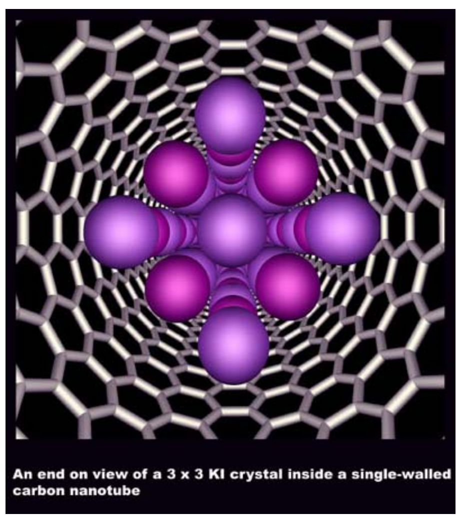
National Science and Technology Council
Committee on Technology
Subcommittee on Nanoscale Science, Engineering and Technology

Nanotechnology Grand Challenge in the Environment: Research Planning Workshop Report

Vision for Nanotechnology R&D in the Next Decade



http://www.chem.ox.ac.uk/nanotemp/info.html

May 8-9, 2003
Arlington, VA

About this document: A visionary planning workshop was held on May 8-9, 2003, in Arlington, VA, to strategize on how nanotechnology research can be used to protect, inform, manage, and improve the environment and how potential harm from nanotechnology can be anticipated and prevented. The workshop was sponsored by the National Nanotechnology Coordinating Office and organized by an interagency group, led by the U.S. Environmental Protection Agency. This report summarizes workshop participants' vision for nanotechnology research and development (R&D) in the next decade.

About the cover: The cover shows an end-on view of a 3 X 3 KI crystal inside a single-walled carbon nanotube. http://www.chem.ox.ac.uk/nanotemp/info.html

Table of Contents

Executive Summary

Introduction

A multidisciplinary group of scientists and engineers met on May 8-9, 2003, in Arlington, VA, for a visionary planning workshop to strategize on how nanoscale science and technology research can be used to protect, inform, manage, and improve the environment and how risk assessments associated with both natural and anthropogenic sources of nanometer-sized objects can be performed. The workshop was organized by an interagency group, led by the U.S. Environmental Protection Agency (EPA), and sponsored by the National Nanotechnology Coordinating Office (NNCO). The May 8 plenary session, held from 8:30 a.m. to 12:15 p.m., was open to the public. The afternoon of May 8 and all day on May 9 consisted of five closed breakout sessions for invited participants. Workshop participants discussed topics in smaller groups to draft a vision for future research related to nanotechnology in the environment. Results of the workshop are contained in this report.

General plenary speakers included Clayton Teague, Director of the NNCO, who welcomed the participants and described the mission of the workshop; and Mihail Roco, Nanoscale Science, Engineering and Technology (NSET) Committee Chairman, who presented an overview of U.S. Government-sponsored activities/programs in nanotechnology R&D. Barbara Karn from EPA presented the charge and goals to the workshop participants, and Alexandra Navrotsky of the University of California–Davis gave a plenary talk discussing the relationship between nanotechnology and the environment.

Plenary speakers for the five broad topics explored during the workshop were:

- Robert Hamers (University of Wisconsin–Madison), who discussed applications for measurement in the environment: sensors, monitors, models, separations, detection, and data gathering and dissemination;
- Debra Rolison (Naval Research Laboratory), who discussed applications for sustainable materials and resources: water, waste (including reuse and recycling), pollution, and energy issues;
- Kenneth Klabunde (Kansas State University), who discussed applications for sustainable processes: bottom-up manufacturing, waste and water treatment, remanufacture and reuse, self-assembling systems, biomimicry, and hierarchical structures;
- Richard Flagan (California Institute of Technology), who discussed implications in natural and global processes: climate change, transport of aerosols, colloids and particulates, biomineralization, and the role of biosystems; and
- Günter Oberdörster (University of Rochester), who discussed implications in health and environmental safety: environmental health, persistence, toxicity, fate and transport, and the wet-dry interface.

Vision Statements and Key Findings

Topic A. Nanotechnology Applications for Measurement in the Environment

> **Vision:** *The unique properties of nanoscale materials will enable the development of a new generation of environmental sensing systems. In addition, measurement science and technology will enable the development of a comprehensive understanding of the interaction and fate of natural and anthropogenic nanoscale and nanostructured materials in the environment.*

Research needs were identified in the following areas: (1) biological sensor technologies that are sufficiently stable to allow detection *in situ* on a continuous basis for high-density usage; (2) a general "array" for detection of a wide variety of potential analytes; (3) information concerning the diversity of chemical composition at the nanoparticle level, and the transformations that occur and measurement techniques that distinguish the chemical composition of particle surface layers from the particle interior; (4) generic nanoscale assembly methods; (5) advances in spectroscopic instrument technologies that allow rapid detection of low signal strength, while probing smaller volumes of a nanoparticulate sample; and (6) advances in sensors for the characterization of environmental nanoparticles in both aerosol and aqueous phases to understand the effects and fates of particles that are already present and to anticipate the impacts of future nanostructure releases.

Nanotechnology offers an opportunity to significantly impact these needs. For example, nanotechnology makes it possible to develop massively parallel arrays of nanoscale sensor elements that can respond to a variety of stimuli (such as a specific chemical, biochemical, or biological analytes) with the simultaneous analyses of a large number of analytes with increased sensitivity, accuracy, and spatial resolution. Nanoinformatics is based on new computational methods for understanding signal transduction in nanoscale systems and for analyzing large amounts of data from nanoscale systems in real time. The rapid transformations that nanoparticles undergo in the environment render traditional approaches to characterizing air or water quality inadequate. The development of simpler, miniaturized particle counting, sizing, and composition analyzers is needed to enable nanoparticle measurements to be distributed to many sites. These measurements should then be coupled to smart electronic processing and decisionmaking systems capable of converting raw data into meaningful information with appropriate validation techniques. Conversely, miniaturization and simplification of particle counters will enable nanoparticles and nanostructures in the environment to be effectively characterized. Finally, hierarchical assembly could enable the fabrication of the arrays described above and allow integration and interfacing of macroscopic and microscopic (i.e. silicon-based) features.

Topic B. Nanotechnology Applications for Sustainable Materials and Resources

> **Vision:** *A society that uses nanotechnology to transform the way it extracts, develops, uses, and dissipates materials and changes the flow, recovery, and recycling of valuable resources, especially in the use of energy, transportation of people and goods, availability of clean water, and supply of food.*

Research goals for this topic were identified as: (1) global sustainable energy systems enabled by photovoltaics and photo-biofuel cells, (2) optimization of the translocation of people and goods utilizing green vehicles and smart infrastructure, (3) global sustainable use and quality of water enabled by superior composite and multifunctional materials, and (4) global sustainable agriculture (optimization of production and distribution of food) enabled by the development of more effective and less environmentally harmful pesticides and fertilizers. There are opportunities for nanotechnology to significantly impact these areas through the development of a knowledge base that relates structure and function at the nanoscale and by designing new materials and architectures with tailored multifunctionality. Nanotechnology offers the opportunity for engineering with synthesis, assembly, and processing at all scales and optimizing control of stability at all scales and conditions of use. Application of life cycle design and interdisciplinary training were identified as key features for achieving these goals and research needs.

Topic C. Nanotechnology Applications for Sustainable Processes

> **Vision:** *Sustainable manufacturing processes based on the use of nanoscale science and nanotechnology—integrated processes and bottom-up assembly—that can serve human needs and are compatible with surrounding ecosystems and the human population*.

Research needs were identified as: (1) optimizing the use of benign processing such as the use of alternative or solvent-free processes; (2) efficient control of manufacturing processes with sensors and actuators to minimize defects, increase fault tolerance, and impart self-healing; (3) controlled selectivity in manufacturing processes using multifunctional catalysts; (4) increased stability of catalysts and sensors to monitor processes, thereby increasing efficiency; and (5) integration of biological processing into nano-driven manufacturing through the utilization of the high enantiomeric selectivity using biological molecules, rational modification of multifunctional materials, and manufacture of self-healing nanostructures.

Opportunities for nanotechnology to significantly impact automatic processes include large-scale production of nanoscale building blocks; manufacturing integrated nanodevices with sensors, actuators, and multifunctional devices; and transformation of unit operations. Additional opportunities include designing innovative manufacturing processes such as just-in-time, just-in-place manufacturing; solar-based manufacturing; and developing theory, modeling, and experimental data on nanoscale materials and processes such as thermo/kinetic/transport fundamental studies at the nanoscale and linking macro/micro/nano/atomic regimes and surface properties. Nanotechnology also can be used to develop new safety and environmental metrics and ethical principles by modifying existing indicators and metrics for use in nanoscale manufacturing, and adapting current ethical principles from professional societies to the needs of nanotechnology.

Topic D. Implications in Natural and Global Processes

> **Vision:** *The ability to understand and quantify nanoparticles in earth system processes to anticipate their impacts and thus optimize and integrate environmental sustainability and nanotechnology.*

Research needs identified were: (1) understanding nanoscale phenomena as they pertain to earth system processes on local, regional, and global scales over a range of time domains; (2) understanding and quantifying the inputs, cycling, and effects of nanoparticles in the environment to anticipate the impacts of future particle release; and (3) optimizing and integrating environmental sustainability and nanotechnology.

Nanotechnology can significantly impact these needs by conducting biological research at all scales of organization to identify, quantify, and predict ecological effects on individual, population, community, and ecosystem phenomena to distinguish between adverse and beneficial perturbations, on both short and long time scales. The design of nanoparticle labels and detection schemes for pollution attribution and use of nanoparticles incorporated into point and distributed emission sources represents another opportunity. The needs also can be addressed by developing broader ecological aspects of nanoscale science and technology by building a broader community of interdisciplinary scientists with particular focus on biologists and ecologists. Additional opportunities to address these needs are developing a database of nanoparticle properties, creating and maintaining an accessible sample repository of model and standard nanoparticles, and developing theoretical and experimental methodologies for real-time characterization of particles in natural waters.

Topic E. Nanotechnology Implications in Health and the Environment

> **Vision:** *Development of nanotechnology responsibly with a full appreciation of its health and environmental impacts.*

Research needs identified were: (1) better understanding of the diversity of anthropogenic nanoparticles through the development of a nanomaterial inventory; (2) development of high throughput/multi-analyte toxicological methodologies, focused on mechanisms and fundamental science of particle toxicity with access to well-characterized nanomaterials by those who are conducting risk assessment research; (3) increased information on exposure to nanomaterials resulting from medical, occupational, environmental, and accidental release of nanomaterials with regard to the concentration of nanomaterials as well as what form(s) they may assume upon release into the environment; and (4) prediction of biological properties of nanomaterials through the toxicological assessment of nanomaterials that includes relevant and scientifically appropriate acute and chronic toxicokinetics and pharmacokinetic studies.

Other research needs include the creation of opportunities for interdisciplinary and leverage-based research involving the private, academic, and federal sectors; knowledge of the biological fate, transport, persistence, and transformation of nanomaterials; increased information on the recyclability, reuse, and overall sustainability of nanomaterials; and mobilization of the research community to address topics of health and environmental importance.

Another research need is to establish an accurate database to access monitoring information derived from nano-based environmental measurements, and to develop new informatics/statistical software to allow effective "mining" of this immense database to identify associations between public health effects and exposure to complex environmental pollutants in a manner that will allow linkages to sources to be determined.

Recommendations

This section includes a summary of key recommendations from each of the issue-specific chapters found in this report.

Nanotechnology Applications for Measurement in the Environment

- Develop the capability for monitoring nanoparticles and nanostructures in the environment with adequate spatial and temporal resolution to elucidate the burden of such materials and to enable studies of their impacts.

- Develop the ability to measure a large number of analytes simultaneously and in real time.

- Construct a massively parallel array of nanoscale sensor elements to provide simultaneous analysis of a large number of analytes and/or probe physical and chemical processes with a very high spatial resolution (thereby essentially becoming a high-resolution imaging detector).

- Develop new nanoscale architectures that will support the transmission of data from multiple probes to multiplexing microscale circuitry. An understanding of the responses of designed nanostructures to chemical and biomolecular stimuli and the development of new mechanisms for transducing these signals will enable high density, low volume sampling on multi-analyte detection chips.

- Develop silicon-based microfluidics that can be used to deliver low volume samples to high-density probe arrays and that can be interfaced with silicon-based microelectronic circuitry.

- Develop methods to understand *in situ* detection kinetics of individual analytes.

- Develop computational methods for analyzing large amounts of data from nanoscale systems in real time. This will enable on-chip data processing and may lead to the creation of a new field—"nanoinformatics."

- Develop measurement techniques that distinguish the chemical composition of particle surface layers from the particle interior. Because most microbial species have not been identified, it also is important to develop measuring and sensing systems that can assess biological diversity in the environment.

- Leverage advances in the ability to prepare and chemically/biochemically modify nanoscale "components" into a more general set of nanoscale assembly methods that would constitute a type of "nano-toolbox" for fabricating more complex structures.

- Develop low-power and/or solar-powered techniques for usage with unattended remote sensing technologies.

Nanotechnology Applications for Sustainable Materials and Resources

- Improve nanoscale understanding of photovoltaic processes and photo-biofuel cells based on improvements in biocatalysts or biomimetic catalysts and biosystems.

- Use developments in nanocomposite materials and corrosion-resistant materials to update the transportation infrastructure.

- Develop point-of-use supply and closed-loop systems to address the problems of an outdated water supply system.

- Use nanotechnology-driven approaches to optimize the production and distribution of food (e.g., develop nanoparticles for direct nitrogen fixation, develop photocatalysts to facilitate the breakdown of biocides and smart dust to identify and locate biocides).

- Adopt a life cycle approach to nanotechnology R&D.

- Develop a knowledge base that relates structure and function at the nanoscale; design new materials and architectures with tailored multifunctionality; optimize control of stability at all scales and conditions of use; address engineering as well as synthesis, assembly, and processing at all scales; and create research tools that bridge the molecular scale and ordered bulk.

Nanotechnology Applications for Sustainable Processes

- Optimize the use of benign processing, which may include alternative or solvent-free processes, using the unique reactivity and properties of nanoscale materials, and using enzymes to develop benign material feedstocks and multifunctional, smart nanoscale catalysts.

- Control manufacturing processes with nanosensors and actuators, for defect minimization, fault tolerance, and self-healing materials.

- Use controlled selectivity in manufacturing processes, through multifunctional catalysts or using stability of catalysts, as well as sensors to monitor processes and make them more efficient.

- Integrate biological processing into nano-driven manufacturing, including high enantiomeric selectivity using biological molecules, rational modification of multifunctional materials, manufacture of self-healing nanostructures, and programmable "death."

- Maximize recyclability, recovery, remanufacturing, and reuse of products.

- Reduce the number of unit operations in manufacturing using combined catalysis and separations.

- Continually evolve practices and metrics that enable and define sustainability.

Nanotechnology Implications in Natural and Global Processes

- Further develop the interaction between nanotechnology and ecosystem biology to identify, quantify, and predict ecological effects on individual, population, community, and ecosystem phenomena.

- Quantify, both theoretically and experimentally, nonclassical behavior at the nanoscale, which affects the kinetics and thermodynamics of nucleation, growth, and dissolution in the environment. Develop molecular-scale models of the structures, reactivity, and solubility of nanoparticles as dependent on composition, size, and external conditions.

- Further develop experimental approaches for studies of hydrated nanoparticles, including measurement with high resolution in space and time of particle number, composition, and morphology as well as predictive models validated by such data.

- Design nanoparticle labels and detection schemes.

- Develop broader ecological aspects of nanoscale science and technology, possibly by building a broader community of interdisciplinary scientists, with a particular focus on biologists and ecologists.

- Establish a database of nanoparticle properties and create and maintain an accessible sample repository of model and standard nanoparticles.

- Develop theoretical and experimental methodologies for real-time characterization of particles in natural waters.

- Develop sensors to enable mapping the state of the environment to a greater degree.

- Use natural biota for the sustainable production of tailored nanoparticles.

- Involve stakeholders, especially the public, in the discussion of the impacts of nanotechnology on the environment.

- Understand nanoscale phenomena as they pertain to earth system processes on local, regional, and global scales over a range of time domains.

Nanotechnology Implications in Health and the Environment

- Develop a better understanding of the health and environmental impacts of nanomaterials due to the ever-increasing applications of nanotechnology in society.

- Develop distributed sensor networks suitable for determining the concentrations, size distribution, and composition of airborne nanoparticles with sufficient spatial and temporal resolution to quantify exposures to these short-lived aerosols.

- Categorize nanoparticles by types, volumes, and applications, and provide\disseminate classification schemes to the broader research community.

- Create high throughput screening and/or combinatorial approaches to toxicological studies to allow evaluation of a greater diversity of nanomaterials.

- Provide investigators with access to well-characterized nanomaterials to facilitate risk assessment research.

- Obtain information regarding the exposure to nanomaterials resulting from medical, occupational, environmental, and accidental release of nanomaterials for conducting nanotechnology risk assessment.

- Address the critical gap in knowledge related to toxicological assessment of nanomaterials so that nanotechnology can develop in a safe and environmentally friendly manner.

- Utilize interdisciplinary and leverage-based research approaches to determine the impact of nanotechnology on health and the environment.

- Determine how nanomaterials interact with their environment as a result of intentional or unintentional release, including their distribution, fate, and transformation processes as well as their biopersistence.

- Establish an accurate database to access monitoring information derived from nano-based environmental monitoring measurements, and develop new software to allow effective "mining" of this database to identify associations between public health effects and exposure to complex environmental pollutants so that linkages to sources can be determined.

Infrastructure Needs for R&D and Education

- Foster an educational system that links the biological sciences, physical sciences, engineering, and computer sciences at all levels, from K-12 through the faculty level.

- Develop undergraduate and graduate curricula to provide the knowledge base required for interdisciplinary research, including an introduction to the unique properties of nanostructured materials.

- Establish a summer research program for K-12 students and teachers that focuses on nanotechnology and environmental sciences.

- Create funding mechanisms to link K-12 students with industries, and support outreach programs to enable K-12 students to visit universities and other sites that are actively engaged in nanotechnology research.

- Develop a more complete set of instructional materials and hands-on demonstration tools that K-12 teachers could use to teach students about nanotechnology.

- Promote communication and networking, including scientific meetings, colloquiums, and workshops that bring together various disciplines using nanotechnology.

- Generate appropriate health, safety, and environmental guidelines based on sound science for handling and employing nanomaterials.

- Establish a public communications program that clearly presents the risks and benefits of nanotechnology in nonscientific, layman's terms.

- Create an interagency group to effectively support inter-institutional, interdisciplinary research, curricula design, and evaluation.

- Provide longer term support (4–5 years) for interdisciplinary projects, and increase support for tightly knit, small collaborative groups (3–4 Principal Investigators) in focused areas of research.

- Create a mechanism for providing mid-sized instrumentation grants ($100K–$1M) to small groups without requiring matching funds.

- Build an infrastructure for training scientists, engineers, and researchers from other subject areas to enhance their ability to work together in an interdisciplinary manner.

- Incorporate the concept of sustainability into current and future educational activities related to nanotechnology.

Introduction to Nanotechnology Grand Challenge in the Environment

Nanotechnology is the creation and utilization of materials, devices, and systems through the control of matter on the nanometer-length scale—at the level of atoms, molecules, and supramolecular structures. The essence of nanotechnology is the ability to work at these levels to generate larger structures with fundamentally new properties and molecular organization. These "nanostructures," made with building blocks understood from first principles, are the smallest human-made objects and exhibit novel physical, chemical, and biological properties and phenomena. Nanotechnology's goal is to exploit these properties and efficiently manufacture and employ the structures.

Nanotechnology has the potential to significantly impact environmental protection through understanding and control of emissions from a wide range of sources, development of new "green" technologies that minimize the production of undesirable byproducts, and remediation of existing waste sites and polluted water sources. Nanotechnology has the potential to remove the finest contaminants from water supplies and air as well as continuously measure and mitigate pollutants in the environment.

Nanotechnology will be a strategic branch of science and engineering for the next century and will fundamentally restructure many current technologies. Control of matter on the nanoscale already plays an important role in scientific disciplines as diverse as physics, chemistry, materials science, biology, medicine, engineering, and computer simulation. A number of environmental and energy technologies already have benefited substantially from nanotechnology in the areas of reduced waste and improved energy efficiency, environmentally benign composite structures, waste remediation, and energy conversion.

Complex physical processes involving nanoscale structures are essential to phenomena that govern the sequestration, release, mobility, and bioavailability of nutrients and contaminants in the natural environment. Processes at the interfaces between physical and biological systems have relevance to health and biocomplexity issues. Increased knowledge of the dynamics of processes specific to nanoscale structures in natural systems not only will improve understanding of transport and bioavailability, but also lead to the development of nanotechnologies useful in preventing or mitigating environmental harm.

This report, which is based on discussions and recommendations resulting from a workshop addressing the vision for nanotechnology R&D in the next decade, focuses on the following areas: (1) nanotechnology applications for measurement in the environment, (2) nanotechnology applications for sustainable materials and resources, (3) nanotechnology applications for sustainable processes, (4) nanotechnology implications in natural and global processes, (5) nanotechnology implications in health and the environment, and (6) infrastructure needs for R&D and education. Appendix A contains a list of participants and contributors; Appendix B includes reference materials; and Appendix C contains a report from the "Emerging Issues in Nanoparticle Aerosol Science and Technology (NAST) Workshop, held June 27–28 at the University of California, Los Angeles (UCLA). A glossary and index are found in Appendices C and D, respectively.

Chapter 1

Nanotechnology Applications for Measurement in the Environment

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1.1 Vision

The unique properties of nanoscale materials will enable the development of a new generation of environmental sensing systems. Examples include: (1) distributed arrays of smart sensor networks that could be used to quantify the spatial, chemical, and biological dynamics of an ecosystem in real time; (2) small, inexpensive, low-power, multifunctional sensor arrays, distributed in public places, homes, or on individuals, that could be used to warn of pollutants and other environmental hazards; and (3) improved characterization of the life cycle of natural and anthropogenic nanoparticles in the environment.

Measurement science and technology will enable the development of a comprehensive understanding of the interaction and fate of natural and anthropogenic nanoscale and nanostructured materials in the environment. Examples of uses of these measurements include identifying conditions for safe manufacturing, use, and disposal of nanotubes, nanoparticles, and other nanoscale materials; and understanding how the morphology, size, composition, surface reactivity, and transport of combustion-generated particles affect human health and global climate change.

1.2 Current Scientific and Technological Advancements

Recent findings indicate that nanoscale dimensions play a critical role in determining particle transport in human tissue, and therefore, are key to understanding health effects. Significant gains have been made by coupling studies of environmental interactions to nanostructured material research and device design. The last few years have witnessed dramatic improvements in the fabrication of nanoscale materials of interest for environmental analysis. The use of electric fields and flowing fluids to align carbon nanotubes during and/or after growth has made it possible to produce nanoscale sensors, which have been noncovalently linked to biomolecules and used as nanoscale sensor elements.[1-10]

Electrochemically fabricated metallic nanowires has been another major advance. By changing the composition of the electrolytic solution during deposition, it is possible to fabricate nanowires that have complex structures akin to bar codes.[11]

The size- and shape-dependent properties of nanostructured materials give rise to new electrical and optical properties that have been incorporated into new chemical and biological sensors. For example, individual nanoparticles fabricated from semiconducting materials have been used as new types of fluorescent tags that are far superior to molecular fluorophors.[12-16] Collective effects of nanostructured materials are being used as the basis for new types of optical and electrical sensing (e.g., the “artificial nose”). Direct electrical sensing of chemical and biological molecules using individual nanowires and nanotubes has been demonstrated.[17-21] New methods for controlling and guiding the growth and assembly of nanoscale materials and monolayer films also have been developed.

1.3 Goals for the Next 10–15 Years: Barriers and Solutions

The biotechnology revolution has led to rapid advances in the detection of biomolecules. Nanotechnology provides a way to strongly leverage these advances toward the development of environmental sensing systems that can operate on a continuous mode. The important role of microbes in controlling a large number of environmental processes has been known for many years; however, only recently has it been possible to use genomic analysis to understand biological diversity in environmental systems.[22] To fully understand the relationships of biological systems in the environment, it will be necessary to identify biological species through genetic analysis and assess what proteins are being expressed. This will require the ability to conduct biological analysis at extremely low concentrations, below the detection limits of existing biological sensors. Moreover, to fully understand environmental systems, it will be necessary to measure large numbers of chemical and biological species simultaneously and correlate such measurements over many length scales, from sub-micron to hundreds of kilometers.

The events surrounding the *Bacillus anthracis* (Anthrax) releases of 2001 highlighted the fact that good sensor technologies do not yet exist for rapid (ideally, real-time) analysis of microbes and their constituent biomolecules. Important underlying technical issues include: (1) existing biological sensor technologies are not sufficiently stable to allow usage on an *in situ*, continuous basis; (2) most chemical sensors use methods that are optimized for detection of single species (array methods are fairly well developed for DNA, but the use of RNA arrays and antibody arrays is only now becoming widespread and there is not a general array for detection of a wide variety of potential analytes); and (3)sensitivity remains an issue, because many molecules of interest are present at extremely low concentrations.

From the standpoint of environmental measurement, problems exist in measuring anthropogenic and natural nanoparticles that are present in the soil, air, and water. Particles in liquid phases present unique measurement challenges. Little is known about the diversity of chemical composition at the nanoparticle level and the transformations that occur.

Human health, epidemiological and toxicological studies of the impact of combustion-generated nanoscale particles in ambient air on human cardiovascular health are inconclusive when health effects (health endpoints) or physiological response are correlated with the bulk chemical composition of particles. Therefore, measurement techniques are needed that distinguish the chemical composition of particle surface layers from the bulk particle interior.

Most existing biological measurement systems are based on targeting a specific compound/ molecule. Because most microbial species have not been identified, there is a need for measurement and sensing systems that can assess biological diversity in the environment. Similar problems exist in detecting anthropogenic and natural nanoparticles which are present in soil, air, and water.

A major challenge in using nanotechnology for environmental analysis is the need for generic nanoscale assembly methods. The usefulness of rapid advances in the ability to fabricate and functionalize individual nanoparticles and nanotubes will be realized when these materials are integrated into more complex assemblies (i.e., dense arrays) and combined with macroscopic materials (i.e., silicon-based microelectronics) in a cost-effective manner. Nanoscale materials such as carbon nanotubes can be fabricated on silicon, but *in situ* chemical/biochemical modification of these structures in an array format has not yet been demonstrated.

It is unclear whether it will be possible to achieve the needed nanoscale fluid handling to selectively modify nanoscale materials in a high-density array format. An alternative approach would involve the modification of nanoscale materials in bulk, followed by directed assembly and integration of these materials into more complex assemblies. Directed assembly may be achieved using weak forces such as the viscosity of flowing fluids, electrostatic interactions, or magnetic interactions to direct functionalized nanoscale materials (e.g., biologically-modified nanotubes or nanowires) to specific locations as part of the assembly process. As the cost and resolution of electron beam lithography continue to improve for silicon-based submicroelectronic devices, opportunities will arise for nanosensor fabrication.

Other challenges exist in collecting spectroscopic data for analysis at smaller spatial scales in a timely manner. Existing methods for analyzing nanoparticles, for example, are prohibitively slow and generally nonquantitative. In addition, the analytical cost of reducing the interaction volume of the spectroscopic probe (e.g., electrons) to achieve smaller scale measurement is a decrease in the signal-to-noise ratio. Thus, advances in spectroscopic instrument technologies must allow rapid detection of adequate signal strength, while probing increasingly smaller volumes of the nanoparticulate sample.

Refinement of methods to measure density, shape, and surface area also are needed. Measurement tools for nanoparticles in liquids are even less developed than for those in the gas phase.

1.4 Opportunities

In biology, microsensors have provided a wealth of new information about biochemical and neurological processes, but typically only under a very strict set of experimental conditions. To understand the environment, it is necessary to dramatically expand the range of analytes detected and to characterize the inorganic, organic, and biochemical composition of the environment in a nonintrusive manner. Nanotechnology provides the opportunity to achieve this goal in at least two ways. First, nanoscale sensing elements can provide improved sensitivity compared to conventional sensors.[23] Second, nanotechnology makes it possible to create a massively parallel array of thousands or millions of high-sensitivity nanoscale sensing elements.

A massively parallel array of nanoscale sensor elements (such as chemically or biologically modified carbon nanotubes or quantum dot structures) could be used in two distinctly different modes. If each element were tailored to respond to a different stimulus (such as a specific chemical or biochemical analyte), then the array would provide simultaneous analysis of a large number of analytes. If each element were tailored in an identical manner, then a massively parallel array of sensor sites would provide the ability to probe physical and chemical processes with very high spatial resolution, essentially becoming a high-resolution imaging detector. The combination of high-density nanoscale sensor arrays could be combined with advanced nanofluidics and artificial intelligence to create a reconfigurable, adaptable array that could, for example, modify its specificity or function under changing conditions.

From the standpoint of chemical and biochemical detection, massively parallel sensor arrays would provide several important advances. For biological detection, the ability to measure relatively weak biomolecular interactions, such as protein-binding events and antibody-antigen interactions, is crucial. However, biochemical responses often are dictated not by individual molecules, but by combinations of molecules and combinations of processes. A high-density array could be functionalized with a large number of molecular recognition sites. By using smart data analysis software to look for patterns of response, such a sensor system would provide vastly improved selectivity, in a manner similar to that by which the human olfactory system can identify large numbers of odors using only a limited set of receptors.

A massively parallel sensor would also yield improvements in sensitivity. Using an array of nanoscale sensor elements separated by a distance greater than the diffusion length, it should be possible to achieve significantly improved sensitivity for electrochemical detection compared with today's planar sensor.[24-26]

Nanoscale systems also can be expected to achieve higher sensitivity due to intrinsic quantum effects. For example, there has been a great deal of attention paid to single-molecule or single-particle detection and single-electron transistors. In an analogous manner, a chemically-modified quantum dot or other nanoscale structure should be able to achieve single-molecule sensitivity. A single molecule interacting with the quantum dot, in turn, can relay the sensing signal in terms of an optical property or electrical conductivity.

As an imaging detector or sensor, a high-density array would provide greatly improved spatial resolution for specific physical or chemical/biochemical phenomena. An array of quantum dot structures could act as an array of optical detectors or even nanoscale optical sources, providing a way to characterize the optical properties on nanometer-length scales. An array of biosensing elements may be able to examine the spatial distribution of biological molecules within more complex, small structures (such as a cell or a microbial community). Imaging detectors may be particularly important for characterization of nanoparticles. Existing methods for characterizing particulates are slow and do not provide good statistical information about chemical composition and structure. It also should be possible to fabricate an array of field-emission electron sources and electron detectors that would provide a way to image and perform electron-based spectroscopies, such as energy-loss spectroscopy with nanometer-scale spatial resolution. This would greatly aid characterization of individual nanoparticles present in complex environmental systems.

New assembly methods would allow for the miniaturization of particle counters and particle composition analyzers, based on the use of field emitters for particle charging and separation as well as ultrasensitive single-charged particle detection. High field emitters could be used to generate fields sufficient to form microplasmas and, when coupled to arrays of quantum dot structures, could be used to detect by atomic emission from the nanoparticle. Miniaturization also would enable the deployment of personal monitors for epidemiologic studies.

Nanoinformatics

The use of massively parallel arrays brings with it a need for the development of new computational methods for understanding signal transduction in nanoscale systems and analyzing large amounts of data from nanoscale systems in real time. This may lead to a unique field of "nanoinformatics," analogous to the explosion of interest in bioinformatics. There are several aspects of nanoinformatics applicable to nanotechnology and the environment. New challenges in understanding signal transduction and data analysis in nanoscale arrays and networks, systems issues for deployment, communication networking, and software are areas of fundamental interest.

The fabrication of thousands or millions of "perfect" sensing elements will be extremely difficult or impossible. The need for perfection in the sensor "hardware" can be avoided by using advanced computer training and measurement methods. This approach essentially shifts the need for perfection from nanoscale hardware and places it on software. Such training is similar to a calibration process, but would be much more extensive and involve measuring sensor response to a wide range of stimuli, followed by mathematical analysis of the results to provide a well-defined stimulus-response function. By using redundant sensor elements and individualized training, the need for absolute perfection in each sensor array can be eliminated. Reducing the need for strict perfection of thousands or millions of sensing elements may be an important way to develop nanoscale arrays in a cost-effective manner.

The data content provided by these arrays could be overwhelming, and smart electronic processing and decisionmaking systems would need to be developed to convert these raw data into meaningful information. In the case of sensor arrays, methods such as principal component analysis, neural network analysis, or other linear and nonlinear methods would be used to characterize the response of multiple chemical or biological receptor elements and extract the identity and concentration of species present in the sample. Ideally, these computer methods could provide optimized information content (such as chemical composition, biological identity, or physical properties) on an as-needed basis to an individual user or as part of a real-time control system.

Hierarchical Assembly

The development of nanoscale sensor arrays ultimately requires the ability to fabricate, integrate, and interface them with the macroscopic world. Furthermore, this must be achieved in a cost-effective manner. Recent advances in the ability to prepare and chemically/biochemically modify nanoscale "components" need to be leveraged into a more general set of nanoscale assembly methods that would constitute a type of "nano-toolbox" for fabricating more complex structures. One of the fundamental problems in using nanoscale materials is that "bottom-up" fabrication processes, in which complex nanoscale assemblies are made in a linear, sequential manner, are extremely susceptible to failure because of the large number of steps involved. In contrast, by using a convergent, hierarchical assembly process in which prefabricated "nano-elements" are constructed (such as nanowires or nanotubes that are modified with specific chemical or biomolecular recognition elements) and then assembled, single points of failure are reduced or eliminated. This process distributes the complexity of fabrication among a larger number of elements that can be independently purified, verified, and then assembled in a small number of steps, thereby leading to more reliable methods of fabrication.

Recent experiments have shown that direct current and alternating current electric fields can be used to translate and align nanotubes and nanowires; magnetic fields can be used in a similar way to manipulate nanoscale materials such as nickel nanowires and quantum dots.[27,28] These results suggest that it should be possible to use electric and magnetic fields, together with fluid flow and other methods, to control the assembly of nanoscale objects into more complex two- and three-dimensional assemblies. Hierarchical assembly of nanoscale components with each other and with traditional materials is required to yield complete systems and leverage the unique properties of nanoscale materials and integrate them with macroscopic materials, such as silicon-based microelectronics and micro- or nanofluidic systems.

1.5 Scientific and Technological Infrastructure

Infrastructure needs include: (1) long-term (4-5 years) support for interdisciplinary projects; (2) increased support for tightly knit, small collaborative groups (3–4 Principal Investigators) in focused areas of research; and (3) a mechanism for providing mid-sized instrumentation grants ($100K–$1M) to small groups without requiring matching funds.

1.6 R&D Investment and Implementation Strategy

Research Needs

The research needs for developing high-density sensor arrays for *in situ*, real-time, multiple-analyte quantification in the environment are categorized as follows.

Development of High-Density Sensor Probes

High-density sensor probes require the development of complex nanoscale molecular architectures and an understanding of their responses to chemical/biomolecular stimuli. It also is necessary to develop an understanding of how to control, manipulate, and immobilize nanoscale materials to fabricate integrated sensor architectures. A greater understanding of how weak forces such as electrostatic forces, magnetic fields, hydrophobic-hydrophilic interactions, and hydrogen bonds affect and control the behavior of molecules and nanoscale systems is needed. It also is essential to understand the collective properties of nanoscale materials.

Research is needed to achieve optimal chemical and biological modifications on the sensor surface to permit specific and robust binding, and therefore, detection, for each analyte. Additionally, different sensing environments (e.g., air, water, and soil) can pose limitations on certain transduction mechanisms. To best suit different sensing environments, diverse transduction mechanisms such as electric, optic, magnetic, piezoelectric, magnetoresistive, and so on require exploration. Understanding how chemical and/or biomolecular interactions translate into optical, electrical, or other transduction signals is critical.

Integration With Silicon-Based Microelectronics

To achieve simultaneous detection of a large number of analytes, research on the integration of sensor probes with silicon-based microfluidics and microelectronic circuitry is needed. This will allow: (1) simultaneous data acquisition, (2) an easy computer interface for real-time analysis, and (3) reduction in the sensor system's size and increased potential for portable, hand-held devices.

Model Development, Analysis, and Validation

A thorough analysis must be performed to gain an understanding of the *in situ* detection kinetics of each individual analyte. Such information will help quantify the concentration of each analyte. In addition, it is necessary to develop models that will help characterize and predict the response of high-density, possibly nonlinear and potentially interacting sensor arrays in the presence of multiple analytes. The models must be incorporated in a communication network to allow crosstalks and feedbacks, and integrated with smart and interactive software for decision-making. Such models and software development will help optimize the specificity of the response produced by the analytes of interest. It also is critical to develop, test, and validate protocols for calibrating the response of measurement systems.

Research needs for a new generation of nanoparticle detectors include the development of: (1) low-cost miniaturized instruments that integrate physical and compositional characterization (such devices could be used to provide dosimetrics for personal and area monitoring for both epidemiological and environmental monitoring needs); (2) instruments for studying gas- and liquid-nanoparticle interactions (these studies are needed to unravel the complex interrelationships between nanoparticles, such as those generated by combustion sources and the natural environment); and (3) particle detectors and counters that improve the state-of-the-art in liquid samples to a level comparable with that for gas-dispersed nanoparticle detection.

1.7 Examples of Recent Achievements and Paradigm Shifts

Inspiration for this vision derives from recently acquired understanding of the properties of nanostructured materials which, in turn, is a consequence of advances in synthesis and characterization of nanostructures. Realization of the vision is dependent on the development of libraries of ultrasensitive and selective sensing components and advances in the fabrication of integrated parallel sensing and signal transduction devices. A sampling of breakthroughs that support the vision include demonstrations of: (1) molecular detection using biomolecule-functionalized metal and semiconducting nanoparticles or bar-coded metallic nanowires,[11,29] (2) pathogen detection using piezoelectric cantilevers,[30] (3) field- and flow-controlled assembly of aligned carbon nanotubes,[2-5] and (4) transport of electrical and optical signals through designed nanostructures.[31]

Breakthroughs that speak to the environmental impact of both natural and anthropogenic nanostructures include the recent demonstration that precise nanoscale dimensions play a critical role in determining particle transport in human tissue and, therefore, are key to understanding health effects. This breakthrough highlights the importance of coupling studies of environmental interactions to nanostructured material research and device design.

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Chapter 2

Nanotechnology Applications for Sustainable Materials and Resources

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2.1 Vision

A society that uses nanotechnology to transform the way it develops, uses, and dissipates materials and the flow, recovery, and recycling of valuable resources, especially in the use of energy, transportation of people and goods, availability of clean water, and supply of food. Materials and technology sustainability has become a topic of great interest.[1] Materials have been an integral part of addressing environmental quality over the past 30 years. Materials scientists have had a great impact on the improved quality of released effluent and exhaust plumes, the use of catalysts to avoid unwanted byproducts in chemical processes, and the treatment of waste. They also have led the way in moving from the use of solvents in industrial processes to the use of biodegradable materials and the generation of cleaner energy.

Designers of materials for such purposes, however, have not always considered the environmental impact as well as material functionality, and "the costs and benefits of synthesizing and processing".[1] For example, efforts at greening vehicles, such as battery-powered vehicles, fall short of impacting the environment in a positive way. The vehicles appear to be a cleaner choice when compared with gasoline-powered vehicles because there are no tailpipe emissions produced during operation. However, large quantities of toxic and hazardous materials are used to make batteries, and this must be considered in the assessment of environmental benefits of this technology.[2] Thus, applications must address societal needs with respect to sustainability over their entire lifecycle. To develop these applications, it will be necessary for nanoscientists to collaborate with scientists and engineers from other disciplines.

Applied research must be balanced with basic research. Basic research that will support the development of sustainability applications for nanotechnology include development of a knowledge base that relates structure and function at the nanoscale; design of new materials and architectures with tailored multifunctionality; methods for optimizing control of stability at all scales and conditions of use; engineering as well as synthesis, assembly, and processing at all scales; and creation of research tools that bridge the molecular scale and ordered bulk.

2.2 Current Scientific and Technological Advancements

This section explains research needs and directions to be taken that address future needs, with considerations for sustainable material design and resource use.

Energy and Transportation

In the near term, fossil fuels will be used as the main source of energy. Improvement in the performance of both gas and diesel engines is needed. To enable the production of more super ultra-low emission vehicles, higher quality fuels are needed. This will require advances in catalyst technology to: improve catalyst reactivity, selectivity, and yield; optimize and reduce active species loading levels; improve catalyst durability and stability under exposure to the operating environment; reduce reliance on precious metal-based and corrosive catalysts; and produce lower cost, less energy-intensive, and more environmentally friendly catalysts. In essence, catalytic processes are nanoscale because reactions take place on the surface.

To realize the above improvements, continued research and development are needed to advance understanding of molecular and particle behavior in catalytic reactions. Basic research to develop methods and approaches for optimizing control of stability at all scales and conditions of use will be critical to achieve these advances. Basic research in synthesis, assembly, and processing will be required to develop fabrication techniques for controlling surface area, cluster and particle structure, component dispersion, and other defining characteristics.[3,4] Advances in nanoscale science that enable sequestering of CO_2 and separations applications also will be beneficial.

Alternative energy transduction, storage, and transmission materials can be improved in the near term. Ultracapacitors and batteries will benefit from moving to the nanoscale. Breakthroughs in the performance of thermoelectrics have already occurred due to advancements at the nanoscale. Methods for assembling nanoparticles need to be explored in more depth, as does nanoscale wiring to move electrons when designing new energy-conversion devices. Photovoltaics can be greatly improved by implementing photonic crystals concepts, which improve light collection and emissivity. Quantum effects made possible by nanotechnology might lead to increases in efficiency. Bridging the molecular scale and ordered bulk will be particularly important for space-efficient energy storage.

Water and Agriculture

More effective approaches for treating and remediating water for human consumption and other uses are needed. Removing organics represents a significant challenge. Use of nanoparticles (e.g., modified TiO_2) as photo-oxidants is promising.[5] Nanotechnology also may play a role in the development of passive separation processes such as in mesoporous membranes, filters, and sorbents. Heavy metals could be applied to the use of derivatized surfaces to target specific contaminants. Reactive nanoparticles appear to be useful in remediating groundwater and, thus, also may prove useful in removing pesticides and herbicides in the environment.[6] Nanoparticles also may provide a more efficient and controlled delivery/release method for the application of pesticides and fertilizers. A knowledge base relating structure and function at the nanoscale will be useful for both environmental remediation and agricultural applications.

2.3 Goals for the Next 10–15 Years: Barriers and Solutions

Maintaining and improving soil, water, and air quality represent some of the most formidable challenges facing global society in the 21st century. The earth's population is expected to reach between 10 and 11 billion by 2050.[7] The materials and resources required to sustain such a population are staggering. Furthermore, increasing amounts of pollutants from a variety of sources enter the atmosphere and hydrosphere on a daily basis. For example, at the current rate of fuel consumption, global energy consumption is expected to double by 2050 to nearly 30 TW, and atmospheric levels of carbon dioxide are expected to double by the end of the 21st century.[8] It has been suggested that materials and resource use be reinvented. An interdisciplinary and life cycle design approach will be required to achieve the goals of developing and deploying sustainable materials. This section describes goals for materials and resource development, use, and life cycle in the context of the future needs of the human population.

Global Sustainable Energy System: Photovoltaics and Photo-Biofuel Cells

Although fossil fuels are expected to remain abundant for the next 10–20 years, R&D of alternate energy technologies that are "safe, secure, clean, and affordable" are extremely important in achieving sustainability.[7,8] All energy technologies require improved materials to achieve higher performance. In particular, an improved scientific understanding of nanoscale phenomena and control of material design at the atomic level could enable high-efficiency, low-cost materials for transducing, storing, and transporting energy. Researching, developing, and commercializing carbon-free primary power technologies capable of 10–30 TW by the mid 21st century could require efforts, perhaps international, pursued with the urgency of the Manhattan Project or the Apollo Space Program.[9]

A suggested goal is to acquire the total electricity needs of the planet (12 TW worldwide or 20 TW by 2020) through solar energy. The overall practical solar energy potential is 600 TW worldwide, with current photovoltaic technology able to provide a 10 percent conversion efficiency, or 60 TW. Although this is a sufficient supply, it is very costly ($0.35–1.50/kW) compared to energy resources such as fossil fuels, (approximately 8–10 times higher) and would require approximately a 0.1 percent area of the globe, or 5 percent area of the United States, to produce this amount of electricity.

A greater understanding of nanoscale photovoltaic processes could lead to significant improvements in this energy technology. Improvements are required not only to raise efficiency, but also to lower costs, integrate materials into new or existing infrastructure, and provide point-of-use supplies. Photo-biofuel cells present an alternative to current photovoltaic technology, although they are only in the stages of exploratory research at present. To fully realize the potential of this technology, improvements are needed in the R&D of biocatalysts or biomimetic catalysts (isolation, stability, turnover numbers) and biosystems (identified/designed, stability, efficiency). This area represents a potentially comprehensive and integrated use of nanotechnology (e.g., photoactive particles, membranes, bioactive surfaces, design of antenna systems, non-precious metal-based catalysts). Developing an extensive photovoltaic and photo-biofuel cell infrastructure will require design of new materials and architectures with tailored multifunctionality; methods for optimizing control of stability at all scales and conditions of use; and creation of research tools that bridge the molecular scale and ordered bulk.

Optimizing the Translocation of People and Goods: Green Vehicles and Smart Infrastructure

Many of the material and resource requirements are intimately linked with how people and goods are transported on roads, across rails, in the air, and on the water. Substantial amounts of materials and resources are used inefficiently for this burden. Thus, it is necessary to rethink the design of vehicles used to transport people and goods, as well as the very structure of how materials and resources are delivered to their point-of-use.

Lowering the costs of alternative fuel sources and energy storage is a significant challenge. Current technology provides approximately 100 kW/$1,000.[10] Improvements in power cost will come from a greening of the powertrain of vehicles (use of fuel cells, ultracapacitors, flywheels, batteries) and utilization of lightweight but strong and multifunctional materials for the physical structure. Nanocomposite materials that are high strength, low weight, and multifunctional (i.e., self-cleaning, self-healing) hold great potential for obtaining such properties.[10] Improved electrocatalysts and materials for hydrogen storage will enable the development of new green fuel sources.

The current transportation infrastructure is designed for the 19th century; a complete redesign for 21st century realities is needed. Developments in nanocomposite multi-functional materials (self-healing, smart, energy harvesting, photovoltaic, piezoelectrics, passive remediation of air and water) and corrosion-resistant materials will play a significant role in updating this infrastructure. The transportation system also might be revolutionized and made more sustainable by creating a virtual infrastructure that eliminates the need for unnecessary and inefficient travel and transportation of goods. Nanoelectronics (computation, memory, communication) and on-demand production and recycling of goods at their point-of-use could reduce the physical requirements for travel and transportation.

Global Sustainable Water—Optimize the Use and Quality of Water

New purification schemes, such as microfiltration, reverse osmosis, and photocatalysis, are needed to replace current techniques. New highly distributed and smart water monitoring schemes are needed, as are new membrane technologies (self-assembling pores, adaptable, smart, photoactive, reporter functionality) and new models for nanofiltration/nanoseparations. New composite materials, water purity sensors, e.g., for chemical speciation, and adaptive multi-functional materials will help to achieve this goal. Use of new water purity sensors will greatly enhance purification schemes. Current water systems suffer from the same problems as roadways and the overall transportation infrastructure. In the 21st century, point-of-use supply and closed-loop systems are required to address the problems associated with a water system that was designed to meet the needs of the 19th century.

Global Sustainable Agriculture*—Optimize the Production and Distribution of Food

Current technology requires use of fertilizers or crop rotation to provide nutrient fixation to agricultural crops.[11] Nutrient optimization is needed to avoid this excess; nanoparticles for direct nitrogen fixation might prove revolutionary, or there may be opportunities to engineer soil for fertilization improvement. Excessive use of pesticides, herbicides, and rodenticides is another area that may benefit greatly from R&D at the nanoscale. It will be a great challenge to eliminate or optimize delivery and use of these polluting materials for pest-management applications. Nanotechnology may add benefit to the development of photocatalysts to facilitate the breakdown of biocides and smart dust to identify and locate biocides. Development of a knowledge base that relates structure and function at the nanoscale and design of new materials and architectures with tailored multifunctionality will aid in the development of agricultural applications.

2.4 Scientific and Technological Infrastructure

Interdisciplinary Training

A key feature to achieving the goals outlined in this chapter will be the ability of scientists, engineers, and researchers from diverse subject areas to collaborate in an interdisciplinary manner. In general, research in engineering as well as synthesis, assembly, and processing will be required to scale-up production of the new materials. Collaboration with other fields will be necessary to develop specific applications. Solar energy/photovoltaic applications for example, will require that chemists work with materials scientists as well as architects and urban planners to optimize and integrate photovoltaic technology into existing and future physical infrastructure. Work on creating virtual transportation, however, will require a different set of collaborators, such as computer scientists and engineers, manufacturing engineers, and urban planners.

Life Cycle Design

Another essential aspect to achieving the goals for sustainable materials and resources is taking a life cycle design approach to R&D. Considering the photovoltaic example, durable functionality, recyclability, and use of benign materials in developing the products must be considered. In the area of nutrient optimization, green manufacturing and global nitrogen/phosphorous cycles need to be addressed.

2.5 R&D Investment and Implementation Strategies

Interdisciplinary funding strategies are needed to meet the goals and challenges outlined in this chapter. Changing current thinking about materials development and resource use will require a carefully thought out scientific research agenda. A knowledge base that relates structure and function at the nanoscale must be developed; new materials and architectures need to be designed with tailored multifunctionality; control of stability at all scales and conditions of use should be optimized; and engineering must be addressed along with synthesis, assembly, and processing at all scales. In addition, research tools that bridge the molecular scale and ordered bulk are needed.

* Note: there were no agriculture experts in the group.

2.6 Examples of Recent Achievements and Paradigm Shifts

Rechargeable Magnesium Alloy Batteries—Cheaper, Lighter, and Greener

A prototype rechargeable magnesium alloy battery generates 0.9–1.2 volts—about the same as a nickel-cadmium battery—and can be discharged and recharged many times without losing significant power capacity.[12,13] Researchers used an alloy of magnesium, AZ-31, which is 3 percent aluminum and 1 percent zinc.

Multifunctional Alloys

Most metals would be permanently deformed if stretched up to 2.5 times their original length; however, new alloys based on nanotechnology spring back again, and therefore, have been termed "super elastic." When pulled harder, they extend by an additional 20 percent before snapping.[14] This degree of elasticity is most unusual for a metal, and has been dubbed "superplasticity."

Nature-Inspired Smart Material

The Fuji Xerox team makes tiny, contractible pigment bags from a polymer known as NIPAM. Its long, chainlike molecules can be crosslinked to form a soft gel, the volume of which is controlled by temperature. At approximately 34°C, the polymer molecules suddenly contract, and the gel collapses to 10 percent or less of its original volume. Akashi and colleagues make particles consisting of NIPAM pigment bags that are only 20–200 thousandths of a millimeter across when swollen.[15] The researchers load these particles with large amounts of pigments such as carbon black (used in Indian ink) without significantly affecting their temperature-triggered shrinking. Therefore, it should be possible to construct smart windows that respond to all types of triggers.

Two additional advances that represent examples of potential paradigm shifts include a biofuel cell that runs on metabolic energy[16] and thin-film thermoelectric devices with high room temperature figures of merit.[17]

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Chapter 3

Nanotechnology Applications for Sustainable Processes

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3.1 Vision

Sustainable manufacturing processes based on the use of nanoscale science and nanotechnology—integrated processes and bottom-up assembly—that can serve human needs and are compatible with the surrounding ecosystems and human population. Nanotechnology has significant potential to impact conventional and future manufacturing processes. However, these processes may carry environmental and social impacts as well, so it is necessary to try to foresee and prevent negative impacts as new processes are developed.

3.2 Current Scientific and Technological Advancements

To accomplish the vision stated above, the current state of nanoscale processing technology must be examined. Current examples include commercial sunscreens, composed of ZnO or TiO_2 nanoparticles and the production of carbon nanotubes or diamondoids. Some of these products can be produced only in limited quantities, and consequently, the price is prohibitive for most practical applications at the present time. Another example is the production of electronic devices. Components can be on length scales from microscale to large nanoscale and are developed using top-down processing methods that require huge quantities of material and energy. As a result, large volumes of solid and liquid wastes are produced.

3.3 Goals for the Next 10–15 Years: Barriers and Solutions

Recent developments have suggested a new paradigm for manufacturing, which requires the following objectives: (1) eliminate material waste; (2) reduce resources used in manufacturing processes; (3) minimize energy use; and (4) assess the safety, environmental, and ethical aspects of nanoscale manufacturing.

3.4 Scientific and Technological Infrastructure

The specific goals outlined in this section require interdisciplinary research funding. The development of sustainable manufacturing processes will require a carefully thought out scientific research agenda. Characterization of nanomaterials at the nanoscale must be developed, and engineered solutions must be developed with consideration for sustainable production processes.

3.5 R&D Investment and Implementation Strategies

A number of specific strategies can be used to accomplish these objectives. One such strategy is optimizing the use of benign materials such as alternative or solvent-free processes, using the unique reactivity and properties of nanoscale materials, and using enzymes to develop benign material feedstocks and multifunctional, smart nanoscale catalysts. Others include: (1) efficient control of manufacturing processes with sensors and actuators, which may include defect minimization, fault tolerance, and self-healing; (2) controlled selectivity in manufacturing processes, including multifunctional catalysts and stability of catalysts, as well as sensors to monitor processes and increase their efficiency; and (3) integration of biological processing into nano-driven manufacturing, including high enantiomeric selectivity using biological molecules, rational modification of multifunctional materials, manufacture of self-healing nanostructures, and programmable "death." Maximizing recyclability, recovery, remanufacturing, and reuse of products; reducing the number of unit operations in manufacturing using combined catalysis and separations; and continually evolving practices and metrics that enable and define sustainability are additional strategies.

Challenges in Sustainable Manufacturing Processes

Between the current state of manufacturing processes and the vision described at the beginning of this chapter are a number of hurdles in the research of nanoscale manufacturing processes. One challenge is designing and manufacturing nanomaterials, including: (1) large-scale production of nanoscale building blocks (e.g., nanotubes, diamondoids, quantum dots); (2) design and production of complex, nanostructured materials (e.g., nanocomposites, multifunctional catalysts, electrolytes); and (3) the possible creation of a federally funded user facility in bottom-up processing for pilot-scale synthesis and production of nanomaterials.

Another challenge is manufacturing integrated nanodevices, such as: (1) sensors, actuators, and multifunctional devices (e.g., a catalytic reactor that also performs separations); (2) transformation of unit operations (e.g., building nanosize reactors, pumps, mixers, and separators) moving from micro- to nanofluidics and constructing "factories on particles"; and (3) self-assembly, bottom-up manufacturing, directed assembly, and use of both weak and covalent forces. In addition, the design of manufacturing processes based on nanotechnology is another hurdle. This includes just-in-time, just-in-place manufacturing (e.g., mobile and low power), rather than "here-and-now moving to there-and-then"; novel architectures (e.g., bio-inspired, three-dimensional); and solar-based manufacturing (e.g., hydrogen generation, artificial photosynthesis).

Developing theories, models, and experimental data on nanoscale materials and processes of are additional hurdles in the research of nanoscale manufacturing processes. These activities include: (1) thermo/kinetics/transport fundamental studies at the nanoscale level; (2) linking macro/micro/nano/atomic regimes using quantum, molecular, and continuum modeling; and (3) surface properties (intermolecular forces, surface area, surface charge, surface chemistry). Similarly, another hurdle is the development of safety and environmental metrics and ethical principles appropriate for nanotechnology, such as modifying existing indicators and metrics for use in nanoscale manufacturing (e.g., research decision tools, considering particle aspect ratio, surface area, and reactivity) and adapting current ethical principles from professional societies to the needs of nanotechnology (e.g., what determines responsible use of nanotechnology). Finally, it also will be challenging to incorporate the concept of sustainability into current and future educational activities related to nanotechnology.

3.6 Examples of Recent Achievements and Paradigm Shifts

Sunscreens composed of ZnO or TiO_2 nanoparticles are produced at a commercial level, as are nanostructured sorbents for environmental remediation purposes, and nanostructured polishing agents. If the challenge of designing and manufacturing nanomaterials is achieved, it will be possible to produce bulk quantities of other nanoparticles such as carbon nanotubes, diamondoids, and fullerenes. At present, electronics are produced using photolithography, a material- and energy-intensive process. However, bottom-up techniques that use self-assembly and directed assembly could produce molecular electronic devices that are smaller and use the quantum effects inherent in the nanoparticles.[1] Thus, the architectures would be as novel as the particle properties. DNA functionality could be used to drive assembly.

Current efforts in pharmaceutical delivery have included drug delivery and laboratory-on-a-chip techniques. One paradigm shift envisions a "factory on a particle," in which small-scale pharmaceutical production occurs inside the body.[2-4] The nanoscale factory that produces the drug could be implanted, and benign raw material could be injected. Sensors in the "factory" would determine when to turn it on and when to turn it off. Transportation, production, and legal costs could be greatly reduced. The factories would be distributed spatially, as each patient would have a personal factory.

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Chapter 4

Nanotechnology Implications in Natural and Global Processes

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4.1 Vision

The ability to understand and quantify nanoparticles in earth system processes in order to anticipate their impacts and thus, optimize and integrate environmental sustainability and nanotechnology. The intentional and unintentional release of nanoparticles and nanomaterials into the environment poses challenges and potential dangers. Nanoparticles and nanoscale processes impact such long-term phenomena as climate change, ore and petroleum deposition, paleomagnetism, and groundwater composition.[1] Environmental science and technology link the concentrations of both anthropogenic and natural constituents to their effects on the well-being of humans and other organisms. Quantifying these links is especially needed when assessing the effects of nanoparticles and the uses of nanotechnology. The concepts of nanoscale science and the tools of nanotechnology offer unique opportunities for understanding and monitoring these links. Environmental and biological sciences at all levels of organization must be closely integrated because human survival requires robust and diverse ecosystems.

4.2 Current Scientific and Technological Advancements

Advances to date have been identified from several different perspectives, such as technology for detection and characterization of nanoparticles, how molecular and nanoscale events trigger processes at all scales important to the environment, and discoveries of new and different properties inherent at the nanoscale. However, experts still do not know how to anticipate the fate of nanoparticles in most environmental systems (soils, groundwater, bed sediments, lakes, etc.).

Technology that led to the understanding of particles in the atmosphere (mobility measurements) has allowed size resolution of particles from a polydispersed system and quantification of particles within a size class, allowing for rapid determination of particle size distributions in real time.[2-9] Recent advances in the physical characterization of atmospheric nanoparticles now allow for the detection of these nascent particles when they are only hours old (corresponding to diameters of approximately 3 nm), and thus, correlate local meteorology and gas-phase atmospheric chemical composition to new particle production.[10] This capability has enabled direct observation of homogeneous nucleation events over boreal forests and tidal zones, in the free troposphere, and even in the polluted urban atmosphere, as well as the detection of nanoparticles in the on-highway emissions from diesel engines.[11] Such data have stimulated advances in modeling the dynamics of atmospheric nanoparticles. These physical characterization techniques already are undergoing rapid advances that are decreasing the detectable particle size, even to the molecular scale.

Thermodynamically stable crystal structures are different at the nanoscale than at macroscales. For example, transport of aluminum in aqueous solution occurs through a series of labile clusters that aggregate to form larger particles, eventually defining the reactivity of the bulk phase.[12-14] This phenomenon occurs in many environments, such as water treatment plants where aluminum sulfate is used in coagulation, a critical step for efficient removal of particles, pollutants, and pathogens affecting human health.

Understanding the distributions of chemical species in aquatic systems among dissolved, colloidal, and larger particle phases has been a major success in the field of geochemistry. An improved knowledge of nanoscale species has explained periodic failures of filtration-based water treatment. The discovery that small nanoparticles and their chemical burdens pass through the filters led to improved water treatment processes.[15] Further, recognition of colloidal phases enabled great improvements in knowledge of solid-solution partitioning.[16] Likewise, this improved understanding has allowed experts to anticipate how subsurface transport of contaminants (e.g., radionuclides) can be facilitated by suspended nanoparticles.[17-19]

Nanoscale signal processing controls the replenishment of some biological populations. As a result, researchers successfully have harnessed the signals that control reproduction and recruitment of a commercially exploited and critically depleted marine shellfish (abalone), providing the key to restoring abundances in the wild and launching an aquaculture industry.[20-24]

4.3 Goals for the Next 10–15 Years: Barriers and Solutions

Current Questions and Needs

Future advances as a result of changing technology will help to develop predictive models of the spatial and temporal distribution, transport, transformations of nanoparticles in the environment, and impacts on organisms. The ultimate goal of these models is to predict the effects of nanoparticles on earth system processes, local-to-global ecology, and human health. One key product will be predictions of the likely sources, types, and concentrations of nanoparticles released to the environment.

The interaction between nanotechnology and ecosystem biology is insufficiently developed. Biological research at all scales of organization is essential to appropriately address the environmental impact of nanoscale science and technology. Goals are to identify, quantify, and predict effects on individual, population, community, and ecosystem phenomena. Then, it will be possible to distinguish between adverse and beneficial perturbations on both short and long time scales.

Nonclassical behavior at the nanoscale affects the kinetics and thermodynamics of nucleation, growth, and dissolution in the environment. This effect must be quantified both theoretically and experimentally. Molecular-scale models of the structures, reactivity, and solubility of nanoparticles as dependent on composition, size, and external conditions are needed. In addition, theoretical and experimental methodologies for the real-time characterization of particles in natural waters should be developed.

Further development of experimental approaches for studies of hydrated nanoparticles is required. This includes measurement, with high resolution in space and time, of particle number, composition, and morphology as well as predictive models validated by such data. In addition, nanoparticle labels and detection schemes are needed. One possible application of this technology is pollution attribution, which can be achieved through the use of nanoparticles of signature chemical compositions incorporated into point and distributed emission sources. These markers also will be important in distinguishing anthropogenic from natural nanoparticles.

Although nanobiology currently emphasizes human health, the broader ecological aspects of nanoscale science and technology need to be developed. This could be accomplished by building a broader community of interdisciplinary scientists, with a particular focus on biologists and ecologists. Furthermore, a database of nanoparticle properties should be developed, and an accessible sample repository of model and standard nanoparticles should be created and maintained. Discussions involving the relevant stakeholders could contribute to the identification of a limited set of nanoparticles and nanomaterials in the near term. Over the long term, the database could be extended through a combination of targeted experiments, combinatorial studies, and model predictions.

Major industry sectors that produce large amounts of nanoparticles, such as carbon black and fumed silica, exist. An active start-up industry sector that manufactures novel nanoparticle products has developed over the last 10 years. The experience of the large-scale manufacturers should help guide the development of the start-up industry. It will be important to identify trends in the development of the start-up sector to forecast the effects of this new sector on the environment.

Long-Term Targets

Today, only a very small portion of the atmosphere and hydrosphere can be characterized. Currently available sensors are extremely limited in their coverage. If sensors and instrumentation are developed that are inexpensive, rugged, long-lived, real-time, autonomous, and deployable by buoys, subsurface objects, balloons, and remotely operated vehicles in the atmosphere, the state of the environment can be mapped to a degree not previously possible. Using data continuously obtained from deployed instrumentation, it is possible to go back and identify sources of unexpected appearances of deleterious materials in the environment; time and place emissions to minimize deleterious effects; understand the evolution of problems in time; and develop and validate models that will allow experts to predict, anticipate, and prevent future pollution.

A number of vital rates govern population dynamics in the ecosystem. Using knowledge of nanoscale signaling and nanotechnology to manage ecosystems will mitigate deleterious effects. One primary strategy could be to employ nanotechnology to regulate the vital rates of individuals, which control population growth, by harnessing key environmental signals that govern the rate-limiting process.

Biological systems are natural sources of nanoparticles, and there is an untapped potential to use natural biota for the sustainable production of tailored and technologically useful nanoparticles. In addition, there is a need to effectively involve stakeholders, especially the public, in the discussion of the impacts of nanotechnology on the environment.

4.4 Scientific and Technological Infrastructure

Long-term research support for interdisciplinary projects is critical. In addition, research on the development of novel manufacturing techniques on the nanoscale for sustainable processes is needed.

4.5 R&D Investment and Implementation Strategies

The following goals emerge from the challenges and opportunities described above: (1) understand nanoscale phenomena as they pertain to earth system processes on local, regional, and global scales over a range of time domains; (2) understand and quantify the inputs, cycling, and effects of nanoparticles in the environment to anticipate the impacts of future particle release; and (3) optimize and integrate environmental sustainability and nanotechnology.

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Chapter 5

Nanotechnology Implications in Health and the Environment

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5.1 Vision

In 30 years, nanotechnology will be pervasive and incorporated into all aspects of daily life. This emerging technology will develop responsibly with a full appreciation of its health and environmental impacts. Nanotechnology can provide novel ways to enhance human health as well as protect and clean the environment. Developing these applications, which range from sensors to catalysts, has been the objective of ongoing research efforts discussed elsewhere in this report. This chapter addresses the implications of nanotechnology on health and the environment. Currently, a limited number of reports exist on this critical topic, and its development will spawn an exciting new discipline at the intersection of nanochemistry, ecology, geology, and toxicology.

5.2 Current Scientific and Technological Advancements

Information describing the relative health and environmental risk assessment of nanotechnology and associated nanomaterials is severely lacking. Due to this knowledge gap, it is uncertain whether one can extrapolate nanomaterial health and environmental risk assessments from information derived from natural or pollution-derived nanoparticles. Only recently have studies assessed the relative toxicities of nanomaterials.[1] Comparative inherent pulmonary toxicological assessments of single-wall carbon nanotubes have been undertaken by two groups led by Dr. Chiu-wing Lam of Wyle Laboratories, Johnson Space Center, Houston, TX, and also by Dr. David Warheit, DuPont's Haskell Laboratory for Health and Environmental Sciences, Newark, DE.[2,3] Both studies reported similar pathological findings demonstrating the ability of single-wall carbon nanotubes to induce the formation of granulomas. An interesting finding from these studies was, in contrast to quartz particles, the formation of granulomas without evidence of ongoing pulmonary inflammation. However, artifacts due to administration of high doses of aggregated nanostructured materials have to be considered when interpreting results. These results further suggest that it may be difficult to extrapolate the toxicity of synthetically generated nanomaterial using the existing particle toxicology databases.

5.3 Goals for the Next 10–15 Years: Barriers and Solutions

Understanding the health and environmental impacts of nanomaterials will be essential given the ever-increasing applications of nanotechnology in society. Several research challenges need to be addressed for the applications of nanotechnology to proceed in a safe and "environmentally friendly" manner. There are significant research challenges to understanding the implications of nanotechnology on health and the environment, both because of its youth as well as its broad interdisciplinary content. The following research challenges represent significant issues that must be addressed for the implications of nanotechnology on health and the environment to be as beneficial as possible.

The diversity of nanomaterial and its derivatives represent a significant challenge for risk assessment research. The challenge associated with engaging in this research before a manufacturing base is mature is that no one nanomaterial system becomes standard in impact studies. This leads to a significant problem because nanomaterials can be organic and inorganic materials, in a variety of shapes, sizes, and formats. This is further complicated by the multitude of surface coatings available. A complete understanding of the environmental and health impacts for such a broad class of systems requires strategies for handling this intrinsic diversity. The following paragraphs describe specific research needs.

Nanomaterial Inventory

This broad class of materials cannot be studied unless it is first defined and inventoried. It is critical to categorize nanoparticles by types, volumes, and applications, and to provide/disseminate such classification schemes to the broader research community.

High Throughput/Multianalyte Toxicological Methodologies

High throughput screening and/or combinatorial approaches to toxicological studies would allow a greater diversity of nanomaterials to be evaluated.

Mechanism and Fundamental Science of Particle Toxicity

One of the most powerful ways to combat the problem of nanomaterial diversity is to focus initial research on basic scientific issues. For example, if general principles for governing how nanomaterials are transported into and out of cells can be developed, then these principles can be extended to all nanomaterial classes. Similarly, if accurate models for the environmental fate and transport of nanoscale materials are developed, then ecological distribution could be predicted from particle size information.

Well-Characterized Nanomaterials

To conduct risk assessment research, it will be necessary for investigators to have access to well-characterized nanomaterials.

Exposure Assessment of Nanomaterials

Nanotechnology will be pervasive and incorporated into all aspects of daily life. Therefore, information regarding the exposure to nanomaterials resulting from medical, occupational, environmental, and accidental release of nanomaterials is critically needed for nanotechnology risk assessment. Information with regard to the concentration of nanomaterials as well as what form(s) they may assume upon release into the environment is needed. Nanotechnology exposure assessment will provide critical information on the routes of exposure to nanomaterials.

Due to the size and physiochemical characteristics of nanomaterials, new monitoring methods and instrumentation will be needed to perform nanomaterial exposure assessments. Nanomaterial exposure assessments in the medical, occupational, and environmental areas using instrumentation that can accurately detect nanomaterials in each of these settings are needed.

Unpredictable Biological Properties of Nanomaterials

The paucity of toxicological assessment of nanomaterials is a critical gap in knowledge within nanotechnology that must be addressed for the field to develop in a safe and environmentally friendly manner. Toxicological studies conducted thus far indicate that nanomaterials may pose a unique toxicity that cannot be extrapolated from the existing particle toxicological databases.[4] The research portfolio for nanomaterial toxicological assessment should include relevant and scientifically appropriate acute and chronic toxicokinetic and pharmacokinetic studies. The nanomaterial toxicological assessment research portfolio also should include studies that determine the inherent and comparative toxicological assessment of nanomaterials that are derived naturally, environmentally, and chemically; that contribute to understanding the mechanisms of nanomaterial toxicity; and that identify susceptibility factors that may enhance nanomaterial toxicity. The ability to detect and monitor the fate of nanomaterials in biological systems may require the development of unique measurement instrumentation capabilities. Therefore, support for the detection of nanomaterials in biological systems should be part of the nanomaterial toxicological assessment research portfolio.

Research Needs in Uncertainty in the Biological Fate, Transport, Persistence, and Transformation of Nanomaterials

To assess the impact of a nanomaterial, it will be critically important to determine how nanomaterials interact with their environment as a result of intentional or unintentional release. Determining their distribution, fate, and transformation processes will be vital. It will be especially critical to know the biopersistence of nanomaterial, how much of it there is, where it is, and in what chemical form. Currently, very little is known about how nanoscale materials move in the environment. The following paragraphs describe specific research needs:

Methods and Devices for Sensing Nanoparticles

It is critical that new methods for detecting nanomaterials in biological and environmental systems be developed. Without these tools, this research is severely limited. Needs in this area are discussed in Chapter 1.

Extending Existing Models of Particle Transport to the Nanoscale

For physical transport, nanoparticle movement through soil, air, and water may be extrapolated from larger colloidal systems. Existing models for these processes (e.g., colloid-mediated transport) should be tested and modified to describe the behavior of nanoscale materials. Some needs in this area are described in Chapter 4.

Study and Quantification of Biotransformation Processes

Biological systems can have a powerful effect on the surface chemistry and state of particulate matter in the environment. Nanomaterials should be subjected to standard biotransformation tests using appropriate organisms to evaluate whether such processes are modified on the nanoscale; in particular, it will be important to evaluate if nanoparticle solubility and aggregation state are influenced by such processes.

Characterization of Bioaccumulation of Nanomaterials

Bioaccumulation is a major pathway for molecular contaminants to concentrate in higher organisms. Some nanomaterials by virtue of their amphiphilic surface character may be highly susceptible to this process. Bioaccumulation should be quantified for key nanomaterial systems, and this information should be incorporated into an understanding of their effective environmental exposure.

Characterization of Biodegradation Processes

Facile biodegradation provides a means for nanomaterials to disperse in the ecosystem. Because of their high surface areas and small sizes, nanomaterials may be susceptible to these effects. The degradation of nanomaterial, both by naturally occurring organisms as well as organisms designed specifically for remediation, should be evaluated.

Considerations for Health and Environmental Impacts

For many nanotechnologists, money and recognition are achieved through the development of new applications. In contrast, the health and environmental impact research of nanotechnology does not provide this type of caché. Success in impact research depends on: (1) targeted and sustained research funding for examining the health and environmental implications of nanotechnology; (2) communication and networking, including scientific meetings, colloquiums, and workshops that bring together various disciplines using nanotechnology; and (3) access to well-characterized nanomaterials for risk assessment.

For nanotechnology to develop in a rapid and responsible manner, it will be critical to generate the appropriate health, safety, and environmental guidelines based on sound science for handling and employing nanomaterials.

Application of Nanotechnology To Improve Health and the Environment

Advances in nano-based environmental monitoring will lead to real-time, rapid, multimedia measurements of thousands of pollutants. The ability to "mine" this immense database will provide epidemiologists with an unprecedented ability to associate adverse health effects associated with exposures to complex mixtures of pollutants. This application of nano-based monitoring can be broadened to include applications to monitor medical health conditions. Research needs include: (1) establishing an accurate database to access monitoring information derived from nano-based environmental monitoring measurements, and (2) developing new informatics statistical software to allow effective "mining" of this immense database to identify associations between public health effects and exposure to complex environmental pollutants to allow linkages to sources to be determined.

5.4 Scientific and Technological Infrastructure

Interdisciplinary and leveraged research approaches will be required to determine the impact of nanotechnology on health and the environment. With regard to research needs, a strong and highly interactive network model for funded programs would be most suited to address this challenge, rather than a central paradigm. This network would involve private, academic and government cooperation. To conduct risk assessment research, it will be necessary for investigators to have access to well-characterized nanomaterial. In addition, support for the detection of nanomaterials in biological systems should be part of the nanomaterial toxicological assessment research portfolio.

5.5 R&D Investment and Implementation Strategies

Near-term research challenges, as described in this chapter, include: (1) diversity of anthropogenic nanoparticles (high priority); (2) exposure assessment of nanomaterials, specifically, instrumentation and procedures to detect/monitor nanoparticles (high priority); (3) unpredictable biological properties of nanomaterials (high priority); (4) interdisciplinary and leverage-based research (medium priority); (5) uncertainty in the biological fate, transport, persistence, and transformation of nanomaterials (high priority); and (7) mobilization of the research community (high priority). There also are a number of long-term research challenges. These include: exposure assessment of nanomaterials; unpredictable biological properties of nanomaterials; unknown recyclability, reuse, and overall sustainability of nanomaterials; and application of nanotechnology to improve health and the environment.

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Chapter 6

Infrastructure Needs for R&D and Education

Educational Needs

There is a general need to foster an educational system that links the biological sciences, physical sciences, engineering, and computer sciences. This need exists at all levels, from K-12 through the faculty level, where fundamental barriers in terminology and approach can inhibit vital cross-disciplinary interaction. Undergraduate and graduate curricula are needed to provide students with the broad knowledge base required for interdisciplinary research, while including an introduction to the unique properties of nanostructured materials. The natural interest of young people in nanotechnology and environmental science should be cultivated and used as a motivation for basic science learning and the development of knowledge-based interaction with the world of technology. An opportunity also exists to incorporate the concept of sustainability into current and future educational activities related to nanotechnology.

Curricula that emphasize the unique properties of materials at nanometer-length scales also are needed. One recommendation is to develop a summer research program for K-12 students and teachers that focuses on nanotechnology and environmental sciences. Funding mechanisms to link K-12 students with industries should be developed, and support is needed to create outreach programs to enable K-12 students to visit universities and other sites that are actively engaged in nanotechnology research. In addition, support is needed for the development of a more complete set of instructional materials and hands-on demonstration tools that K-12 teachers could use to teach students about nanotechnology. This could be accomplished with a 1-day course in nanotechnology, involving in-house and outside experts. Local media could be invited to broaden the outreach effort beyond the participants.

Communication Efforts

There are needs to generate appropriate health, safety, and environmental guidelines based on sound science for handling and employing nanomaterials and creating an increased awareness of the importance of interactions with the media for scientists in nanotechnology through programs that assist or train scientists to interact with the news media. There also is a need to create an awareness of the importance of the news media in clearly presenting the risks and benefits of nanotechnology in layman terms.

Development of an Interagency Group To Foster Research, Curricula, and Evaluation

The enormous challenges presented by nanotechnology and its environmental implications for education at all levels as well as the imperative for rational decisionmaking in the face of these challenges, requires state-of-the-art education and research-funding management. A necessary ingredient is the creation of an interagency group that could effectively support interinstitutional, interdisciplinary research, curricula design, and evaluation. Such a group could develop, design, and advocate for the diverse set of programs essential for creation of a technologically and environmentally literate population and a highly functional nanotechnology workforce. Examples of activities that this group might oversee include: (1) a summer research program for K-12 students and teachers focusing on nanotechnology and environmental sciences; (2) a funding mechanism that would promote linkage between K-12 students and industry, academic organizations, and others where nanotechnology research is being pursued, including programs that would bring the students and K-12 teachers to the research sites; (3) the development of a more complete set of instructional materials and hands-on demonstration tools that K-12 teachers would be able to use to teach nanotechnology; and (4) a variety of 1- or 2-day programs for continuing teacher education that would involve government laboratory and industry experts as well as local media.

Infrastructure Support

Longer term support (4–5 years) is needed for interdisciplinary projects, as is increased support for tightly knit, small collaborative groups (3–4 investigators) in focused areas of research. Additionally, it is recommended that a mechanism be developed for providing mid-sized instrumentation grants ($100K–$1M) to small groups. A key component to any approach that strives to achieve the goals outlined in this report also will include building an infrastructure for training scientists, engineers, and researchers from other subject areas to enhance their ability to work together in an interdisciplinary manner. Another infrastructure need is incorporating the concept of sustainability into current and future educational activities related to nanotechnology.

Appendix A

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Appendix B

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Appendix C

Report of the Workshop on "Emerging Issues in Nanoparticle Aerosol Science and Technology (NAST)"

This Workshop was held on June 27–28, at UCLA, and was sponsored by the National Science Foundation and the Southern California Particle Center (EPA supported).

Chair: S.K. Friedlander, UCLA
Co-Chair: David Y. H. Pui, University of Minnesota

The field of aerosol science and technology covers the basic principles that underlie the formation, measurement and modeling of systems of small particles in gases. These systems play an important role in nature and industry. Many government agencies including EPA, NIOSH, DOE and NOAA have substantial aerosol research activities. EPA is responsible for the establishment of ambient air quality standards for particulate matter, NIOSH is concerned with workplace exposure to particulate matter, and the DOE has responsibility for nuclear reactor safety which includes emissions of radioactive particles in reactor accidents. Aerosol technology plays an important role in inhalation therapy and in counter-terrorism, fields likely to be of interest to NIH including NIEHS. Industry uses aerosol processes for the manufacture of powdered materials of many different kinds including reinforcing fillers, pigments and catalysts and in the manufacture of optical fibers. The Particle Technology Forum, sponsored by AIChE, includes industry participation and has an interest in aerosol technology. Finally, the American Association for Aerosol Research (AAAR), the principal professional society in the field, with a membership of about one thousand, sponsors regular research meetings in this field.

Aerosols of interest to government agencies and industry cover a wide range of particle sizes, shapes and chemical compositions. The Workshop focused on NAST, a new subdiscipline in which a basic understanding of the relevant science and technology is only now emerging. Nanoparticle aerosols refer to particles smaller than 100 nanometers (0.1 micrometers) which may be present as individual particles or as aggregates. Nanoparticles may have unusual mechanical, optical, biochemical and catalytic properties that make them of special interest. Novel experimental and theoretical methods are under development and/or needed to characterize their formation and behavior.

Advances in NAST have applications in many fields that include (but are not limited to) (1) characterization and control of ultrafine aerosols emitted by air pollution sources, (2) industrial production of nanoparticle reinforcing fillers such as carbon black and fumed silica and catalysts such as titania, (3) start-up companies that manufacture specialty nanoparticle products by aerosol processes, (4) atmospheric dynamics of fractal-like nanoparticle aerosols (e.g. diesel emissions), (5) nanoparticle emissions from aerosol control technologies including filters and electrostatic precipitators, (6) nanoparticle formation in the upper atmosphere by entry of bodies from space and by emissions from solid fuel rockets, (7) control of workplace exposure to ultrafine aerosols, (8) manufacture of optical fibers, (9) manufacture of composites composed of blends of nanoparticles and molecular polymers (e.g., rubber), (10) fabrication of nanoparticle coatings, (11) on-line measurement of nanoparticle chemical composition and (12) contamination control in the microelectronics industry as line features shrink.

These applications are undergoing rapid changes. To help develop a coordinated effort, about 40 participants from university research groups, government agencies and industry with backgrounds in nanoparticle aerosols were brought together at the Workshop. The goals were (1) to review the current status of the field and identify research needs and (2) to set up a group that can serve as a prototype to promote research and development in NAST. The Workshop structure was as follows: As a scientific discipline, NAST depends on: (1) Nanoparticle aerosol characterization methods (2) Basic principles of nanoparticle aerosol formation and (3) Computational simulation of nanoparticle aerosol behavior. Two major fields of application of these methods and principles include: (4) Aerosol reaction engineering and (5) Atmospheric nanoparticles (ultrafine aerosol). Thus, the Workshop was organized into five Panels that covered the basic areas and two major fields of application. The Panel reports constitute the main body of the Workshop document. They are preceded by an Executive Summary that includes all of the Panel recommendations and brief statements on their applications. Also included in the report are a Terminology section and an Epilogue that puts the results in perspective. The 119-page Workshop report can be accessed at the following Web site: http://dalton.chemeng.hosted.ats.ucla.edu/nanoaerosol_workshop/.

Appendix D

Glossary

Aerosol:
A cloud of solid or liquid particles in a gas.

Array:
An arrangement of sensing elements spaced to give desired characteristics/results.

Catalyst:
A chemical species or other structure that facilitates a chemical reaction without itself undergoing a permanent change.

Diamondoids:
Molecules with structures that resemble diamond in a broad sense, strong stiff structures containing dense, three-dimensional networks of covalent bonds, formed chiefly from first- and second-row atoms with a valence of three or more. Many of the most useful diamondoid structures will in fact be rich in tetrahedrally coordinated carbon.

Earth System Processes:
Interactions (cycles) among the atmosphere, hydrosphere, cryosphere, biosphere, and geosphere from a global to local point-of-view, and across the time scales (minutes to eons) in which these spheres interact.

Ecosystem:
The system of interactions between organisms and their environments. An ecosystem is a dynamic and interrelating complex of plant and animal communities and their associated nonliving environments.

Electron Beam Lithography:
Lithographic patterning using an electron beam, usually to induce a change in solubility in a polymer films. The resulting patterns can be subsequently transferred to other metallic, semiconductor, or insulating films.

Exposure Assessment:
The determination or estimation (qualitative or quantitative) of the magnitude, frequency, duration, route, and extent (number of people) of exposure to a chemical or microorganism.

Grand Challenges:
Topics that focus on nine specific R&D areas of the National Nanotechnology Initiative that are directly related to applications of nanotechnology and that have been identified as having the potential to realize significant economic, governmental, and societal impact.

Hierarchical Assembly:

A process in which multiple subunits are independently fabricated and assembled in later stages of manufacture into a final product. Similar to folding cells into tissues, tissues into organs, and organs into organisms.

Microelectronics:

The term that describes a group of 10 technologies that integrate multiple electronic devices into a small physical area, generally a silicon (or other) wafer. Microelectronics is an enabling technology.

Microfiltration:

Filtration is filtration down to colloidal and polymeric molecular size (0.01–20 µm). Ultrafiltration and hyperfiltration usually involve diffusion across a membrane but often are considered to be filtration down to molecular and ionic sizes.

Microfluidics:

The science of designing, manufacturing, and formulating devices and processes that deal with volumes of fluid on the order of nanoliters or picoliters. The devices themselves have dimensions ranging from millimeters down to micrometers.

Nanobiology:

A new field of study combining biology and physics that examines how nature works on the nanometer scale, particularly how transport takes place in biological systems. The interaction between the body and nanodevices are studied, for example, to develop processes for the body to regenerate bone, skin, and other damaged tissues.

Nanodevices:

Functional nanoscale components.

Nanomaterials:

Materials with a basic nanometer-sized structure, usually less than 100 nm.

Nanoparticles:

Particles with diameters in the nanometer range consisting of between a few hundred to hundreds of atoms (greater than 100 nm).

Nanotechnology:

See the National Nanotechnology Initiative Web Site, at http://www.nano.gov.

Nanotube:

Most commonly, carbon nanotubes, in which a graphitic sheet is curled up into a seamless cylinder; can be multi- or single-walled.

Nanowire:

A cyclindrical material with a large aspect ratio and a diameter of 1,000 nm. Nanowires can be filled (nanorods) or hollow (nanotubes) and can be made from conducting or semiconducting materials. The term often is used to refer to nonconducting materials of this same shape, so that the term "conducting nanowires" must be used to clarify whether the term implies that the objects are conductive or not.

Photo-Biofuel Cells:

Renewable energy sources from living things or from the sun that convert optical energy into electrical energy using biomolecular reactions.

Photocatalysis:

A substance that is able to produce, by absorption of light quanta, chemical transformations of the reaction participants.

Photolithography:

Pattern definition method common in semiconductor manufacturing that uses ultraviolet (UV) radiation to expose the resist in printed circuit boards.

Photovoltaics:

Solar cells that absorb sunlight and convert it directly into electricity.

Piezoelectric Cantilever:

A device that integrates sensing elements that utilize the piezoelectric effect, where a voltage is created between surfaces of a solid dielectric when mechanical stress is applied.

Quantum Dots:

Also called nanocrystals, they are tiny clumps of semiconductor material, amounting to a few hundreds or thousands of atoms each. In bulk, these materials do not fluoresce, but in the form of these tiny particles—each only a few billionths of a meter, or nanometers, in diameter—they glow brightly when illuminated by a light source. Depending on the size and composition of each particle, they can fluoresce in a variety of colors.

Quantum Effects:

Changes in the interactions of atoms or molecules due to wave/particle duality of quantum mechanics rather than classical mechanics laws. These interactions occur for nanometer-scale materials.

Self-Assembly:

The ability of objects to assemble themselves into an orderly structure. Routinely seen in living cells, this is a property that nanotechnology may extend to inanimate matter.

Signal Transduction:

Conversion of information from one form to another. For example, the translation of information about the presence of a biological molecule into an electrical signal whose magnitude, frequency, or other property depends on the presence/absence of a biological molecule.

Smart Infrastructure:

Systems of public works, such as telecommunication and mass transportation, using information technology as a catalyst for transforming life and work to meet the challenges of the new millennium.

Sustainability:

Of, or relating to, a method for using or harvesting a resource so as to not deplete it or permanently damage it. The implication is that the resource will be available to future generations.

Thermoelectrics:

Electrical phenomena occurring in conjunction with a flow of heat.

Appendix E

Index