular responses. Cellular events such as membrane fusion are specifically associated with lysomal disease, viral infection, and neuromuscular pathologies. Understanding these signaling events could lead to more effective treatments.

These kinds of analyses will require development of specific probes that cover a range of length scales and of spectroscopies that cover a range of time regimes (nanoseconds to days or years). High-resolution electron microscopy, optical techniques that surpass diffraction limits, chemically sensitive scanned-probe spectroscopies, and high-resolution positron emission tomography need to be adapted to nanometer-scale imaging of biological systems. Superior computational capability and software development will be required for organizing information and modeling.

Indicators of progress in analysis of molecular and subcellular events at the nanometer scale will include:

- Development of drugs and medical procedures from insights into sub-cellular events
- Contributions to realistic, quantitative models of cells (systems biology)

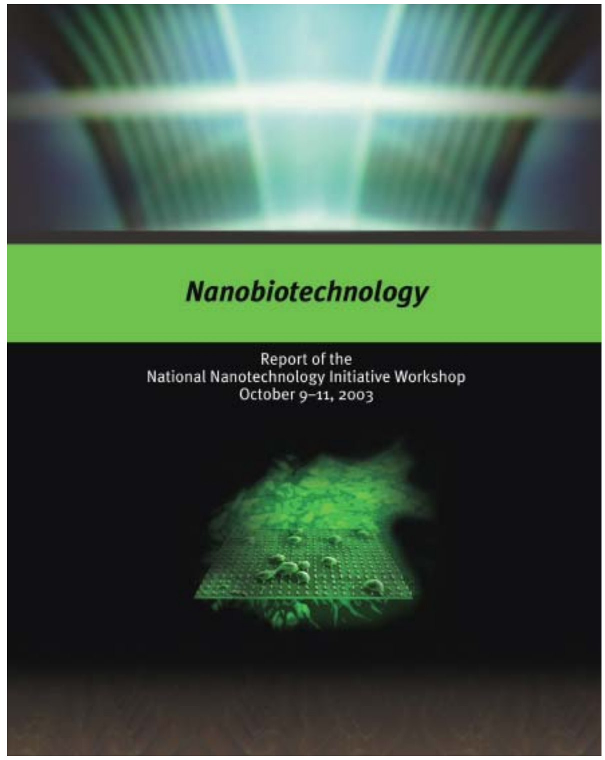


Figure 4.1. The Nanobiotechnology workshop explored how nanotechnology can be used to study life processes and to develop effective interventions for promoting human health. Report available at http://www.nano.gov/html/res/pubs.html.

Smart Nanoparticles

Nanostructures can be loaded with multiple functionalities that are tailored to specific needs—so-called "smart particles." At a minimum, these can be contrast agents, for example, fluorescent tags or probes for magnetic resonance imaging, that can target specified locations in the cells of humans, plants, and animals. These structures could contain sensors that probe the immediate environment and can be actuated to release drugs. Even greater sophistication will include sensing the response to drugs and releasing additional factors that are regenerative. These smart particles may also be enabled to communicate wirelessly with an external operator or computer. Applications include early detection of and intervention for cancer and other diseases, regeneration or improvement of function, and use of nanoparticle sensors to recognize pathogens for easy detection or capture and removal.

Individuals must be trained to integrate medical knowledge with an understanding of the regulatory processes necessary for approval for use of these kinds of engineered functional nanostructures in humans and animals. Also needed is the industrial infrastructure to produce these in an efficient and economically viable manner.

Indicators of progress in the use of smart nanoparticles will include:

- New contrast agents for medical diagnostics derived from engineered nanoparticles
- Successful treatment of human patients or animals using nanotechnology-derived therapeutics
- Improvements in food safety derived from nanotechnology

Hybridization of Biological and Physical Systems

The materials, structures, and processes that have evolved in nature to enable life can be used for new applications after reconstruction or hybridization with synthetic materials and nanofabricated structures. On the other hand, manufactured materials can restore structures and functions in organisms if they are biocompatibly interfaced and, possibly, enhanced with specialized functions. An example might be biomechanical/electronic/optical interfaces that emulate how plant leaves harvest solar energy. Another example might be electronic devices for therapeutic brain stimulation. Yet another application might be development of biologically compatible materials for bone or neural implants, or new materials, inspired by living systems, that act like enzymes or collagen. Some new nanotechnology-inspired systems and structures could be tailored to target only specific and undesirable plants or animals. Other specific nanostructures might be developed to track metabolic processes in plants or in animals.

To develop these kinds of hybrid nanostructured materials, special resources must be employed; these include facilities that better enable nanofabrication and characterization of biological and hybridized materials (wet, soft samples, salt solutions, and others).

Indicators of progress in the development of hybrid biological and physical systems will include:

- Materials that specifically target unwanted or invasive species in agricultural production, reducing the use of conventional chemical pesticides
- Successful and functional implants using engineered nanomaterials

Safety Assessment

The development of nanoparticles and hybridized materials as probes, sensors, and therapeutics in medicine can have extraordinary beneficial effects and may revolutionize the development of current therapies. However, it is conceivable that therapeutic strategies could lead to unintended adverse effects that could result in the failure of a given product. For example, injected nanoparticulates could be sequestered in a bystander organ. The potential toxicity of a new drug or sensor could be discovered in late-stage, preclinical testing. Therefore it is prudent to integrate safety testing into earlier, shorter-term efficacy studies. In this regard, it will be important to develop a general framework for considering relevant toxicological issues and to develop a generic understanding of risk analysis for nanomaterials at an early stage in their development.

To expedite the development of early safety assessment strategies, rapid screening methodologies could be extremely helpful for identifying toxicological properties. These might include animal-on-a-chip gene arrays and *in vitro* systems. A thorough evaluation could more readily lead to safe, effective nanobiomaterials. This toxicological information would also facilitate development of realistic simulations and model systems for addressing toxicology and provide rigorous risk/benefit analyses of therapeutic applications.

Indicators of progress in safety assessments for nanobiomaterials will include:

- Expedited commercialization (including regulatory approval) of engineered, nanotechnology-derived diagnostics and therapeutics
- Accepted standards for evaluating potential toxicity or health impacts of engineered, nanotechnology-derived therapeutics

5. NANOMANUFACTURING, NANOMACHINES, AND NANOSYSTEMS

Session Chair: C. D. Montemagno

INTRODUCTION

The ultimate success of nanotechnology depends on manufacturability, that is, on the ability to successfully transition advances in the nanosciences from the laboratory bench to the marketplace. The challenges are formidable. Transforming nanoscale scientific phenomena into deployable technologies necessitates the establishment of manufacturing processes and systems that bridge ten orders of magnitude in size. Furthermore, it now seems credible that through the precise manipulation of matter, systems and materials can be engineered that intrinsically manifest complex behaviors, thus providing challenges to commercially produce highly engineered complex systems with performance and capabilities previously only imagined. The overarching manufacturing research challenge over the coming years is to establish a framework for integrating nanoscience advances with requirements emanating from many science and engineering disciplines. Nanomanufacturing will have to integrate elements of surface chemistry, electrostatics, fluid flow, adhesion, and numerous other fields in order to control the assembly and integration of nanoscale elements into commercial products.

Significant advances in manufacturing have already occurred. These include synthesis and processing of nanoscale components such as nanotubes, nanoparticles, nanofibers, and quantum dots. Progress has also been made in the dispersion, patterning, and templating of two- and three-dimensional structures. Simple nanodevices have been fabricated. Some tools for positioning, imaging, and measuring with nanometer resolution have been invented. However, much of what has been accomplished falls into the category of passive devices and structures. Less progress has occurred in manufacturing of active nanoscale devices and structures such as transistors, sensors, and actuators. In the future, active devices, biologically assembled devices and systems, and ultimately three-dimensional networked systems, all engineered at the nanoscale to have new functions, will have to be accommodated in standard manufacturing processes. This chapter focuses on barriers to high-volume, high-throughput manufacturing, with an emphasis on implementing new and widely applicable processes, rather than on the production of specific devices or structures.

RESEARCH TARGETS

The participants in this session anticipated a path to developing multiscale systems that bridge from the nanoscale to the macroscale. With this in mind, they recommended that emphasis be placed on the following technology challenges and research targets:

- Tool development
- Nanomanufacturing processing techniques
- Multifunctional and adaptive materials
- Fundamental research on mesoscale mathematics and physics

Tool Development

New metrology and manufacturing tools are needed to measure and manipulate material at the nanometer scale. Tool development should focus on the development of multiscale design software, high-throughput characterization tools, and manipulation instruments from a systems perspective. Software should be developed to enable the detailed design of multiscale systems. The software must incorporate accurate physical models of processes that occur at nanometer scales and must be able to predict emergent system properties with size. A concerted effort must be made to develop tools for both the precision characterization and the precision manipulation of matter. These efforts should focus on the development of tools for manufacturing to facilitate the transition from nanoscience to nanotechnology. High throughput, repeatable precision, and ease of use must be the standards for these investigatory efforts.

Outcomes from the tool development effort should be used to support the development of a framework of technology standards for defining interfaces between scales, both in size and in time. Enabling the commercial production of true multiscale systems requires the establishment of a suite of physical technology standards to communicate both function and information up and down size-scales. This will greatly reduce both the time and the costs associated with translating new nanoscience breakthroughs from the lab bench to the marketplace.

Many of the new research and development tools will be expensive. Moreover, these instruments will require highly trained technicians to operate and maintain them. Such complex instrumentation is often best housed in large, dedicated user facilities and research centers. Ideally, these nanomanufacturing research centers and nanofabrication facilities should be strategically distributed throughout the country. Efficient integration of these resources into the existing scientific and engineering research infrastructure will ensure greater efficiency and promote lower-cost production.

Indicators of progress in tool development for nanoscale manufacturing will include:

- New tools
  - manufacturing
  - testing and measurement
  - modeling, simulation, and analysis
- Cost-effective, commercially viable production
- Technology standards for functional interfaces

Nanomanufacturing Processing Techniques

Reliable manufacturing processes are critical to commercial success in the development of nanotechnology-based products and devices. Instrumentation and metrology are important components of these new processes. New manufacturing processes are needed that have the capacity for atomically accurate three-dimensional fabrication, positioning, and manipulation at room temperature.

The diversity of manufacturing environments required for new nanotechnology-based products will place added challenges on tools and techniques. For example, manufacturing of many nanoscale materials occurs in the liquid phase, and thus tools and instruments compatible with liquid-phase processing are required. New classes of process monitors must be designed for mass production of large-sized samples such as semiconductor wafers; the monitors must be able to work on the fabrication line and provide fast analysis and real-time feedback to the manufacturing process.

Advances are needed in understanding materials properties at the nanometer scale, modeling multiscale behavior, systems-level description of manufacturing, and analysis and visualization of process data.

Indicators of progress in developing new nanomanufacturing processes will include:

- Full device inspection with nanometer resolution
- Process monitors for liquid-phase manufacturing of nanomaterials
- Increased number of viable commercial products incorporating nanotechnology

Multifunctional and Adaptive Materials

The engineering of multiscale systems that originate at the supramolecular scale and progress to the macroscale is where the true power and opportunities of nanotechnology will be realized. Biological systems often demonstrate functionality that seemingly belies their component makeup. Through the precise manipulation of matter, nanotechnology clearly presents the opportunity to engineer system functionalities that mirror those found in living systems. Defining and engineering nonlinear interactions among physical entities at the same size scale will enable the creation of systems with functionality greater than that of their component elements. This will facilitate the engineering of environmentally responsive materials and systems that are able to incorporate and react to information communicated by their local environment via defined stochastic interactions that originate at the supramolecular scale and cascade up to the macroscale.

Indicators of progress in development of multifunctional and adaptive materials will include:

- Creation of heterogeneous nanostructures
- Integration of nanometer-scale functionality into macroscopic systems

Fundamental Research on Mesoscale Mathematics and Physics

Building systems with designed functionality will require a significant research effort to expand our fundamental understanding of the mathematics and physics associated with these processes. It is imperative to establish general rules that predict emergent behavior. Much of the present research effort focuses on discovering new phenomena in single nanostructures, such as a single molecule, nanotube, nanowire, or nanoparticle. This is critical, because without being able to predict the behavior of simple nanostructures, it is difficult to exploit the novel behaviors of these systems. However, in order to develop nanotechnology-enabled systems, that is, systems that will include many nanostructures or nanostructures integrated into a unit, broader research is necessary.

The research community needs to start addressing fundamental issues related to collective effects in assemblies and systems of nanostructures. The complex behavior of collective systems formed from seemingly simple parts—a behavior often termed “emergent”—is generally unpredictable from a lower-level description. This emphasizes the need for experimental and theoretical study of collective phenomena. Only with this type of knowledge will it be possible to design multicomponent, nanotechnology-driven systems. As our understanding of these systems evolves, nanotechnology tools will be required to both verify and implement this new knowledge. Consequently, funding of investigations in this area should be executed using an

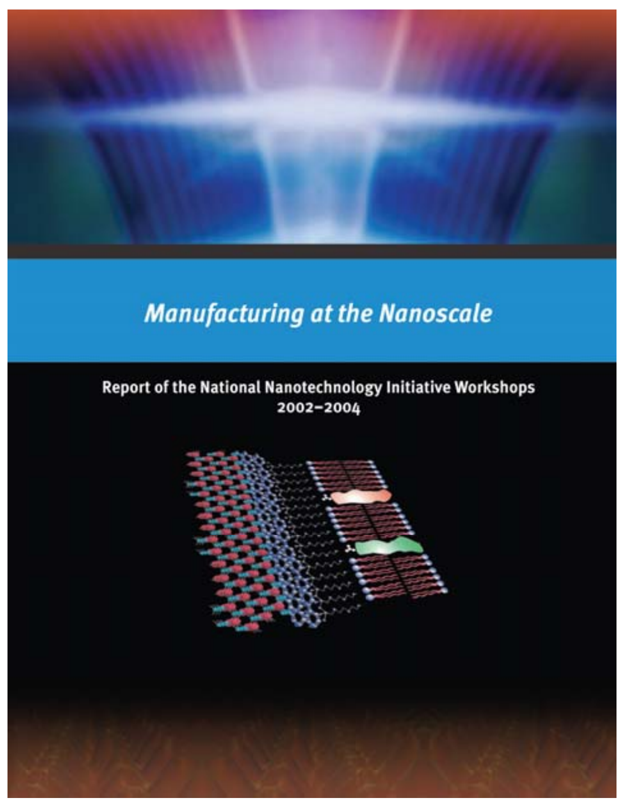


Figure 5.1. The Manufacturing at the Nanoscale workshops explored the challenges and opportunities of scalable production of nanotechnologies. Report available at http://www.nano.gov/html/res/pubs.html.

interdisciplinary, team approach. Problems should be defined through a wide-ranging dialog in the nanotechnology community.

Indicators of progress in fundamental research on mesoscale mathematics and physics will include:

- Understanding the translation of nanoscale functionality to macroscale systems
- Predicting complexity of systems (i.e., emergent properties not predicted by the behavior of the parts)
- New nanotechnology-derived products and/or services motivated by modeling

6. INSTRUMENTATION, METROLOGY, ADVANCED ENVIRONMENTS, AND SIMULATION

Session Chair: R. J. Hocken

INTRODUCTION

The issues in instrumentation, metrology, advanced environments, and simulation are crosscutting in that they affect every aspect of nanotechnology. Effective advances in these fields will be key enablers of progress in nanotechnology, without which fundamental research discoveries will slow or stall and laboratory breakthroughs will not progress to manufacturing. Instrumentation, metrology, advanced environments, and simulation are the technical tools that enable research, development, and even more critically, commercialization. Powerful new instruments such as the scanning electron microscope, the scanning tunneling microscope, and the atomic force microscope have enabled recent progress in nanotechnology. Furthermore, very large scale integration, one of the most successful technologies at length scales less than 100 nanometers, could not exist without state-of-the-art metrology for measuring position, overlay, film thickness, and critical dimensions.

In the nanoscale domain, instruments and manufacturing tools are limited by subtle environmental disturbances that have not been an issue for instruments in the macroscale domain. As such, they require advanced buildings or individually controlled environments in order to function properly. Finally, computer systems capable of simulating very large scale integration are among the most sophisticated in the world. Such simulations need to be extended to all of nanotechnology from biology to new materials.

RESEARCH TARGETS

The participants in this session recommended that emphasis be placed on the following technology challenges and research targets:

- Robust, high-speed instruments, models, and standards
- Increased simulation capability
- Development of advanced facilities

Robust High-Speed Instruments, Models, and Standards

The current inability to examine complex structures in three dimensions is a key barrier that must be overcome. Incremental improvements on existing technology may eventually address certain nanometer-scale characterization needs. Most needs, however, can be met only with a new generation of robust, high-speed instruments supported by comprehensive models and standards. These instruments must provide two- and three-dimensional maps of interfaces and of material structures and properties. They should be able to map out chemical composition in heterogeneous samples with atomic resolution and be able to establish the phase of the various components. They should have dimensional resolution, and thus accuracy, of < 0.01 nm. They must be able to measure mechanical properties such as stress, elasticity, hardness, and friction with a spatial resolution of < 10 nm. And they must be able to measure electrical and magnetic properties with spatial resolution at < 1 nm and optical properties at < 10 nm resolution.

The need for new instruments with spatial resolution beyond the diffraction limit is especially critical. Spectroscopic measurements provide a wealth of information on structure and dynamical properties of bulk materials and at interfaces. Standard optical microscopies, however, have a spatial resolution that is diffraction-limited to about half the wavelength of the applied radiation or particle used in the measurement. New instruments for measuring beyond the diffraction limit, such as the near-field methods currently being developed at optical wavelengths, need to be extended to other parts of the electromagnetic spectrum (microwave, ultraviolet, x-ray) and to particle microscopies (neutrons, electrons).

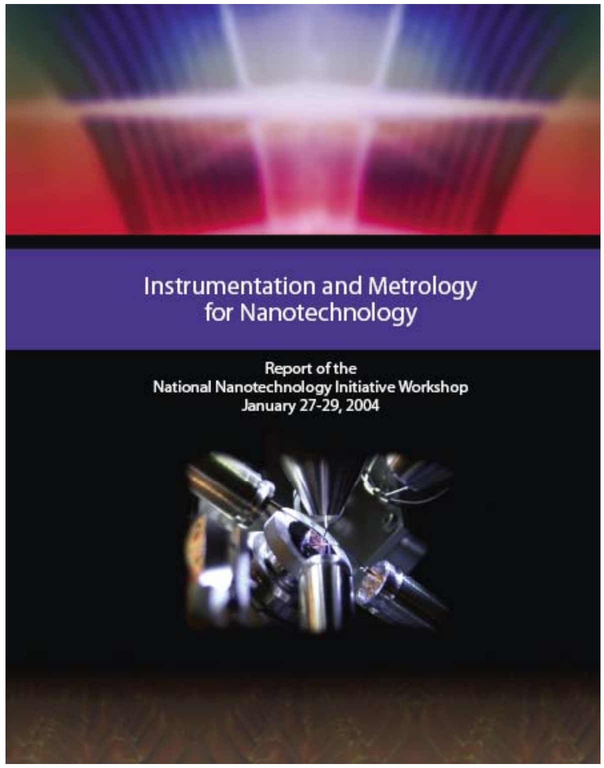


Figure 6.1. The Instrumentation and Metrology for Nanotechnology workshop addressed the unique measurement requirements for manufacturing and characterizing nanotechnology products and processes. Report available at http://www.nano.gov/html/res/pubs.html.

These measurement systems will, inevitably, be complex and will probe a rich variety of physical and chemical processes. As such, these measurements must be interpreted and understood through rigorous physical models that simulate the operation of the instruments and the physics and chemistry involved in measurement processes. Furthermore, reference standards and established protocols will also be essential to obtain artifact-free results. Only these measures will ensure scientifically sound results.

Nanotechnologies use a wide variety of materials: biological, inorganic, organic, and combinations thereof. Ideally, a single characterization instrument and method could be compatible with all these materials; more likely, a set of instruments will be required. Whenever possible, characterization should be done *in situ*. Techniques should produce statistically significant results.

Indicators of progress in developing robust, high-speed instruments, models, and standards will include:

- Patents for new metrology tools that support nanometer-scale manufacturing
- New physical artifact standards that support calibration of nanoscale metrology instruments
- Instruments with spatial limits lower than the diffraction limit

Increased Simulation Capability

Simulation and modeling have emerged as significant tools in technology research and development and can be expected to play an important role in the advancement of nanotechnology. The key roles of simulation and modeling are to provide insight into the operation of metrology tools, aid in the interpretation of nanoscale measurements, provide virtual measurement capabilities, and visualize nanoscale processes.

Simulation requirements lie in two general areas. First, new multiscale models need to be developed for characterization of material properties and nanomanufacturing to facilitate the development of new materials and new nanomanufacturing processes; models also need to be developed for interfaces between dissimilar materials. Second, advanced modeling capability requires new hardware and software development, along with better methods for managing and using the inevitably large and complicated data sets. Close interactions between experimentalists and theorists will be required to validate new methods.

Indicators of progress in increasing simulation capability will include:

- Funding of collaborative proposals in nanotechnology
- New research directions guided by simulation
- Computational infrastructure dedicated to nanotechnology
- An emerging workforce educated in use of simulation tools

Development of Advanced Facilities

Achieving the targets discussed above will only be possible with a wide range of state-of-the-art facilities. The NNI agencies should continue to develop advanced facilities and infrastructure that support development of new instruments, manufacturing processes, and simulation capabilities. These facilities must be able to rigorously control variables such as vibration, radiation, humidity, temperature, and air quality. Tools should provide their own microenvironments if possible. The facilities should be available to industrial partners as a means to accelerate commercial development.

Indicators of progress in facilities development will include:

- Development of a new infrastructure with advanced nanofabrication capabilities
- Use of new facilities by a broad spectrum of users
- Partnerships between industry, government, and academia at new facilities

7. FUNDAMENTAL SCIENTIFIC ISSUES

Session Chair: A. Majumdar

INTRODUCTION

Science at the nanoscale is truly unique for a variety of reasons. First, there are fundamental length scales in nature that lie in the range of 1 nm to 100 nm. Some examples include the wavelength of electrons, phonons, and photons; Debye screening length of ions in liquids; dislocation spacing in solids; and structure and structural variations of biomolecules.

Second, it is now possible to pattern and confine matter with almost atomic-scale precision with at least one dimension in the < 100 nm range. By patterning matter to cross these fundamental length scales, a transition occurs and new science is generated. This change is manifest in the form of new properties and phenomena. Some examples include quantum effects, molecular-scale phenomena that rely on fluctuations, collective effects, chemical reactivity, and size-dependent mechanical, thermal, electronic, optical, and other properties. New science can also emerge when soft matter (for example, biomolecules and liquids) is integrated with hard matter (for example, nanoparticles) to create structures with extraordinary recognition capabilities and novel physical properties.

Finally, nanostructuring produces high surface-to-volume ratios, which has significant influence on surface-related phenomena such as catalysis, adhesion, and friction.

Nanotechnology exploits this new science to produce devices and systems that are useful and beneficial to society. But the bedrock of this technology is the uniqueness of nanoscience, based on the uniqueness of materials phenomena at the nanometer length scale. To truly achieve the promise of nanotechnology, it will be necessary to understand and control these properties. Hence, it is extremely important to examine the fundamental scientific issues and identify areas of greatest opportunity.

RESEARCH OPPORTUNITIES

Since the 1990s, there has been an explosion of new scientific discoveries and inventions in nanoscale science and engineering. While this is indeed creating a foundation for new technology, many fundamental scientific issues remain unexplored, without which nanotechnology cannot develop to the potential that scientists envision. The following are specific research priorities:

- Single and collective effects
- Self-assembly
- Hard-soft interfaces
- Biologically inspired materials and devices
- Catalysis
- Instrumentation

Single and Collective Effects

As indicated earlier, most of the nanoscience research in the past has focused on discovering new phenomena in some single nanostructures. Understanding the science of and acquiring the ability to predict single nanostructure behavior will be fundamental to exploiting the novel properties of nanostructures in systems. In addition, if we are to develop nanosystems that include many nanostructures, or nanostructures integrated with microstructures, more work needs to be done to address fundamental issues concerning collective effects in assemblies and systems of nanostructures. Examples of these collective effects include phase transitions, interference and localization due to multiple wave scattering, and self-organization. It is vital to understand these effects not only because is it important that systems are predictable, but also because it may be possible to exploit them to produce new functionality.

Self-Assembly

The process of self-assembly or programmed assembly of nanostructures is undoubtedly the most promising cost-effective approach for manufacturing devices and systems. In order to develop robust and rapid self-assembly protocols, it will be necessary to understand the thermodynamics of self-assembly. For example, to estimate kinetics and predict pathways, it will be necessary to understand the free-energy landscape of the reactions involved in self-assembly. Biology is replete with examples of coded assembly, and it could provide clues for understanding and designing synthetic approaches.

Hard-Soft Interfaces

It is clear that interfaces between soft and hard matter will be important in nanotechnology and deserve much attention. However, given the complexity of surface chemistry combined with surface structure, most of the early research has led to empirical knowledge. A fundamental focus on understanding the dynamics, spreading, and wetting of fluids and on understanding the structure of single molecules and assemblies of molecules on surfaces is critical because these kinds of attributes underlie many aspects of interfacial phenomena such as adhesion, friction, and molecular binding.

Biologically Inspired Materials and Devices

It has long been recognized that the molecular encoding in biomolecules, as well as the novel approaches biology uses to generate cellular function, can be harnessed for nonbiological purposes. These include directed assembly, extremely precise manufacturing using biomolecular scaffolds, molecular recognition, energy conversion, signal amplification, and regulatory feedback mechanisms. Biomolecules combine structure, chemistry, and fluctuations to generate function. To develop synthetic approaches, it is essential to develop a fundamental understanding of how this occurs.

Catalysis

Catalysis is vitally important in many industrial processes. A unique aspect of nanostructured catalysts is that the reactants and nanocatalysts can synergistically modify structures that can produce or yield new reactions and higher specificity.

Instrumentation

Instrumentation is a crosscutting requirement for addressing many fundamental scientific issues and thus deserves attention. Near-field techniques are critical for probing and studying nanometer-scale phenomena. New tools are needed to explore the behaviors of soft materials.

IMPLEMENTATION STRATEGIES

Fundamental research is required for nanotechnology-derived products to move from the laboratory into manufacturing. This research should be knowledge-driven but focused on the areas and projects most likely to lead to useful new products and technologies. Government, industry, and academia should leverage their respective resources to support a broad range of both basic and applied R&D projects that are focused on meeting shared, complementary goals.

8. APPLICATION OPPORTUNITIES AND TECHNOLOGY TRANSFER

Session Chair: C. T. Hunt

INTRODUCTION

Energy, disease therapy, biology, new materials, and computation are some of the application areas potentially impacted by nanotechnology. The National Nanotechnology Initiative could rejuvenate existing industries and create fundamentally new products and services. But all this promise is currently far from realization. The NNI agencies must implement a strategy to maximize the economic, societal, and scientific benefits of investments in nanotechnology, based on understanding the fundamentals and translating this understanding into the design, demonstration, and delivery of new products.

This chapter discusses potential high-impact application opportunities for nanotechnology. Each opportunity relies on the development of an essential facet of nanotechnology infrastructure, including instrumentation, metrology, advanced environments, simulation technologies, and nanomanufacturing capabilities. Success will also require an extraordinary level of coordination across the research and development community, and a higher level of industry involvement than is usual in the precompetitive phase of R&D. Scientifically based health and safety standards and regulatory policies that foster commerce while protecting workers, the public, and the environment are also needed. The ultimate objective is viable commercial products that result in an increase in jobs, improved global competitiveness, and enhanced quality of life.

APPLICATION OPPORTUNITIES

The participants in this breakout session identified the following application opportunities as having the highest potential to benefit the U.S. economy and improve human quality of life:

- New nanomaterials
- New information technologies
- High-density, multianalyte sensors
- Alternative, nonpolluting energy
- Human health assessment and remediation

New Materials

New nanomaterials have the potential to impact all areas of nanoscience and nanotechnology. The objective is to be able to design and synthesize these materials so that specific functions and properties are incorporated. The key to realizing this goal will be to understand the fundamental chemistry and physics of these materials through basic experimental and theoretical research.

Several types of new nanostructured materials applications are envisioned. One type is intelligent, adaptive coatings; researchers can imagine self-healing car surfaces, self-actuating and repairing composites, materials of variable resistance or permeability, and structures with adaptable shapes. Energy-related material types include materials to harvest, transport, and store energy, as well as materials enabling economically viable fuel cells and photovoltaics. High-strength, lightweight, multifunctional polymers and composite nanomaterials for stronger and self-regulating buildings and roads are yet another potential nanomaterial type. Another type relates to environmental remediation and waste handling; for example, a new class of filters made from nanomaterials could be used to purify wastewater and exhaust gases. New catalytic nanomaterials should result in lowered cost of monomers and drug precursors, and may ultimately lead to new feedstocks that are not based on petrochemicals. Finally, there are specialty types of materials, such as those with high or low thermal conductivity, high radiation hardness, and high mechanical toughness, that can be applied to impact protection systems or materials of high energy density, both of which are useful in aeronautics and space exploration.

New Information Technologies

The objective of this application area is to sustain the economic engine enabled by Moore's Law. The IT industry projects that even the most advanced lithographic techniques under development will reach fundamental limits within a decade. Beyond that time, continued increases in circuit density will require a paradigm shift in the design, fabrication, and operation of electronic components at the nanoscale. For this shift to happen, developments must take place that enable new component technologies, new logic systems (probably ones that use state variables such as spin state, thermodynamic phase, or polarization), and new fault- and defect-tolerant architectures. Optical interconnects may reduce the need for electrical wiring within processors. Novel computational systems and terabit processing capability will provide unprecedented computing power for image processing, data transfer, voice recognition, and human-machine interfacing.

High-Density, Multianalyte Sensors

The principal target of this application area is molecular recognition materials that are sensitive to specific chemical compounds or biological agents. Engineered nanometer-scale materials can easily provide single-molecule sensitivity, although selectivity will be a major challenge. These kinds of technologies can be used to develop sensors for national defense and homeland security purposes. Optimally, these sensors will have long lifetimes and be networked using the advanced information systems discussed above. They should be able to work unattended in remote locations and operate in harsh environments. They may require energy-scavenging capability for harvesting energy from the sensing environment.

Another use of sensors is in smart textiles. Such fabrics could, for example, be incorporated into garments to sense the physiological state and/or local environment of the wearer and provide appropriate alerts or responses. In battlefield applications, sensors might be embedded in uniforms to sense chemical or biological agents and trigger actions to neutralize them.

There are also potential transportation, construction, and energy applications for nanosensors. For example, sensors embedded in pavement might monitor and report street and highway conditions, or harvest and transform the heat absorbed by the pavement to generate clean energy.

Alternative, Nonpolluting Energy

Nanotechnology research offers an avenue for strengthening U.S. energy security and independence. The objective of R&D in this area should be to improve the transformation, transmission, and storage of energy. New materials will enable photochemical technologies for splitting water to produce hydrogen as the fuel for new, nanomaterial-based fuel cells. Novel nanomaterials should result in improved capacitors, more efficient batteries, thermoelectric conversion devices, wind turbines, and photovoltaic devices. Electrical transmission lines made from nanomaterials, perhaps carbon nanotubes, could result in an ultra-low-loss electrical distribution network.

Human Health Assessment and Remediation

Nanotechnology offers the opportunity to develop new tools to study biological systems at the molecular level, to detect disease at earlier stages of development than traditional methods, and to treat disease at the cellular level. Highly specific probes made from nanomaterials can allow single molecules or molecular assembles to be tagged and followed; this will make it possible to follow events such as protein folding and to develop diagnostics that detect specific aberrant cellular events or foreign materials. Engineered testing or therapeutic nanostructures could be made to serve multiple purposes. These structures could serve as contrast agents (for fluorescent or magnetic resonance imaging probes) specific to certain cells or disease states. They could contain sensors that recognize when attachment to a cell has occurred and actuate the release of drugs. "Nanoagents" could perform noninvasive intervention when activated by an external energy source. Nanomaterials could be used to direct cell separation, growth, proliferation, and differentiation for tissue engineering. Nanomaterials and information processing will enable a new generation of "smart" prostheses.

IMPLEMENTATION STRATEGIES

Appropriate policies can facilitate realization of the objectives discussed above. To begin with, information and knowledge transfer must occur across the nanotechnology community, including university labs, government research facilities, industrial labs (both large and small), and industrial manufacturing works. A coordinated, interagency effort would be helpful to achieve high-profile goals. These goals should incorporate concrete objectives rather than general research aims. It is important to have direct industry involvement and rigorous peer review in selecting and prioritizing goals.

A critical element of the process will be streamlining the intellectual property transfer processes. In order to maximize economic impact, there must be a simplified pathway from invention to innovation and commercialization. This will require new intellectual property practices, since current practices are often a hindrance to technology transfer. Throughout the streamlining process, it will be important to experiment with different procedures, study which work best, and disseminate best practices. Success will require an extraordinary level of coordination across the research establishment, and a high level of industry involvement.

Rapid and efficient technology transfer is a necessary part of the innovation process. Several steps may improve existing mechanisms. For example, a streamlined Small Business Innovation Research (SBIR) process could spur nanotechnology research. Encouraging universities to create commercialization incubators focused on nanotechnology would bring small business and fundamental research into closer contact and could prove valuable for enabling technology transfer.

The technology transfer process could benefit from better interfacing between industry, academia, and government. State and local governments should coordinate their investments in nanoscience and nanotechnology R&D funding with those of industry, academic institutions, and Federally-funded government labs. Access to funding for fundamental research should be available to all three sectors. In addition, mechanisms need to be established that ensure availability of funding to collaborations between industry, universities, and government

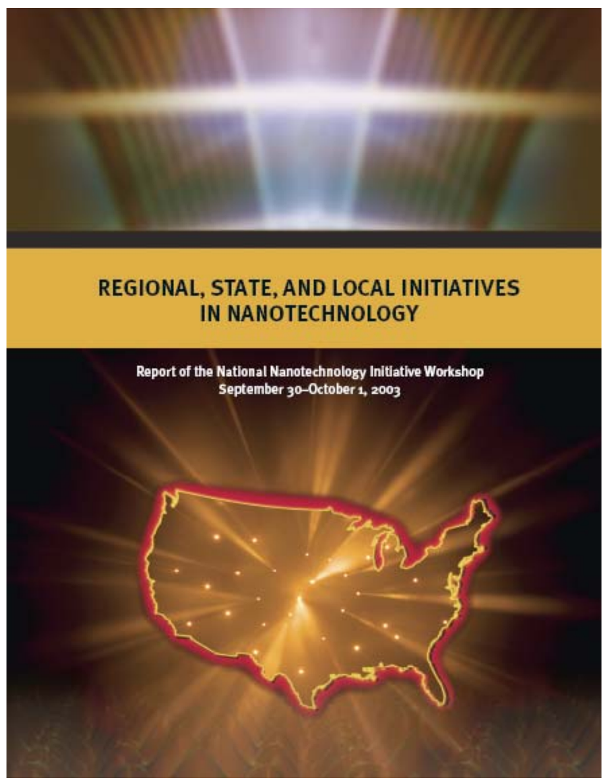


Figure 8.1. The Regional, State, and Local Initiatives in Nanotechnology workshop explored strategies for accelerating the commercialization of nanotechnology. Report available at http://www.nano.gov/html/res/pubs.html.

labs for applied, high-risk development projects. Government can also foster more collaboration between entities by establishing industry-university-government lab cooperative research centers and national user facilities with open access and equitable intellectual property policies. Creation of fellowships for industry researchers to work at government labs or universities—and vice versa—would provide a more seamless industry/academic interface. More government-funded programs should require industry partnering.

New policies for negotiating intellectual property rights resulting from industry-sponsored academic research should help accelerate interactions and technology transfer. Clear and consistent intellectual property policy for government-sponsored activities would also accelerate technology transfer. Benefits could be considerable from enhanced engagement of academia with industry, and could lead to university research that is more relevant to industry. Students would be better trained for jobs in industry. In short, the result would be accelerated technology transfer and more rapid commercialization of new products.

Commercialization of new products also requires that regulatory structures be put in place that promote the development of commerce-based and science-based environmental, health, and safety standards. This will require both industry and government input.

Across the nanotechnology enterprise, clear channels of communication will be essential between industry and Federal policymakers and program managers. Mechanisms for implementing this include establishing industry consultative boards to guide and advise the Federal nanotechnology effort, increased industry participation at Federal agency strategy and planning workshops and program reviews, and information dissemination at professional society and industry association meetings.

9. INFRASTRUCTURE NEEDS

Session Chair: T. A. Michalske

INTRODUCTION

Building the technology infrastructure to meet the goals of the NNI is an important aspect of U.S. investment strategy. Federal, state, and local governments as well as higher education institutions and private industry recognized the potential of nanotechnology early on and made some serious investments in the now burgeoning nanotechnology infrastructure. Ongoing investment in infrastructure will allow the United States to translate scientific success into new commercial applications. A long-term investment approach should recognize the great strides and new opportunities accomplished by infrastructure investment to date as well as focus on tailoring future investments to capitalize on newly identified opportunities with the greatest potential advantages.

Infrastructure development should not be limited to facilities and instruments; it must include computing, communications, and human resources as well as policies and programs designed to deliver the required funding. In order to leverage public investment against investments by other stakeholders, it will also be important to properly catalogue the infrastructure resources already available and share that information with all stakeholders. Given the early stages of current nanotechnology research and development, pooling such resources will eliminate duplication of effort and reap benefits more quickly.

One of the stated goals of the NNI is to develop the supporting infrastructure and tools (e.g., facilities, instrumentation, and computational capacity) needed to advance nanotechnology R&D. In order to tailor a balanced investment strategy, infrastructure needs should be weighed against other goals of the NNI: exploring the fundamental phenomena of the nanometer scale, developing applications of nanotechnologies, understanding societal implications of nanotechnology, education and training of a skilled workforce, and enhancing U.S. economic competitiveness. This section identifies ways in which the present infrastructure investment portfolio may need to be refined in order to properly capitalize on the opportunities ahead.

INFRASTRUCTURE DEVELOPMENT NEEDS

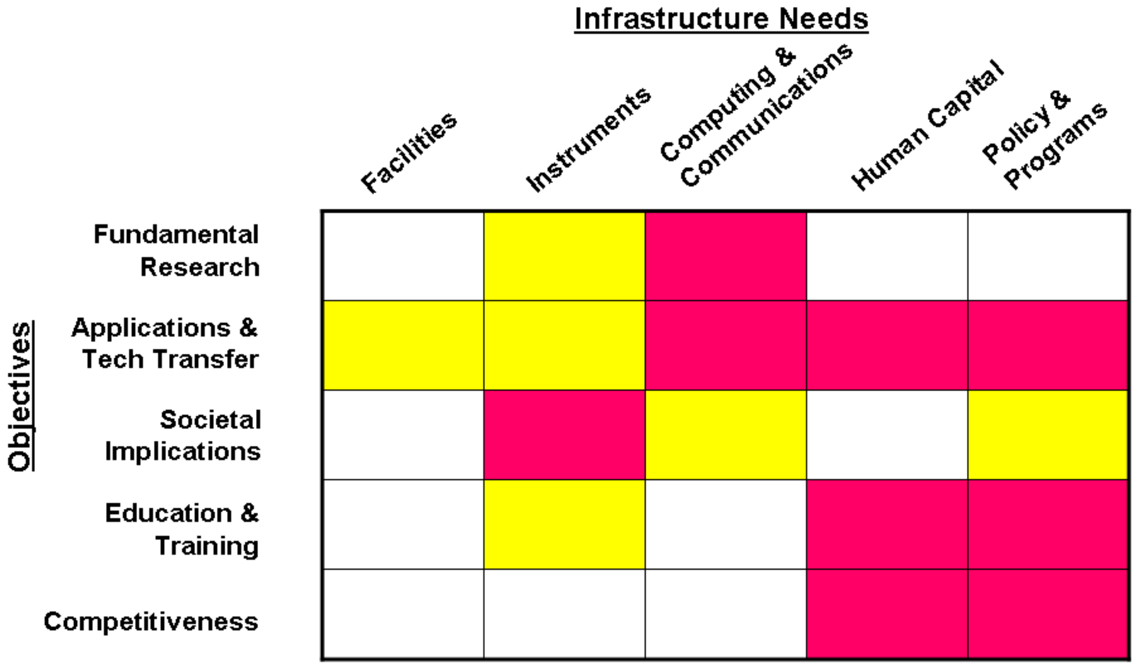
Table 9.1 gives a summary assessment of nanotechnology infrastructure investment priorities, where the investment areas are weighted in three levels of priority with respect to program opportunities current at the time of the Research Directions II workshop. Participants in this breakout session identified the following high-priority infrastructure development opportunities, needs, and challenges:

- Facilities, instrumentation, and tools
- Computing and communications
- Human resources, policy, and programs

Facilities, Instrumentation, and Tools

The initial NNI investments directed toward construction of new facilities and acquiring advanced instruments and tools have provided a strong foundation for U.S. nanotechnology research. Several NNI agencies are already funding new research and development centers, which when complete will provide a nationwide network of resources that are openly available to the nanotechnology community. In addition, many more topically focused centers are adding needed instruments for nanoscience research.

Table 9.1. Summary Assessment of Infrastructure Investment Priorities



Key

White:	Investment consistent with current nanotechnology opportunity
Yellow:	Additional investment required to capitalize on opportunities
Red:	Major investment increase needed to exploit as significant opportunity

In addition to Federal NNI investments, many new facility and instrument investments are being made through regional and state funding. It is important to recognize the strong leveraging function of these investments, especially when coupled with existing major science infrastructure investments, including Federally funded synchrotron and neutron science centers.

In considering future facilities investment, it will be important to identify the particular needs of facilities to support prototype development and nanotechnology manufacturing. Great progress has been made in designing facilities that meet the vibration, temperature, and cleanliness standards needed to conduct nanotechnology research. As focus shifts to include manufacturing and commercialization, the design of facilities must include considerations for the demands of a manufacturing environment and the health and safety of the nanotechnology workforce. It is essential to set priorities for these investments. Important in budget considerations will be opportunities to leverage Federal, state, and local investments with new and existing private sector facilities infrastructure.

The NNI has made major improvements in the available instrumentation for basic nanotechnology research. As the program moves into its second decade, it will be important to address the needs for upgrading major instrumentation so that it remains at the cutting edge. It is also important to acknowledge the difficulty in keeping current in the area of midlevel instrumentation such as atomic force microscopes, advanced laser systems, and the like. Purchase of such instrumentation is often not prestigious enough to garner targeted research funding, and yet its cost is too great to take it out of a research grant.

Of particular importance for future investment will be the development of instruments for high-throughput analysis of nanomaterials; they will be critical for commercialization of nanotechnology. In addition, high-throughput instruments capable of characterizing nanomaterials in the environment will be critical to establishing a technical basis for environmental health and safety policies and for programs and procedures to safely introduce nanomaterials into the workplace and the environment.

Computing and Communications

Advances in high-performance computing and other broadly distributed computational resources are providing much-needed capability in support of nanotechnology research. The need for computational nanotechnology crosscuts all facets of current nanotechnology research (electronics, photonics, magnetics, material design and manufacturing, characterization, fabrication, environmental consequences, and health effects). Computational resources currently available to the nanotechnology community are estimated to be oversubscribed three-fold. As NNI stakeholders look towards the next phase of development, we will need to be able to address an even broader set of problems and more complex, multi-length-scale systems that span from the nanoscale to predict macroscopic properties and performance. When addressing the computational needs of nanotechnology research, NNI agencies should consider investing in a dedicated computational capability for nanoscience; this consideration should include evaluating the merits of constructing a single, large "nanoSimulator" machine rather than pulling together high-end computing capability as a distributed resource.

Investments in computing hardware must also be accompanied by investments in software development, user-friendly interfaces, and available human expertise to help researchers in a range of disciplines apply advanced theory and computation to a broad spectrum of problems. Along with large computational applications will come large data sets that will need to be stored and shared across teams of nanotechnology researchers; this will require investments in high-bandwidth networking and data visualization.

As NNI investments are adjusted to better capitalize on opportunities in technology applications and commercialization, it will be important that computational investments begin to meet the needs of design engineers. Specifically, research tools will need to evolve into predictive design tools that can be used to reliably predict performance of nanoscale materials and systems in the context of integrated engineering systems. The development of nanotechnology design tools represents a strong opportunity for leveraging with private sector software and manufacturing suppliers. An area of particular opportunity is in computational toxicology. This is an excellent target for leveraging against the investments by Federal agencies that have health-related missions.

Human Resources, Policy, and Programs

In the coming years, the United States will face challenges to its position in the international marketplace for high-technology manufacturing areas such as electronics and communications. Many nanotechnology discoveries made under the NNI are pointing toward possible solutions to these and other difficult challenges. In order to capitalize on the opportunities presented by nanotechnology, the NNI agencies must examine the infrastructure requirements associated with transferring new knowledge and discovery into technological solutions and commercial applications. While it is clear that a physical infrastructure will be needed, the most important need is for outstanding intellectual talent.

Among the issues that must be addressed are how to train, assemble, and motivate superb human talent; how to establish appropriate deliverables and metrics that will create focus for distributed activities; and how to establish fair and equitable ownership of resulting intellectual property. How would the NNI agencies measure the value of their contribution to such a highly leveraged activity? Answers to these questions are obviously beyond the scope of this report. However, workshop participants do recommend that the NNI agencies take broad, creative approaches to address this issue of vital importance to U.S. success in nanotechnology.

Of all the forms of nanotechnology infrastructure investment, human capital may be the most critical to U.S. economic competitiveness. Human resource needs cover the spectrum from research staff on the cutting edge of scientific discovery, to manufacturing and systems engineers addressing applications and commercialization, to workers engaged in high-volume, nanometer-scale precision production. Development of human resources is intimately linked to development of sound policies. While some education programs are providing important nanotechnology and training opportunities, more needs to be done to ensure that an adequately trained nanotechnology workforce is prepared to make the United States the world's most competitive nation in terms of manufacturing, applications, and commercialization of nanotechnology.

IMPLEMENTATION STRATEGIES

The challenge at hand is to leverage Federal NNI investments, regional and state infrastructures, and private sector capabilities to construct a distributed infrastructure able to bring together the physical, financial, and human resources to successfully tackle complex application-driven problems. While this challenge is not unique to nanotechnology, it is clear that the vast potential of nanotechnology to provide completely new approaches to existing technological problems will not be realized without development of policies and programs that facilitate this distributed model.

Participants in this breakout session identified several measures that can be taken to meet the infrastructure needs and requirements identified above. First, in the area of physical infrastructure, it would be helpful to catalog the total U.S. investment in facilities and instrumentation and make that information available to the nanotechnology research community. This data will also be valuable in setting detailed strategies for further investment. A strong priority should be placed on investments that will lead to high-throughput instruments to monitor and assess nanomaterials in the workplace and in the natural environment.

Second, in the area of computation infrastructure, participants recommended that a large computational resource be dedicated to high-priority nanotechnology research problems. In particular, there needs to be an increased emphasis on computer modeling to produce design tools that can expedite commercialization of nanotechnology.

Third, in the areas of physical infrastructure and computational resources, the Federal government should work with regional and state governments as well as the private sector to develop a structure for highly distributed approaches to tackling large nanotechnology challenges. Federal investments should be leveraged with other Federal, regional, state, and private sector investments to create facilities for nanotechnology manufacturing and prototype development, with special attention given to the nanotechnology worker.

Finally, the full spectrum of education and training programs available must be assessed in order to ensure that the human resource needs are being met, including the development of a highly trained U.S. nanotechnology workforce.

10. SOCIETAL IMPLICATIONS

Session Chair: D. W. Baird

INTRODUCTION

The societal interactions between nanoscience, nanotechnology, and the many stakeholders in the public, commercial, and research sectors have the potential for spectacular benefits, but also risks. For this reason it is imperative that the United States continue to pursue aggressive and proactive research, education, and outreach programs focused on societal aspects of nanotechnology development. The work of the nanotechnology community to date has been responsive to societal concerns and ahead of the curve in gaining a degree of public trust. The proposals below aim to build on and develop these successes as we move toward integrating nanotechnology into the fabric of society.

OPPORTUNITIES FOR SOCIETAL INTERACTIONS IN NANOTECHNOLOGY

The overarching fundamental goal is for the nanotechnology R&D community to earn and retain the public trust and to engage the public in joint creation of the nanotechnology of the future.

The participants in this breakout session identified the following overarching opportunities for societal issues related to nanotechnology:

- Preserve and nurture public trust
- Research, assess, and manage exposure to engineered nanometer-scale materials
- Research the full spectrum of societal interactions that nanotechnology portends
- Develop educational programs about nanotechnology and its societal implications

Preserve and Nurture Public Trust

The members of this group felt that it is important to preserve and enhance public trust in nanoscale science and technology. Public trust in science and technology has been strong in the past. But it is important to take steps to preserve and nurture this trust through open and informed discussion of the benefits and risks of nanotechnologies as they enter the marketplace. It is far easier to sustain the public's initial trust in new science and technology than it is to rebuild lost trust.

The trust-building process could begin with programs to measure public understanding of and attitudes toward nanoscience and nanotechnology. Several efforts exist now to produce ongoing time series measurements of public perceptions of science and technology. These should be supplemented with measures of public perceptions of nanotechnology specifically. This information will provide important feedback to the scientific community and to policymakers.

Forums should be held to foster dialog among all stakeholders, including universities, corporations, government regulators, various interest groups, and the general public. It will be important to provide a breadth of information about nanoscience and nanotechnology that addresses the full range of citizen interests, levels of prior understanding, cultural backgrounds, and needs. For scientists unused to communicating with the public, it would be helpful to create an information clearinghouse about nanoscience and nanotechnology that would include guidance on best practices for communicating effectively with citizens and groups of different backgrounds and interests. This will help the nanoscience community to more effectively engage the broad range of stakeholders in meaningful dialog about developments in nanotechnology and about individuals' beliefs, values, hopes, and fears tied to these developments. All such communication must be responsible and informed.

For dialog venues, this group recommended using existing structures where possible, including existing nanotechnology centers, extension programs, museums and science centers, public libraries, community colleges, chambers of commerce, and civic groups. Members of the nanoscience and nanotechnology communities must participate in these dialogs, both to explain their work and to listen to the questions and concerns of others.

Research, Assess, and Manage Exposure to Engineered Nanometer-Scale Materials

This group recognized that there is both the opportunity and the need to study risk assessment and risk management associated with nanomaterials. It is critical to manage proactively the risks associated with new nanomaterials and to develop safe practices for those in the workforce exposed to new materials. Risk-related research must be multidisciplinary, must address the full spectrum of issues that bear on human and environmental risks and benefits of new nanomaterials, and must speak to hazard assessment, exposure assessment, and management issues. It should incorporate all of the research in this area, including that by scientists, social scientists, and ethicists.

Because of the interrelationship between the future success of nanotechnology and public trust in the safety of nanomaterials, topics related to safety need a substantial amount of research. Toxicology research and health risk management personnel are just beginning to evaluate both risks and exposure levels of natural and man-made nanoparticles. Exposure assessment methodologies and toxicity data sets for these new materials are just beginning to be developed. The extent to which nanoparticle toxicity evaluations may be extrapolated from existing data concerning atoms, molecules, and bulk materials is not known; much more research is needed. Standardized and tiered hazard assessment methodologies must be developed and validated for nanomaterials. Also, effort must be made to assess the toxicological mechanisms of selected, generic, standardized nanoscale particulate types. When these steps have been taken, businesses and labs can deploy instruments to accurately measure—and respond to—any exposures of workers to nanoscale particulates.

In addition to human health studies and of equal importance is research on the environmental fate of engineered nanoscale particulates to determine how they enter the environment, whether they are persistent and bioaccumulative, and/or whether they undergo transformations in the environment. Estimates of the potential for nanoparticulate exposure in the environment will require information about releases, emissions, transport, distribution, and transformation. All of this research should be coordinated and the information fed into a program for managing risks from nanomaterials.

Since risk assessment managers and government agencies must also establish effective ways to communicate with the public about exposures and potential risks of nanomaterials, social science research must be coordinated with the natural science assessments of hazards. In general, development of accurate hazard and exposure data should lead to better assessments of health risks and to better regulation of nanomaterials. Done correctly, these measures should reassure the public that new nanotechnology-derived products are safe.

Finally, an essential part of the responsible management of risks tied to nanotechnology will be to provide guidance on best practices for safe handling of nanomaterials to those in the workforce who handle these materials. Personal protective equipment requirements must be determined, and standards must be established for filters and respirators that remove nanometer-sized particles.

Research the Full Spectrum of Societal Interactions that Nanotechnology Portends

Specific scientific and engineering considerations in nanoscience and nanotechnology interact fundamentally and continuously with social, ethical, and workforce considerations. The members of this group felt that understanding these interactions is essential for society to transition smoothly to a world where nanoscience-enabled products and processes are pervasive. As a society, it is possible to organize the nanoscience research agenda in terms of scientific and technological developments or in terms of various kinds of societal interactions. Here, a second approach can be adopted. But the social research agenda is prompted by current or anticipated developments in nanoscience and nanotechnology; of particular consequence are developments in nanomaterials, information technology, nanomedicine, and nanotechnology-enabled work in energy production, transmission, and consumption.

The overlapping scientific and social considerations that demand concentrated study include environmental health and safety; equity concerns; legal, regulatory, and insurance matters; privacy issues; economic models; and public awareness, attitudes, and trust. Work should begin with examining the likely interactions between new nanotechnologies and human and environmental health. Secondly, we must examine the possible distributions of benefits and risks, broadly understood, that may develop from nanotechnology's interactions with society, and take steps to ameliorate inequities that may occur. Thirdly, we must investigate the adequacy of existing legal, regulatory, and insurance approaches to the safe and equitable introduction of nanotechnologies and develop alternative approaches as required. Fourthly, we must analyze the interactions of new nanotechnologies with current laws and social expectations concerning privacy and take steps to develop legal and other approaches to deal with privacy concerns. We must also investigate the likely economic consequences. In general, it will be important to develop increasingly specific and accurate models of public awareness of, attitudes toward, and trust concerning specific emerging technologies.

Addressing equity concerns is important and relates to addressing health and safety concerns. It is legitimate and proper to worry about inequitable distribution of risks and benefits in the development of new nanomaterials. Workplace safety laws should help ensure that workers do not shoulder an inequitable share of risk while business owners and shareholders enjoy an inequitable share of benefits. Developments in medicine raise equity concerns about access to beneficial new products and devices. Equity questions get more complicated when considered in global geopolitical terms. But equity concerns cover an even broader and more basic social mandate: It is important that the considerations and discussions that will shape nanotechnology's future include points of view from all economic sectors, from all cultures, and from all walks of life. Nanotechnology's promise to provide new economic opportunities to many, for example, must be weighed against nanotechnology's promise to provide new curative medical therapies that may be affordable to only a few. Proactive steps need to be taken to keep the social equity agenda prominent.

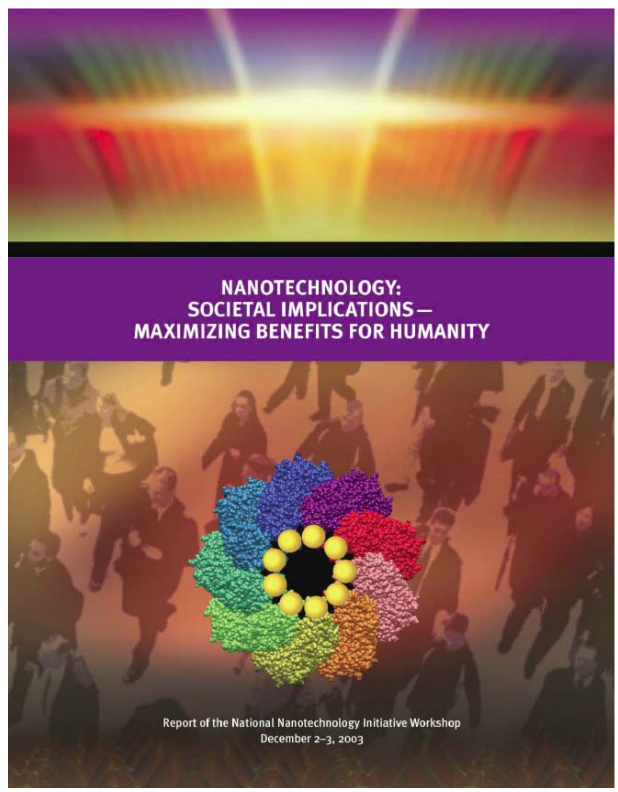


Figure 10.1. The Societal Implications workshop discussed the ethical, legal, education, and workforce implications of nanotechnology. Report available at http://www.nano.gov/html/res/pubs.html.

The push to accelerate technology transfer from the laboratory to the marketplace is redefining previously stable institutions and institutional relationships, particularly with respect to the role of intellectual property in relationships between government, academia, and industry. There are concerns about whether the current patent system is properly promoting the development of new nanotechnologies. It may prove advantageous to seek new and better ways to use the regulatory and insurance systems to distribute risk and benefit when promoting research and entrepreneurial efforts. Intellectual property issues are both national and international. Nanotechnology is developing around the globe, and there is a need to take steps to establish some internationally accepted ground rules with respect to nomenclature, approaches to risk, patents, and protection and dissemination of intellectual property.

Concerns about privacy of individuals and security of information already have surfaced with respect to information technology advances. Nanotechnology developments are likely to sharply accentuate these concerns. The prospect of ubiquitous information technologies connected to multiple and, in some cases, invisible sensors continuously communicating information through wireless networks raises all kinds of privacy concerns. Health-monitoring networks pose a striking example. Embedded diagnostic devices that communicate patient health data by wireless technology could make highly personal information widely available. Increases in the extent of medical information that can be revealed with new diagnostics can have both insurance and personal consequences that will be difficult to resolve.

Nanotechnologies are expected to have enormous economic impacts, some potentially quite disruptive. It is necessary to prepare for this by pursuing a research agenda that will provide details about both macro- and microeconomic consequences tied to the introduction of new nanotechnologies. One can foresee new technologies upsetting the fortunes of those invested in and working with current technologies. The probability of workforce displacement, industrial displacement, and regional economic displacement raises a variety of issues that need examination.

Public opinion is a critical component to the successful introduction of any new technology. The public can hamper nanotechnology progress through lawsuits, political pressure, local activism, market revolt, and social movements. Proactive approaches to problem solving are called for, based on sound knowledge about public concerns and their genesis. Current evidence suggests that the public is excited about nanotechnology opportunities; at the same time some members of the public express great concern that their interests be adequately protected. The present window of opportunity to capitalize on positive public opinion and to thoroughly answer public concerns should not be lost.

It would be helpful to obtain accurate, ongoing information on public awareness, attitudes, and trust. It is necessary to understand how sources of information about nanotechnology drive public views, and action is required to counteract irresponsible or uninformed portrayals that gain public currency. It is equally imperative that to develop and implement successful communication programs to responsibly inform multiple publics about nanotechnology, and that to develop and implement multidirectional forums for dialog on nanotechnology's future. In all cases, metrics for assessing success should be established.

Develop Educational Programs About Nanotechnology and its Societal Implications

This group concluded that broadly based public education in and about nanotechnology is critical. Without increasing the number of students drawn to science and technology subjects and nanotechnology in particular, the nation will be at risk for a serious human resource deficit. The inherent public interest in nanotechnology is a valuable inducement for students to study science and engineering. It is also a motivator for engaging the interest of the broader public in dialog about nanotechnology in society. Thus, the educational mission should run from "K to gray."

There will be several components to this educational enterprise. It will be necessary to develop multidisciplinary teaching methods that can provide practicing scientists and engineers an opportunity to learn about the societal and ethical interactions associated with nanotechnology.

Also required will be opportunities for social scientists to learn about the scientific and technical possibilities presented by nanotechnology. In short, appropriate multidisciplinary approaches are needed to educate and engage in dialog the full spectrum of nanotechnology stakeholders.

To prepare the nanoscience engineers, researchers, and knowledge workers of tomorrow, secondary schools should take steps to develop a nanoscience-based educational design framework aligned with current national science education reform efforts and grounded in the latest pedagogical practices and learning theories. Materials should be developed that could be adapted for local use in school districts throughout the nation. Educational design teams should include input from nanoscience and nanoengineering research expertise, pedagogical expertise, and practitioners who will be among those responsible for implementing curricular innovations.

In addition to developing materials to teach students about nanoscience, the members of this group thought that there is an opportunity to include social studies materials on the societal interactions related to nanotechnology developments. Educational efforts should include provision to assess these efforts, focusing on effectiveness in conveying an understanding of nanoscience, engagement with the materials, and feasibility and scalability. These materials should be freely available.

University education in nanoscience and nanoengineering should strive to increase breadth without a loss of disciplinary depth. Steps should be taken to coordinate educational opportunities from the variety of disciplines that contribute to our understanding of the nanoscale. Steps also should be taken to provide opportunities and encouragement to students in the humanities and social sciences to learn more about science and engineering at the nanoscale, and the converse.

Inherently multidisciplinary in nature, nanotechnology provides an opportunity to bridge disciplinary barriers that exist between the science and engineering disciplines and between the science/engineering disciplines and disciplines in the humanities and social sciences. However, this will not happen unless steps are taken to facilitate and reward interaction on nanotechnology issues between faculty members from these multiple disciplines. Universities should be encouraged to create opportunities for multidisciplinary teaching.

Educational efforts that reach beyond undergraduate and graduate programs need two foci. First, opportunities should be provided to workers moving into nanotechnology-related industries to acquire the necessary skills. Second, a wide variety of informal educational efforts should be undertaken with multiple publics to inform them about nanotechnology and to provide them opportunities to engage with each other and with others interested in nanotechnology's development.

11. Funding Strategy, Interdisciplinary Opportunities, Grand Challenges, Interaction with Other Stakeholders

Session Chair: C. A. Murray

INTRODUCTION

Nanotechnology is still at an early phase of development. Targeted, strategic investments are required to accelerate the innovation process. The inherently multidisciplinary nature of nanotechnology requires shared focus and goals, as well as strong interactions and knowledge sharing among the stakeholders.

RECOMMENDATIONS

Participants in this breakout session identified the following as strategic priorities for advancing nanotechnology research and development:

- Strategic funding of fundamental and applied research
- Focused challenges
- Sharing across sectors; roadmaps
- Internship clearinghouse
- "PubNano Central"

Strategic Funding of Fundamental and Applied Research

The Federal Government invests nanotechnology-related dollars in a variety of ways, including in supporting fundamental research and applied research focused in specific technology areas, building new nanotechnology research centers, developing research infrastructure, and understanding the societal dimensions of deploying nanotechnologies. Historically, a bit less than a third of the Federal nanotechnology research and development funding goes towards fundamental research, and about half goes to applied research. Universities are powerful engines of discovery, and single principal investigators (PIs) or small collaborations execute most of the fundamental research. These small groups also carry out a great deal of the applied research at present. Larger, interdisciplinary teams working at research centers are particularly effective in achieving specific technology goals. However, less than two-tenths of the Federal nanotechnology investment is spent at such centers. A similarly small amount is spent on developing regional user facilities, computational networks, and other infrastructure to support these large, interdisciplinary efforts. Importantly, investment in infrastructure benefits single PIs and large teams, fundamental and applied projects alike. This group recommends sustaining a significant investment in fundamental research and directing a larger portion of the applied research funding towards centers, large teams, and infrastructure.

Fundamental Research

In order to ensure the most rapid commercialization of nanotechnology and maintain U.S. economic competitiveness, fundamental research must remain a major portion of the Federal investment portfolio over the next two decades, at or near current levels. Nanotechnology is in its infancy. We do not understand many of the fundamentals of nanometer-scale interactions at the atomic scale, which differ dramatically from molecular or atomic interactions and also from bulk materials. We also do not yet know how to scale up nanometer-scale devices into functioning complex machines, how to efficiently interconnect devices with each other and with the macroscopic world, how to effectively deal with the stochastic behavior at the nanoscale, how to predict and control device behavior, or how to accomplish manufacturing scale-up. A strong basic understanding of these issues is essential and will greatly accelerate our ability to capitalize on the promise of nanotechnology.

The Federal Government funds the majority of fundamental research, most of that in our nation's research universities, a smaller portion in government and corporate labs. Studies have shown that technology-driven economic development thrives in regions where there are major research universities. Universities both generate new scientific results and create a workforce by training scientists and engineers.

Fundamental research is often best accomplished in single-investigator or small, multiple-investigator grants. These researchers could benefit greatly from collaborations across sectors. When possible, government/industry co-investment in fundamental research, inspired by specific applications, should be encouraged and supported. Industry and venture capital investors should be expected and encouraged to invest in applied research and development of the technology. This will be enhanced if the NNI maintains a strong fundamental research base in the universities. The National Nanotechnology Coordination Office (NNCO) could be a catalyst for academic, national lab, and industry teaming.

It is equally important to ensure that "application- and goal-inspired" fundamental research is a strong component of applied research and engineering centers. Fundamental understanding is an essential component of the best industrial commercialization efforts for revolutionary technologies. For example, the transistor would not have been developed as quickly had it not been for the earlier foundational research into the quantum physics of electronic band structure and electrical transport in semiconductors. These fundamental studies were motivated by the desire to realize the application and were undertaken by the same team as they were experimenting with device geometries. Research in fundamentals carried out simultaneously with and inspired by applied efforts worked effectively in the early days of SEMATECH research across industry and academia, providing the underpinnings of the present U.S. semiconductor industry and maintaining its global competitiveness.

Applied Research

Research centers promote opportunities and support for research in a variety of disciplines and research sectors, including academia, industry, and government laboratories. They are particularly effective in creating strong collaborations with the aim of attaining a particular technical goal. In commercialization efforts, it is essential to have all stakeholders be communicating with each other early on and participating jointly in the effort with a set of aligned goals. If the players have already been part of an applied collaborative effort, commercialization will be much smoother.

Research centers focused on applications should have significant industry collaboration, with on-site industrial researchers at the university or national lab, or have academic or government researchers working at the industrial site (with at least a quarter of funding and researcher contributions from industrial partners in addition to any in-kind contributions). Proposals for centers should be required to have clear intellectual property arrangements and technology transfer mechanisms. Metrics for success of the centers should include the number of technology and patent licenses and new products or businesses created. It is important not to dictate the composition of the centers or the intellectual property arrangements, but to experiment with different models for different research challenges. Best practices should be shared. Peer review and site selection committees for the applied research and engineering centers should have at least one-third industrial participation.

Focused Challenges

Federally funded research and development in nanotechnology should collectively focus on a few targets and challenges of greatest probable importance to society. Some aspects of nanotechnology have become sufficiently mature, with their potential benefits to society sufficiently large, that it is now possible for Federal agencies to team together to create a small set of very specific “grand challenges” to the research and engineering community. Each challenge should be designed to solve a particularly important problem of relevance to society, using technological and scientific understanding that is at least an order or two in magnitude better than any capability we have today, and for which commercialization is at least ten to fifteen years out. An example might be to build a nonvolatile 5 nm logic gate or nanoparticles that target, detect, and destroy cancerous cells *in vivo*. These grand challenges should pose a desired outcome but not the way to achieve it (the “what” but not the “how”).

Meeting the grand challenges will require several separate, highly collaborative interdisciplinary research teams pursuing the challenge with different technical approaches. For maximum success, each team must include a wide variety of stakeholders, for example, researchers from several academic disciplines, industry, national labs, and clinical researchers.

Each of several research teams funded for the first phase of a specific program must pose its own intermediate steps, including attaining the fundamental research understanding they believe necessary to achieving the goal, having a technology transfer plan as a part of the proposal in five years, and if renewed in a second-phase program, coming up with a working prototype; intellectual property terms; industry contribution; risk assessment; safety, environmental, and societal issues, as well as public outreach.

A specific grand challenge such as a cure for cancer is an excellent motivation for the best “use-inspired” applied and fundamental research. It provides a good rationale for the work for communicating the importance of nanotechnology, and it helps to improve U.S. global competitiveness by motivating and training graduate students in systems thinking and partnership across disciplines and sectors.

Sharing Across Sectors; Roadmaps

For maximum effectiveness, the members of this group concluded that it is essential to establish a formal, national nanotechnology alliance. This alliance would bring together all regional, state, and local nanotechnology initiatives, the NanoBusiness Alliance, nanotechnology centers, large corporations, and industry groups. Its purpose would be to facilitate communication among these players in nanotechnology. The alliance could provide a single point of contact for access to U.S. research results, nanotechnology websites, and conference listings. Additionally, it would serve as a means for information sharing on best practices, technology transfer, societal issues, intellectual property practices, and innovation efforts. Large issues call for establishment of national working groups; such issues include best practices and proper incentive structure in intellectual

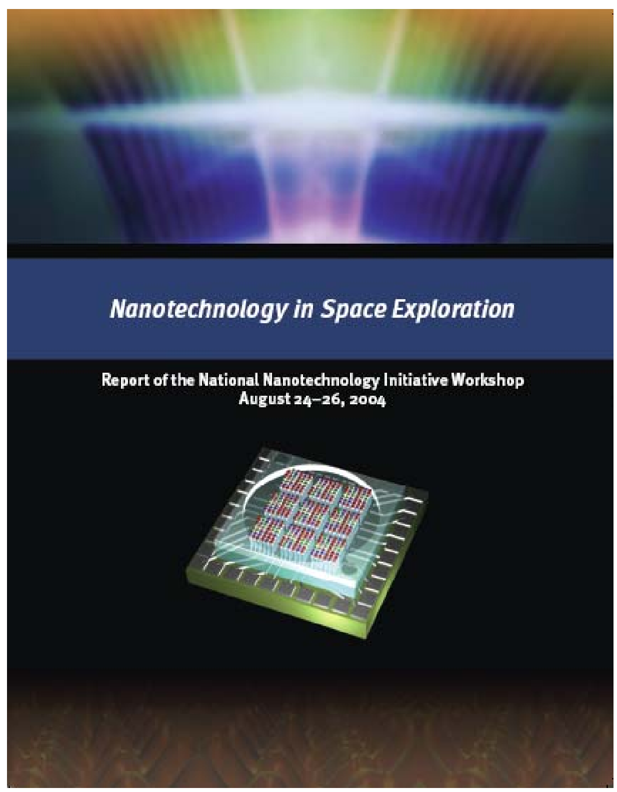


Figure 11.1. The Nanotechnology in Space Exploration workshop considered application of novel nanomaterials, nanosensors and instruments, and nanorobotics to the exploration of outer space. Report available at http://www.nano.gov/html/res/pubs.html.

property sharing, standard nomenclature and measurements, health and safety, "green" manufacturing of nanotechnology products, technology roadmap efforts, and nanotechnology curricula development. An alliance of this type could publish a newsletter that highlights new research results, new companies formed, and new product introduction, and that contains links to other nanotechnology news sources. The alliance could be a focal point for dialog with the public and press and for possible coordination of outreach efforts of centers. The alliance could be a clearinghouse for internships in industry and job listings.

Internship Clearinghouse

Doctoral-level researchers in nanotechnology will need to have knowledge that is both deep in a specific discipline and broad enough to communicate with collaborators in other academic disciplines, as well as with product developers, marketing and sales personnel, and the general public. The nanotechnology workforce of the future will need to be highly flexible, capable of lifelong learning, and skilled in systems thinking, that is, the ability to look at the big picture and optimize the system under a number of often conflicting constraints and boundary conditions. Developing a curriculum and research training experience relevant to nanotechnology poses a huge challenge to our universities, especially at the graduate level. A clearinghouse for matching graduate students with internships in industry would be very helpful in addressing these kinds of issues.

The best way to acquire an ability to collaborate with a wide range of people of different technical and business backgrounds as well as to acquire systems thinking skills is to learn through doing. Internships in industry of several months to several years can be an excellent way for graduate students to get this important experience. Likewise, focused student input could be invaluable to the small and large companies alike that would fund the internships. The universities would get a bonus of potential subsequent job placement of their graduate students after graduation as well as technology transfer opportunities.

"PubNano Central"

This group proposed creation of a "PubNano Central" online database to archive all nanotechnology-related published papers resulting from Federal funding, allowing the public free access starting six months after the publication date. The program should be modeled after the policy of the National Institutes of Health that requires authors to upload all sponsored publications to PubMed Central and encourages the medical journals to submit their final redacted version of the papers six months after publication to the central archive with a link to their own archives. Thought must go into designing policies for such a database, as research will be published in a wide range of technical fields. The nanotechnology-related publication rate has begun to accelerate exponentially as we amass scientific knowledge and engineer new devices, do toxicology and sociological studies, and create massive databases. The scientific and economic benefits would be immense of having a central repository of freely accessible journal papers as the nanotechnology field is taking off. This resource must be designed to respect the scholarly journals' need for economic viability.

Appendix A. Workshop Agenda and Charges to Participants

WORKSHOP AGENDA

Wednesday, September 8, 2004

10:30 am	Welcome to the National Academies	W. A. Wulf
10:35 am	Welcome	J. H. Marburger, III
10:45 am	Opening Remarks	P. J. Bond
10:55 am	Charge to Participants	A. H. Carim
11:05 am	Overview of the National Nanotechnology Initiative	M. C. Roco
11:23 am	Overview of the 1999 Research Directions Workshop	R. S. Williams
11:40 am	Overview of Recent Legislation and Implementation	S. L. Hays
11:50 am	PCAST Perspectives on the NNI	E. F. Kvamme
12:00 noon	Lunch and initial small-group discussions	
	Afternoon: NSET "Grand Challenge" Workshop reports:	
1:00 pm	Nanomaterials by Design	R. Hull
1:20 pm	Electronics/Photonics/Magnetics	G. S. Pomrenke
1:40 pm	Chemical, Biological, Radiological, and Explosive (CBRE)	J. S. Murday
2:00 pm	Energy	E. D. Williams
2:20 pm	Environment	B. P. Karn
2:40 pm	Break	
3:00 pm	Advanced Healthcare, Therapeutics, and Diagnostics	B. A. Baird
3:20 pm	Nanomanufacturing	M. V. Tirrell
3:40 pm	Microcraft and Robotics (Nanomachines and Nanosystems)	M. N. Dastoor
4:00 pm	Instrumentation and Metrology	M. T. Postek
4:20 pm	Full-group open discussion on grand challenge areas, research targets, and unifying themes	
5:00 pm	Time reserved for public comments	
6:00 pm	Adjourn	

Thursday, September 9, 2004

8:30 am	Recap of first day, announcements, schedule, instructions	A. H. Carim
	Other NSET-supported or related meeting or workshop reports:	
8:45 am	Ethical, Legal, and Societal Implications	D. W. Baird
9:00 am	State and Local Nanotechnology Efforts and Coordination	S. Murdock
9:15 am	Agriculture and Food Systems	N. R. Scott
9:30 am	ChemVision 2020 Meeting and Chemical Industry Perspective	J. Solomon

9:45 am	SRC Silicon Nanoelectronics Meeting	J. A. Hutchby
10:00 am	Charge to 1st Breakout Session participants	E. C. Teague
10:05 am	Break	

10:20 am — 1st Breakout Sessions (topic clusters; chairs as indicated):

- [S1A] Nanomaterials by Design, Electronics/Photonics/Magnetics, CBRE (S. Williams)
- [S1B] Energy, Environment (R. Hamers)
- [S1C] Nanomedicine, Nanobiotechnology, Agriculture, and Food Systems (B. Baird)
- [S1D] Nanomanufacturing, Nanomachines, and Nanosystems (C. Montemagno)
- [S1E] Tools: Instrumentation and Metrology, Advanced Buildings, and Simulations (R. Hocken)

11:50 am	1st Breakout Sessions writing: draft community input for workshop report;	
	Working Lunch	
1:00 pm	Reports from 1st Breakout Sessions	
1:45 pm	Charge to 2nd Breakout Session participants	C. I. Merzbacher

1:50 pm — 2nd Breakout Sessions (aspects of initiative; chairs as indicated):

- [S2A] Fundamental Scientific Research (A. Majumdar)
- [S2B] Application Opportunities and Technology Transfer (C. Hunt)
- [S2C] Infrastructure Needs (T. Michalske)
- [S2D] Societal Implications (D. Baird & D. Warheit)
- [S2E] Funding Strategy, Interdisciplinary Opportunities, Grand Challenges, Interaction with Other Stakeholders (C. Murray)

3:20 pm	Break
3:35 pm	2nd Breakout Sessions writing: draft community input for workshop report.
4:45 pm	Reports from 2nd breakout sessions.
5:30 pm	Final full-group discussion: research directions, vision, implementation.
5:55 pm	Wrap-up, thanks to participants, and invitation to participate in report-writing.
6:00 pm	Adjourn

Friday, September 10, 2004

8:30 am	Writing group convenes.
12:30 pm	Adjourn; draft report submitted.

CHARGES TO PARTICIPANTS

Charge to Participants (A. H. Carim)

My name is Tof Carim. I'm involved in managing nanoscale science research efforts within the Office of Science at the U.S. Department of Energy, and in the interagency nanotechnology coordination activities.

I'll be introducing today's speakers and trying to keep track of time. As you can see on the agenda, we've got a very tight schedule and so I'll ask you to hold all but the most pressing questions for the breaks, the breakout sessions, or the discussion periods. At the moment, however, my task is to provide the charge to the participants in this workshop, so let me begin by setting the stage and putting this meeting and related activities into context.

As most of you well know, Federal activities relating to the National Nanotechnology Initiative have been coordinated for the past several years by an interagency body, the Nanoscale Science, Engineering, and Technology (NSET) subcommittee of the Committee on Technology of the National Science and Technology Council. Day-to-day technical and administrative operations and some development and dissemination of reports and other materials are handled by the National Nanotechnology Coordination Office. The NNCO also serves as the point of contact for Federal nanotechnology activities.

Let me add my own welcome on behalf of the NSET Subcommittee and the NNCO, and express our thanks to all of you for your participation. This meeting is intended to recap the major outcomes from the series of prior NNI “grand challenge” workshops and other related meetings, indicate bridging themes and activities, identify overlooked areas or those that may need greater emphasis, and provide the research community's input on research directions and implementation of the initiative going forward. The workshop's report will serve as a key input for the development of the NNI’s strategic plan in the near future.

In 1999, the original Nanotechnology Research Directions workshop was held to help define the initiative, which had not yet begun at that time. It produced a very valuable report, which has become a key reference document. You'll hear more about this shortly, but the situation today is a bit different: the initiative is ongoing, has been addressed by the 21st Century Nanotechnology Research and Development Act, signed into law last December, and involves nearly a billion dollars of Federal investment annually. Just as the 1999 Research Directions workshop helped to inform development of an Implementation Plan for the initiative, part of the impetus for the present meeting is in preparation for the crafting of the NNI Strategic Plan.

In this meeting you'll hear several overview presentations, brief synopses of the findings and suggestions from all of the NNI "grand challenge area" workshops, and input from several related activities. Tomorrow we'll have two separate breakout sessions; the first is organized around topical clusters, while the second broadly addresses various aspects of the initiative. There are also full-group discussion periods late in the day today and tomorrow, and a public comment period this evening prior to adjourning for the day.

We want your input on all aspects of the initiative, and in particular your help in identifying the most pressing and promising research targets, and in determining suitable indicators of progress in those areas. We ask you to take e a broad view, going beyond disciplinary and other boundaries to consider the development of this major national investment in science, engineering, and technology.

This is indeed a workshop, with the emphasis on “work.” The expectation is that a full draft report will be complete by the end of the writing session on Friday. En route to this, each of the breakout sessions is being asked to draft written input during their allotted time. Further instruction will be provided in the charges to the breakout sessions. Our expectation is that the final report will include executive summaries of the prior workshops in an appendix.

While we have, in order to ensure sufficient manpower, asked some of you specifically to stay for Friday's writing, any who wish to stay and contribute are welcome. I emphasize, though, that Friday's sessions are intended not as additional time for discussion and debate, but rather to capture and express the discussions held today and tomorrow.

Three principal editors have been asked, and have bravely agreed, to take responsibility for bringing together the report as a whole. They will be available throughout the meeting, circulate among breakout sessions, and lead the writing group on Friday. I'd like to introduce them and offer our special thanks to them in advance at this time. They are:

- Bob Hwang—of Brookhaven National Laboratory
- Judy Stein—with General Electric
- Jim Baker—at the University of Michigan

With that challenge in front of you, let's get started.

Charge to First Set of Breakout Sessions (E. C. Teague)

My name is Clayton Teague and I’d like to add my welcome and thanks for joining us at this important workshop for the National Nanotechnology Initiative. We value your expertise and knowledge highly and greatly appreciate your assistance in setting the research directions for the Initiative.

The aim of this first set of breakout sessions is to solicit your recommendations for specific scientific and technical challenges that should be targeted by the NNI. You will be asked to examine the Initiative from a broader programmatic perspective in the second set of breakout sessions. Here we are asking for your thoughts on the question: Out of the broad areas that nanotechnology encompasses, what research targets should be selected to ensure maximum societal and economic impact by the NNI? Your recommendations are very important since they will serve as input to the interagency coordinating body as it develops the NNI strategic plan for the next 5-10 years. The plan is to be developed between now and the end of the year.

You have been assigned to one of the sessions, based on expertise and the organizing committee’s desire to achieve a balance of viewpoints. For each of the breakout sessions, the organizing committee has grouped two or more of the grand challenge areas as topical clusters. We did so in the hope of facilitating synergies, identifying high-level cross-cutting themes, interdependencies, etc., among the topics. However, we would encourage you to not feel too tightly bound by the clusters. Please consider cross-cuts and synergies that may extend into other grand challenge areas and identify key areas that might not be captured within existing topical clusters.

My assignment is to provide you with information about the specific outputs we would like you to develop. As you work to develop these outputs, we hope you will draw upon the group’s diverse expertise and knowledge. In addition, you have been provided with copies of yesterday and today’s presentations. Finally, executive summaries and selected parts of workshop reports pertaining to recommendations and identified research targets are included in the handouts.

We request that you develop two outputs in your breakout sessions. First, distill and synthesize from the group of workshop presentations, executive summaries and recommendations related to your session’s cluster of topics a total of no more than five key research targets.

By a research target we have in mind a long range—five to ten years out—specific scientific or technological achievement stated in as quantitative a manner as you can agree on. In discussions among the organizing committee, we thought a good initial step toward identifying the research targets would be to select major areas of opportunity and then to choose one or more targets within the opportunity areas. In choosing the opportunity areas and research targets you should consider a number of factors: scientific opportunity, potential technological and societal impact, resources needed to address the target including S&T professionals, facilities, and funding.

As an example, and this is really meant only as an example; using nanotechnology to improve efficiency of energy conversion might be chosen as an area of opportunity. Within this opportunity area there are a large number of possible research targets; improved efficiency of fuel cells, solar cells, thermoelectrics, etc. The group might—might!—agree on one posed during the Energy workshop: develop solar cells with 20% efficiency at 100X reduction in cost. The argument for choosing this target could be that it has a significant science component—tailored absorption of much of solar spectrum with potentially inexpensive materials; addresses renewable energy—a key national goal; and is highly interdisciplinary—needing extensive engagement of the materials, chemistry, physics, and electrical engineering communities.

That's the idea. If your group thinks major targets were not identified during the workshops, feel free to incorporate these into your five targets.

Second, spell out indicators of progress for each of the research targets. Since the term is not self-explanatory, let me use the solar energy example to provide some guidance. One might choose:

- Indicators for scientific discovery—advances in understanding photovoltaic efficiency in nanostructured materials, number of papers, citations in high impact journals
- Indicators for adequate funding—proposal pressure
- Indicators for technological innovation—overcoming technological barriers, operating prototypes, patents, etc.
- Indicators for degree of commercialization – licenses, cooperative R&D, company investments

To be clear, these are explicitly not intended to be milestones. We realize that progress in research is typically an iterative hypothesis-test-learn process, rather than a linear point A to point B process, and that progress should be measured by other means. These indicators of progress are our attempt to recognize the nature of research. Your thoughts on such indicators would be extremely valuable for us in developing the NNI strategic plan.

You have about 90 minutes for these breakout sessions. We definitely know this is a challenge but trust that with this group and your experience in such matters you will be able to accomplish this assignment. Have fun—we look forward to seeing the results!

Charge to Second Set of Breakout Sessions (C. I. Merzbacher)

From the perspective of the Federal Government, the NNI serves to expedite the discovery and development of the benefits of nanoscale science, engineering, and technology, and the transition of those benefits to public or commercial use.

To accomplish this objective, the NNI currently has the following goals:

1. Conduct R&D that will allow realization of nanotechnology's widespread potential benefits
2. Facilitate transfer of the resulting new nanotechnologies into products, processes, and services that benefit the public
3. Develop the supporting infrastructure and tools (e.g., facilities, instrumentation, and computational capacity) needed to advance nanotechnology R&D
4. Understand better the social, ethical, health, and environmental implications of nanotechnology
5. Provide for education of future researchers, training of a skilled workforce, and outreach to the broad public
6. Ensure U.S. global competitiveness and leadership in the development and application of nanotechnology

These goals form the basis of the second set of breakout sessions, which are entitled:

A. Fundamental scientific research
B. Application opportunities and technology transfer
C. Infrastructure needs
D. Societal implications: Ethical; social; legal; workforce and education; and environmental, health, and safety (EHS)
E. Funding strategy, interdisciplinary opportunities, grand challenges, interaction with other stakeholders (including the public)

The charge to these breakouts is:

- Identify and prioritize the opportunities and needs in the breakout session area
- Suggest new, as well as existing, mechanisms to address these opportunities and needs
- Recommend strategies by which the NNI investment in each area might be leveraged against investments by other stakeholders, including by universities and other research institutions, state and local governments, and other nations

The findings and recommendations of each breakout session will be taken into consideration by the interagency coordinating body as it develops the NNI strategic plan for the next 5-10 years. Each of the workshop participants brings a different perspective to these discussions—representing academia, industry, government agencies, etc. The workshop organizers and the members of the interagency coordinating body urge you to take advantage of this opportunity to take a wide-angle view of nanotechnology, and how the NNI, with its emphasis on research and development, can be organized and focused in order to achieve its purpose.

Below are suggested topics for the five breakout sessions. These are not inclusive, but are a starting point for discussions.

A. Fundamental scientific research

- Fundamental research areas of greatest opportunity for discovery and knowledge generation. Are there research areas that are not currently included that should be?
- U.S. areas of strength vs. those of other countries.
- Mechanisms to enhance multi-disciplinary collaborations.
- What fraction of the total NNI budget should be allocated to the topics covered by breakout sessions (A) through (D) today? In five years?

B. Application opportunities and technology transfer

- Applications with greatest potential to impact national needs and quality of life. Are there any applications that are not currently included that should be?
- Given "pre-competitive" nature of Federal R&D, identify 3-5 technology applications (e.g., fuel cells, data storage, or cancer detection & treatment) that would most benefit from Federal support.
- Identify applications that may require Government development for public good (analogous to support for treatment of "orphan diseases").
- Mechanisms for enhancing technology transfer.
- Mechanisms for enhancing communication of industry needs to Federal R&D program managers, and vice verse.
- What fraction of the total NNI budget should be allocated to the topics covered by breakout sessions (A) through (D) today? In five years?

C. Infrastructure needs

- Processing, characterization, and computational requirements for optimal support of future nanotechnology R&D.
- Mechanisms for joint support with other stakeholders, including industry.

D. Societal implications: Ethical, social, legal, workforce and education, environmental, and health

- Unique and similar aspects of nanotechnology compared to previous technologies.
- Mechanisms for addressing societal impacts.
- Mechanisms for sharing environmental, health, and safety (EHS) data (among Federally funded researchers at universities and Federal labs, in industry, and in other countries).
- What fraction of the total NNI budget should be allocated to the topics covered by breakout sessions (A) through (D) today? In five years?

E. Funding strategy, interdisciplinary opportunities, grand challenges, interaction with other stakeholders

- Relative importance of grants to single investigators (< $0.5 million), multi-investigator teams ($0.5–$2 million), and research centers (> $2 million).
- Utility of specific vs. non-specific grand challenge(s)—Should the NNI focus on specific applications at this time?
- Mechanisms and opportunities for bridging traditionally disparate groups, e.g., disciplines, university departments, government agencies, research organizations vs. industry, etc.
- What fraction of the total NNI budget should be allocated to the topics covered by breakout sessions (A) through (D) today? In five years?

APPENDIX B. WORKSHOP PARTICIPANTS*

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* Affiliation at time of workshop. Breakout session participation is indicated after names, where applicable; see Appendix A (agenda) for breakout session list and designations.

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Appendix C. List of Abbreviations

CBRE	chemical, biological, radiological, and explosive
CMOS	complementary metal oxide semiconductor
IT	information technology
ITRS	International Technology Roadmap for Semiconductors
NNCO	National Nanotechnology Coordination Office
NNI	National Nanotechnology Initiative
NSET	Nanoscale Science, Engineering, and Technology Subcommittee of the NSTC's Committee on Technology
NSTC	National Science and Technology Council
PCAST	President's Council of Advisors on Science and Technology
PI	principal investigator

APPENDIX D. LIST OF NNI-SPONSORED WORKSHOPS (2001-2004)

The following is a list of workshops held between 2001-2004 that were organized or supported by the NNCO or agencies participating in the National Nanotechnology Initiative.

- Nanotechnology: Opportunities and Challenge (September 10, 2001).
  Report: http://www.wtec.org/nanoreports/FinalUCLAnanoRpt0302.pdf
- Nanomanufacturing and Processing (January 5-7, 2002).
  Report: http://www.nsf.gov/mps/dmr/nsfec_workshop_report.pdf
- Nanotechnology Innovation for Chemical, Biological, Radiological, and Explosive: Detection and Protection (May 2-3, 2002).
  Report: http://www.wtec.org/nanoreports/cbre/
- Manufacturing at the Nanoscale (May 13, 2002).
  Report: http://www.nano.gov/html/res/pubs.html
- From the Laboratory to New Commercial Frontiers (May 23, 2002).
  Report: http://wtec.org/nanoreports/ACF64.pdf
- Chemical Industry R&D Roadmap for Nanomaterials by Design: From Fundamentals to Function (September 30 - October 1, 2002).
  Report: http://www.chemicalvision2020.org/nanomaterialsroadmap.html
- Nanoscale Science and Engineering for Agriculture and Food Systems (November 18-19, 2002).
  Report: http://www.csrees.usda.gov/nea/technology/in_focus/nanotech_if_workshop.html
- Buildings for Advanced Technology Workshop (January 14-16, 2003).
  Overview: http://www.nanobuildings.com/bat/overview/
- Nanotechnology Grand Challenge in the Environment (May 8-9, 2003).
  Report: http://www.nano.gov/html/res/pubs.html
- Materials by Design (June 11-13, 2003).
  Report: http://www.nano.gov/html/res/pubs.html
- Nanotechnology and the Environment: Applications & Implications (September 15-16, 2003).
  Summary: http://es.epa.gov/ncer/nano/publications/index.html
- Regional, State, and Local Initiatives in Nanotechnology (September 30 - October 1, 2003).
  Report: http://www.nano.gov/html/res/pubs.html
- Nanobiotechnology (October 9-11, 2003).
  Report: http://www.nano.gov/html/res/pubs.html
- Societal Implications of Nanoscience and Nanotechnology (December 2-3, 2003).
  Report: http://www.nano.gov/html/res/pubs.html
- Instrumentation and Metrology for Nanotechnology (January 27-29, 2004).
  Report: http://www.nano.gov/html/res/pubs.html
- Nanoelectronics, Nanophotonics, and Nanomagnetics (February 11-13, 2004).
  Report: http://www.nano.gov/html/res/pubs.html
- Nanoscience Research for Energy Needs (March 16-18, 2004).
  Report: http://www.nano.gov/html/res/pubs.html
- Nanotechnology in Space Exploration (August 24-26, 2004).
  Report: http://www.nano.gov/html/res/pubs.html

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