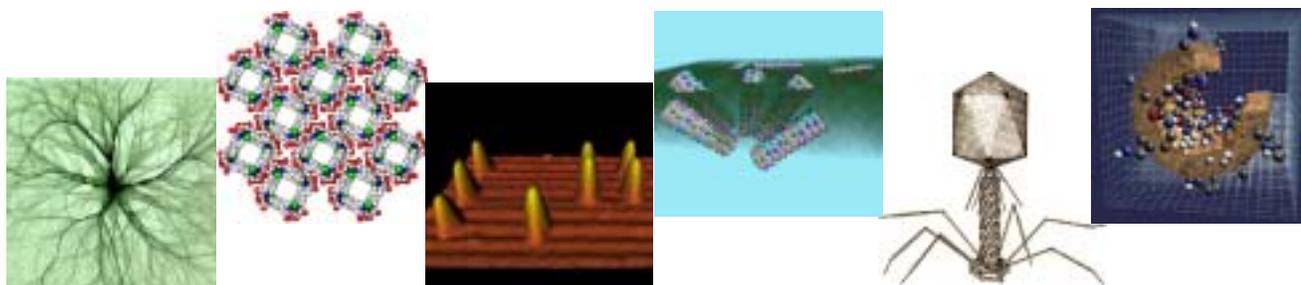


National Nanotechnology Initiative

THE INITIATIVE AND ITS IMPLEMENTATION PLAN



Detailed Technical Report Associated with the
Supplemental Report to the President's FY 2003 Budget

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

June 2002

About the National Science and Technology Council

The National Science and Technology Council (NSTC) was established by Executive Order on November 23, 1993. This cabinet-level council is the principal means for the President to coordinate science, space, and technology policies across the Federal Government. NSTC acts as a virtual agency for science and technology to coordinate the diverse parts of the Federal research and development enterprise.

An important objective of the NSTC is the establishment of clear national goals for Federal science and technology investments in areas ranging from information technologies and health research, to improving transportation systems and strengthening fundamental research. The Council prepares research and development strategies that are coordinated across Federal agencies to form a comprehensive investment package that is aimed at accomplishing multiple national goals.

Please call the NSTC Executive Secretariat at 202-456-6101 to obtain additional information regarding the NSTC, or see http://www.ostp.gov/NSTC/html/NSTC_Home.html.

About the Office of Science and Technology Policy

The Office of Science and Technology Policy (OSTP) was established by the National Science and Technology Policy, Organization and Priorities Act of 1976. OSTP's responsibilities include advising the President in policy formulation and budget development on all questions in which S&T are important elements; articulating the President's S&T policies and programs; and fostering strong partnerships among Federal, state and local governments, and the scientific communities in industry and academe. The Director of OSTP also serves as Assistant to the President for Science and Technology and manages the NSTC for the President.

Call 202-456-7116 to obtain additional information regarding the OSTP, or visit the OSTP web site at: <http://www.ostp.gov/>.

About this document

This supplemental document summarizes the National Nanotechnology Initiative contributions of the participating departments and independent agencies in the President's FY 2003 Budget Request submitted to Congress on February 4, 2002.

About the cover: The cover contains a collection of images that represent nanotechnology research and development activities currently underway among the Federal agencies participating in the NNI. From left to right: (1) Theoretical flow of electrons in a two dimensional electron gas away from a quantum hole electron source at the center (Harvard University); (2) Preprogrammed self-assembly of hollow square or rectangle shaped nanoscale building blocks, followed by condensation of the building blocks into arrays of nanoscale channels (Northwestern University); (3) A pattern of 15 nm gold nanoparticles positioned on a grid with a 100 nm pitch using a scanning probe microscope as a robot (University of Southern California); (4) Polypeptide nanotubes forming a channel through a bacterial cell membrane (The Scripps Research Institute); (5) The structure of phage T4 whose tail fibers of about 3 nanometers in diameters have been engineered from polymers (Tufts University); (6) Simulated biological ion channels — the atom structure (spheres) of an ion channel is represented together with a computational grid (University of Illinois at Urbana).

**NATIONAL
NANOTECHNOLOGY
INITIATIVE:**
The Initiative and Its Implementation Plan

*Detailed Technical Report Associated with the
Supplemental Report to the President's FY 2003 Budget*

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

June 2002
Washington, D.C.

Report prepared by
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL
COMMITTEE ON TECHNOLOGY
SUBCOMMITTEE ON NANOSCALE SCIENCE, ENGINEERING AND
TECHNOLOGY (NSET)

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CONTENTS

EXECUTIVE SUMMARY	5
NATIONAL NANOTECHNOLOGY INITIATIVE	11
1. Definition of Nanotechnology	11
2. Initiative Overview	11
3. A Revolution in the Making: Driving Forces	13
4. Nanotechnology's Impact	13
5. Investment Opportunities.....	16
6. The First Year of NNI (Fiscal Year 2001).....	16
7. Proposed Federal Contribution to the National Nanotechnology Initiative	
A. Fiscal Year 2003	46
Government's role in nanoscience and technology	
Nanotechnology R&D require long-term investment	
Budget summaries for participating departments and agencies	
Funding themes and modes of research proposed in FY 2003	
Priority research areas for increases in nanotechnology funding in FY 2003	
Individual agencies' activities in the initiative in FY 2003	
Collaborative activities in the FY 2003 National Nanotechnology Initiative	
Infrastructure needs for nanotechnology	
B. Outlook for the Future.....	51
IMPLEMENTATION PLAN	54
8. Management Plan.....	54
NNI interagency management objectives	
NSET Subcommittee	
National Nanotechnology Coordination Office	
Establish Grand Challenge and Cross-Cut Champions	
Planning (Roadmaps) for R&D Areas	
Outside Review	
9. Fundamental Research.....	58
10. New Grand Challenges in Fiscal Year 2003	59
A. Manufacturing at the Nanoscale	
B. Nanoscale Instrumentation and Metrology	
C. Chemical, Biological, Radiological and Explosive Detection and Protection (Homeland Defense)	
11. Centers and Networks of Excellence	74
12. Research Infrastructure	74
Metrology (measurement technology)	
Instrumentation	
Modeling and Simulation Infrastructure	
User Facilities	

13.	Societal Implications of Nanotechnology and Workforce Education and Training	76
14.	Transition of Fundamental Discoveries into Innovative Technology.....	79

APPENDICES

A.	National Nanotechnology Initiative Publications	88
B.	Examples of Scientific Achievements in FY 2001	89
	B.1. Nature’s Tools to Assemble Materials with Atomic Precision	89
	B.2. Building DNA Nanomechanical Devices.....	90
	B.3. Simulation of Biological Ion Channels in Human Body.....	92
	B.4. Molecular Circuitry Heralded as “Breakthrough of the Year”.....	93
	B.5. Micro Lens for Nano Research	94
	B.6. Development of the Biological Force Microscope in Geochemistry	95
	B.7. Electron Picometer Ruler to Measure Atomic Displacements in Crystals.....	96
	B.8. Carbon Nanotube Field-Effect Inverters	97
	B.9. Peptide Nanotubes as Antibacterial Drugs.....	98
	B.10. Fluorescent Imaging with Quantum Dots	100
	B.11. Nanopores Distinguish Subtle Differences in DNA Sequence	102
	B.12. Ultrahigh-Density, Radiation-Hard Nonvolatile Memory Based on Silicon Nanocrystals.....	104
	B.13. Explosive Detection by Nano-Thermo-Mechanical Signatures.....	105
	B.14. Nanoparticles for Sensitive, Selective Detection of Chemical, Biological, Radiological, and Explosives (CBRE) Agents	106
	B.15. Nanoparticles for Chemical and Biological Agent Decontamination.....	107
C.	Agencies’ Contributions to FY 2003 NNI Implementation Plan	110
	Department of Defense	111
	Department of Energy.....	114
	Department of Justice	119
	Department of Transportation.....	121
	Environmental Protection Agency.....	124
	National Aeronautics and Space Administration.....	125
	National Institutes of Health.....	132
	National Institute of Standards and Technology.....	136
	National Science Foundation	138
	U.S. Department of Agriculture.....	143
	Agencies’ Contributions to FY 2001, 2002 and 2003 Budgets	149
D.	NNCO Budget Proposal for FY 2003	151

EXECUTIVE SUMMARY

Overview

As part of the fiscal year 2003 Federal budget, the Nanoscale Science, Engineering and Technology (NSET) Subcommittee of the National Science and Technology Council recommends a Federal Government investment of \$710 million for continued funding of nanotechnology research and development through the **NNI (National Nanotechnology Initiative)**. This level of funding increases the current investment by approximately 17%.

The National Science and Technology Council has made the National Nanotechnology Initiative (NNI) a top science and technology priority. The emerging fields of nanoscience and nanoengineering – the ability to fabricate at the molecular level and to assemble large structures/systems with fundamentally new properties – are leading to unprecedented understanding and control over matter at the nanoscale. The nanoscale is not just another step towards miniaturization. The physical, electrical and optical properties of materials with structural features in the range of 1 to 100 nanometers exhibit important differences that are not explained by current theories. Developments in these emerging fields are likely to change fundamentally the existing technology base as well as generating new technologies with a broad range of applications. The initiative will support long-term nanoscale research and development leading to potential breakthroughs in areas as diverse as materials and manufacturing, nanoelectronics, medicine and healthcare, environment, energy, chemicals, biotechnology, agriculture, information technology, transportation, and national security.

The initiative supports a broad range of scientific disciplines including physics, chemistry, biology, materials science, and engineering. More importantly, the NNI creates new opportunities for interdisciplinary research that bridges naturally the physical and life sciences. Agencies participating in the NNI along with their respective funding levels are outlined in Table I. This table also compares the proposed FY03 funding to that in FY02 and tabulates the percentage increase for each participating agency. Roughly 65% of the funding proposed under the NNI will support university-based research and will simultaneously meet the growing demand for workers with nanoscale science and engineering skills.

Table I: Agency Participation and Level of Funding in the NNI

	FY 2002 (\$M)	Proposed Increase (\$M)	FY 2003 (\$M)	Percent Increase
Department of Defense	180	21	201	12%
Department of Energy	91.1	48.2	139.3	53%
Department of Justice	1.4	0	1.4	0
Department of Transportation	2.0	0	2.0	0
Environmental Protection Agency	5	0	5	0
NASA	46	5	51	11%
National Institutes of Health	40.8	2.4	43.2	6%
NIST	37.6	6.2	43.8	16%
National Science Foundation	199	22	221	11%
Department of Agriculture	1.5	1	2.5	67%
TOTAL	604.4	105.8	710.2	17%

Program Management

Funding of the R&D priorities are administered through the participating agencies as a function of their respective missions. A coherent approach has been developed for funding the critical areas outlined above with the express purpose of maximizing the productivity and utility of the Federal Government's investment in nanotechnology. The vision, strategy, agency participation, and agency partnerships for the five priorities are described fully in later sections of this report. A brief overview of the program management is outlined below.

The NNI is managed within the framework of the National Science and Technology Council (NSTC) Committee on Technology (CT). The Committee, composed of senior-level representatives from the Federal Government's research and development departments and agencies, provides policy leadership and budget guidance for this and other multiagency technology programs.

The CT Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) coordinates the Federal Government's multiagency nanoscale R&D programs, including the NNI. The NSET Subcommittee coordinates planning, budgeting, implementation, and reviews to ensure a successful initiative. The Subcommittee is composed of representatives from participating agencies and White House officials. Subcommittee representatives from each agency manage nanotechnology research and/or the nanotechnology infrastructure within their agency. NSET members consist of representatives from DOD, DOE, Department of Justice (DOJ), Treasury Department (DTreas), Department of Transportation (DOT), Environmental Protection Agency (EPA), NASA, NIH, NIST, NSF, USDA, Department of State, and two White House offices – Office of Management and Budget (OMB) and Office of Science and Technology Policy (OSTP).

Under the NNI, each agency invests in those R&D projects that support its own mission as well as the overarching NNI goals. While each agency consults with the NSET Subcommittee, the agency retains control over how resources are allocated against its proposed NNI plan. Each agency then uses their own methods for inviting and evaluating proposals and each agency evaluates its NNI research activities according to its own Government Performance Review Act (GPRA) policies and procedures.

The National Nanotechnology Coordination Office (NNCO) serves as the secretariat to the NSET Subcommittee, providing day-to-day technical and administrative support. The NNCO supports the NSET Subcommittee in the preparation of multiagency planning, budget, and assessment documents. The NNCO serves as the point of contact on Federal nanotechnology activities for government organizations, academia, industry, professional societies, foreign organizations, and others to exchange technical and programmatic information. In addition, the NNCO develops and makes available printed and other material as directed by the NSET Subcommittee, and maintains the NNI Web site. The NNCO Director is an NSTC agency representative appointed by the Associate Director for Technology at the White House Office of Science and Technology Policy, in consultation with the Chair of the NSET Subcommittee and Executive Committee of the Committee on Technology.

The NNI Investment Strategy

The President's Committee of Advisors on Science and Technology (PCAST) strongly endorsed the establishment of the NNI. The PCAST charged the NNI with providing "an excellent multi-agency framework to ensure U.S. leadership in this emerging field that will be essential for economic and national security leadership in the first half of the next century."

The NNI invests in fundamental research to further our understanding of nanoscale phenomena. At the same time, to accelerate the transition of science discovery into innovative technology, the NNI incorporates industrial participation and technology transfer through active participation in SBIR/STTR programs and partnerships with University/National laboratory research programs. The initiative builds upon previous and current nanotechnology programs and is balanced across five generic activities. These activities include the following:

- **Investment in fundamental nanoscience and engineering research** is essential to establishing a fundamental knowledge base of nanoscale phenomena. This activity catalyzes the innovation of new tools/methods to control and manipulate matter at the nanoscale. And provides sustained support to individual investigators and small research groups conducting fundamental research. It promotes university-industry-National laboratory partnerships, and fosters interagency collaborations.
- **Grand challenges** have been identified where the opportunities for the transition of science discovery into innovative technology will be likely and highly valuable. While the NNI emphasis is fundamental science and engineering research, over time it is expected that grand challenge investments will move toward a greater fraction of funding in applied research and exploratory development.
- The establishment of **centers and networks of excellence** provides important user-friendly resources to individuals and institutions that would, otherwise, be unable to participate in nanoscale research. These nanotechnology research centers play an important role in refining and standardizing tools and methods for nanofabrication and measurement. Furthermore, the teams built in the cooperative environment of these centers promote new partnerships and interdisciplinary interactions.
- Building a **research infrastructure** includes funding for metrology, instrumentation, modeling and simulation, and centralized user facilities. The goal is to develop a flexible and enabling infrastructure in support of both fundamental research and of U.S. industry's ability to commercialize the new technologies that arise from this initiative.
- Funding of the **ethical, legal, and societal implications of nanotechnology** is coupled to ongoing efforts to educate and train a new workforce skilled in nanotechnology. This effort is intended to break old education and manufacturing paradigms and introduce new methods that include lifecycle costs and the societal implications of nanotechnology.

Programmatic Structure

At its inception, the National Nanotechnology Initiative established nine “**grand challenges**” to provide a coherent framework to advance the new field of nanotechnology. These grand challenges were as follows:

- Nanostructured Materials by Design
- Nano-Electronics, Optoelectronics and Magnetics
- Advanced Healthcare, Therapeutics and Diagnostics
- Nanoscale Processes for Improving the Environment
- Efficient Energy Conversion and Storage
- Microcraft and Robotics
- Bio-nanosensors
- Applications in Economical and Safe Transportation
- National Security

As shown in this report, significant progress has been made toward meeting many of these challenges (see Chapter 6).

Though the original grand challenges were established as a framework for the NNI program, it is understood that yearly assessments of the program should lead to changes that better address the emerging opportunities and national needs. In response to a survey of NNI participants over the past year, three new operative and/or refocused grand challenges for FY03 are (see Chapter 10):

- Nanotechnology for bio-chem-radiological-explosive: detection and protection (expanded and refocused Bio-Nanosensors)
- Nanoscale instrumentation and metrology
- Manufacturing at the nanoscale

Because they relied so heavily on many of the other grand challenge topics, two of the previous topics – national security, and economical and safe transportation – have been re-designated as special cross-cutting national needs. The total grand challenge number remains at nine.

Transition of Science Discovery into Innovative Technology

While the NNI is only one year old, and has fundamental research as its primary focus, its ancestral programs have already made enormous impact in commercial markets. High electron mobility transistors, vertical surface emitting lasers, and giant magnetoresistance read heads are examples of one-dimensional nanotechnology providing evidence that buttresses the expectation for similar results from the NNI investment. Nevertheless, it is important for the NNI to proactively work toward technology transitions. It must address two questions: what actions are likely to accelerate the rate of transition, and what metrics can be used to measure progress toward the transition goals? The NNI is addressing this transition challenge on several fronts (see Chapter 14) – grand challenge investment strategies to ensure a range of technology options

buttressed by scientific understanding, infrastructure to provide capability for nanoscience measurement / manipulation / metrology, SBIR/STTR programs to foster innovation in companies, outreach efforts to encourage business involvement, and education/training to develop a skilled industrial/technical workforce.

Program Assessment

The PCAST recommended in its letter to the President that a non-government advisory committee review the NNI to assess progress towards NNI's goals. An assessment report is then provided to the Committee on Technology. This year's report has been developed by a National Research Council committee and will be released in June 2002.

Outcomes in Year One

The first year of the NNI witnessed many important contributions to nanoscale science and engineering. A representative listing, all of which are published in peer reviewed archival journals, is contained in Table 6.2. A sampling of significant contributions over the past year include (details available in Appendix B):

- The biological assembly of nanostructures
- Using DNA molecules to construct nanomechanical devices
- The development of molecular nanocircuits
- Invention of a MicroLens for nano research
- Development of the first biological force microscope for geochemistry
- Carbon nanotube field effect inverters
- Fluorescent visualization with quantum dots
- Sequencing DNA with nanoporous membranes
- Development of nonvolatile memory using silicon nanocrystals
- Explosive detection by nano-thermo-mechanical signatures
- Nanoparticles for improved homeland defense

These outcomes are but a small fraction of the scientific and engineering contributions over the past year. It is clear that the field is progressing rapidly and is poised to make important scientific and technological contributions.

Objectives of the NNI

Table II contains a list of specific objectives of the NNI program along with a realization time frame. These objectives were formulated in consultation with leading researchers participating in the NNI program and are expected to have a significant impact on U.S. science and technology. The programs to achieve these objectives are delineated in Chapter 7 and Appendix C.

Table II: Objectives of the NNI

Objectives	Target Date
Fundamental research awarded through competitive solicitations and regular program reviews	FY 2003 -
Establish five new user centers with full range of nanoscale measurement and fabrication facilities	FY 2003 -
Concurrent research on nanoscale metrology and manufacturing to enable rapid technology transfer and industrialization	FY 2003 -
Develop new standard reference materials for electronic applications	FY 2003 -
Establish bio-mimetic paradigms for bio-nano-devices	FY 2003 -
Leverage NNI funds by at least 25% by working with states, universities and private sector	FY 2003 -
Functionalized carbon nanotubes for targeted disease therapy	FY 2004 -
Develop standards for nanocharacterization, nanomanipulation and nanodevices	FY 2004 -
Functionalized nanoparticles for biomedical imaging	FY 2004 -
Build a research infrastructure at 50% of the nations academic research institutions	FY 2005 -
Develop nanoscience and engineering curriculum in at least 25% of research universities	FY 2005 -
Develop 3-D modeling of nanostructures that allows practical system and architecture design	FY 2005 -
Content standards for nanotechnology education for K-12	FY 2005 -
Nanoelectronics: first terabit per square inch memory chip demonstrated in the laboratory	FY 2006 -
Establish best practice manufacturing methods at the nanoscale	FY 2006 -
Reliable devices for monitoring environmental contaminants in air, water, soils	FY 2006 -
The incorporation of conductive organic molecules into electronic devices.	After 2007
Photovoltaic proteins in plants for solar energy conversion	After 2007
Introduce revolutionary technology options to enable meeting the International Technology Roadmap for Semiconductors (ITRS) goals	After 2007

NATIONAL NANOTECHNOLOGY INITIATIVE – LEADING TO THE NEXT INDUSTRIAL REVOLUTION

1. Definition of Nanotechnology

The essence of nanotechnology is the ability to work at the molecular level, atom by atom, to create large structures with fundamentally new molecular organization. Compared to the behavior of isolated molecules of about 1 nm (10^{-9} m) or of bulk materials, behavior of structural features in the range of about 10^{-9} to 10^{-7} m (1 to 100 nm) exhibit important changes. Nanotechnology is concerned with materials and systems whose structures and components exhibit novel and significantly improved physical, chemical, and biological properties – and that enable the exploitation of novel phenomena and processes – due to their nanoscale size. The goal is first to exploit these properties by gaining control of structures and devices at atomic, molecular, and supramolecular levels; and then to learn to manufacture and use these devices efficiently. Maintaining the stability of interfaces and the integration of these “nanostructures” at micron-length and macroscopic scales are all keys to success.

New behavior at the nanoscale is not necessarily predictable from that observed at larger size scales. The most important changes in behavior are caused not by the order of magnitude size reduction, but by newly observed phenomena intrinsic to or becoming predominant at the nanoscale. These phenomena include size confinement, predominance of interfacial phenomena and quantum mechanics. Once it becomes possible to control feature size, it will also become possible to enhance material properties and device functions beyond what we currently know how to do or even consider as feasible. Being able to reduce the dimensions of structures down to the nanoscale leads to the unique properties of carbon nanotubes, quantum wires and dots, thin films, DNA-based structures, and laser emitters. Such new forms of materials and devices herald a revolutionary age for science and technology, provided we can discover and fully utilize the underlying principles.

2. Initiative Overview

The National Nanotechnology Initiative (NNI) represents the Federal Government’s total investment in nanoscale science, engineering, and technology. The NNI supports long-term nanoscale research and development leading to potential breakthroughs in areas such as materials and manufacturing, nanoelectronics, medicine and healthcare, environment and energy, chemical and pharmaceutical industries, biotechnology and agriculture, computation and information technology, and national security. The impact of nanotechnology on the health, wealth, and lives of people could be at least as significant as the combined influences of microelectronics, medical imaging, computer-aided engineering, and man-made polymers developed in the century just past.

The NNI was initiated in FY 2001 with a \$152 million increase to the Federal Government's fiscal year 2000 base nanoscale R&D investment of \$270 million across the six participating agencies. Combined with the FY 2000 base, the total FY 2001 NNI funding was \$422 million. Congress appropriated a total NNI funding of \$604.4 million for FY 2002. The President's NNI request for FY 2003, officially announced in February 2002, was for \$679 million (see <http://www.whitehouse.gov/omb/budget/fy2003/pdf/spec.pdf>). Subsequently, NASA and USDA have identified some additional items within their FY 2003 R&D budget requests as falling under the purview of the NNI, thus the total FY 2003 NNI funding request is now \$710.2 million.

The NNI incorporates fundamental research, grand challenges, centers and networks of excellence, and research infrastructure – activities that are high risk, high payoff, and broadly enabling. The initiative also addresses development of novel approaches to the education and training of future nanotechnology workers, the ethical, legal and social implications of nanotechnology, and the rapid transfer to technology of knowledge gained from research and development. The NNI is coordinated by the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the National Science and Technology Council (NSTC) Committee on Technology. A National Nanotechnology Coordination Office (NNCO) has been created to support the NSET's coordination efforts. In 2001 NSET funded a National Research Council panel to assess the NNI's progress towards its goals. The report is expected in July 2002.

Nanotechnology is in a very early stage of development. Outside of a handful of examples, the creation of commercial nanotechnology-based products is several years away. Therefore, it should come as no surprise that well over half of NNI funding will go towards supporting university-based research. In fact, agencies are receiving such a strong response to their solicitations from the academic community that they are placing restrictions on the number of proposals submitted by any single university. The significant level of research and education activities reflected by the "proposal pressure" for a relatively new field is a key reason why the NSET proposes significant growth in the Federal investment in nanotechnology over the FY 2002 – FY 2006 timeframe.

The creation of the NNI has motivated several states to initiate programs in nanotechnology. California is committing \$25 million per year for 4 years to establish a nanotechnology center at the University of California at Los Angeles (UCLA) and Santa Barbara (UCSB). Pennsylvania has also initiated a program, investing \$10 million over 3 years in a nanotechnology center involving the University of Pennsylvania, Drexel University, and the Ben Franklin Technology Partners (<http://www.sep.benfranklin.org/nanotechcenter.html>). Other states, such as New York, Illinois, New Jersey, Oklahoma, South Carolina, Florida, Indiana, Texas, Virginia, and Georgia have announced their intentions to invest state funds to develop capabilities in nanotechnology. NSET members are meeting with representatives from the Experimental Program to Stimulate Competitive Research (EPSCoR) programs to encourage universities in those states to participate in the NNI. The Oklahoma EPSCoR program recently has established a university consortium identified as NanoNet.

3. A Revolution in the Making: Driving Forces

In 1959 Richard Feynman delivered his now famous lecture, “There is Plenty of Room at the Bottom.” He stimulated his audience with the vision of exciting new discoveries if one could fabricate materials and devices at the atomic/molecular scale. He pointed out that for this to happen a new class of miniaturized instrumentation would be needed to manipulate and measure the properties of these small – “nano” – structures.

The original 2000 proposal for the National Nanotechnology Initiative (see <http://www.nano.gov/nni2.pdf>) set out a plan for realizing Feynman’s vision, and proclaimed a revolution in the making. This plan – and the revolution it promotes – is now beginning to unfold. The promise of nanoscale science and technology has raised the attention not only of researchers in academe and industry, but also in business and venture funding. New challenges have also emerged in the past two years – particularly the threat of chemical, biological, radiological, and explosives (CBRE) use by terrorists. Nanoscale science and technology is rising to meet these challenges. New competition is emerging around the world as well. Virtually every industrialized country in the world has embraced the promise of nanotechnology and has vastly increased its research and development funding for the relevant fields of science and technology. As detailed in the remainder of this report, Federal support for nanoscale science and technology is necessary to enable the United States to take advantage of this strategic technology, provide for national security, and remain competitive in the global marketplace well into the future.

4. Nanotechnology’s Impact

The potential benefits of nanotechnology are pervasive, as illustrated in the fields outlined briefly below (and in more detail in the original NNI proposal, <http://nano.gov/nni2.pdf>):

Materials and Manufacturing. Nanotechnology is fundamentally changing the way materials and devices will be produced in the future. The ability to synthesize nanoscale building blocks with precisely controlled size and composition and then to assemble them into larger structures with unique properties and functions will revolutionize segments of the materials manufacturing industry. Some of the benefits that nanostructuring can bring include lighter, stronger, and programmable materials; reductions in life-cycle costs through lower failure rates; innovative devices based on new principles and architectures; and use of molecular/cluster manufacturing, which takes advantage of assembly at the nanoscale level. Researchers will be able to develop materials and manufacturing processes previously not thought possible.

Nanoelectronics and Computer Technology. The Semiconductor Industry Association (SIA) has developed a roadmap for continued improvements in miniaturization, speed, and power reduction in information processing devices. The current SIA roadmap (see <http://public.itrs.net/Files/2001ITRS/Home.htm>) projects the future to approximately 2016 and estimates that by that date some critical feature sizes (gate lengths) will be as small as 9 nm, well into the realm of fully nanostructured devices. Even more significantly, the 2001 roadmap notes that there are some classes of semiconductor devices for which there are no proven technical

approaches for future manufacturing of the devices. First described as the “Red Brick Wall” in the 1999 report, with predictions that these technical roadblocks will be reached as early as 2005, the 2001 roadmap report now states that segments of the “Red Brick Wall” may be reached as early as 2003. Now that the frontiers of continued progress in the information technology field are clearly in the nanoscale regime, the need for both basic and applied nanoscale science and technology research applied to information technology is greater than ever.

Medicine and Health. Living systems are governed by molecular behavior at nanometer scales where the disciplines of chemistry, physics, biology, and computer simulation all now converge. Such multidisciplinary insights will stimulate progress in nanobiotechnology, with impact in virtually all areas of biomedicine. Opportunities in this arena include the following:

- Dramatic increases in the speed and efficiency of genome and protein sequencing through use of nanofabricated surfaces and devices
- New approaches to the delivery of drugs, enormously broadening the number of drugs that could be effectively administered and improving their therapeutic potential
- Application of new nanoscale tools to benefit basic studies of cell biology and pathology
- Development of new biocompatible, high-performance nanostructured materials
- Bio-inspired nanosystems and materials formed by self-assembly that could be used in diagnostics (e.g., quantum dots in visualization), or even in therapeutic applications
- Increasingly sophisticated nanoscale modeling and simulation of new drugs and other medical products, accelerating their introduction and reducing their cost

Aeronautics and Space Exploration. NASA’s driving considerations for developing advanced technology in pursuit of the agency’s goals and missions are to reduce cost, increase safety and achieve greater performance. These objectives will be enabled through the application of nanotechnology in the development of new generations of safer, lighter, and more efficient vehicles. NASA believes the convergence of nanotechnology, biotechnology and information will provide unprecedented benefits and solutions to its myriad mission challenges. Nanostructured materials and devices promise solutions to many of these challenges. Moreover, the low-gravity, high-vacuum space environment may aid development of nanostructures and nanoscale systems that cannot be created on Earth. Applications include (a) low-power, radiation-tolerant, high performance computers; (b) nano-instrumentation for microspacecraft; (c) wear-resistant nanostructured coatings; (d) enhanced safety through deployment of novel sensors and electronic mentors; and, (e) in the long term, technologies leading to the development of intelligent autonomous spacecraft.

Environment and Energy. Nanotechnology has the potential to significantly impact energy efficiency, storage, and production. It can be used to monitor and remediate environmental problems; curb emissions from a wide range of sources; and develop new “green” processing technologies that minimize the generation of undesirable by-products. The impact on industrial control, manufacturing, and processing will result in energy savings through market driven practices. Current and emerging industrial applications include (a) use of crystalline materials with pore sizes in the 1 nm range as catalyst supports, now the basis of a \$30 billion/year industry; (b) removal of ultrafine contaminants in the oil industry through the use of the mesoporous material MCM-41, with pore sizes in the range of 10-100 nm; (c) development of nanoparticle-reinforced polymeric materials that can replace heavier metallic components in the

auto industry (use of which could greatly reduce gasoline consumption and carbon dioxide emissions); and (d) the replacement of carbon black in tires by nanometer-scale particles of inorganic clays and polymers, leading to the production of more environmentally friendly, wear-resistant tires. Potential future breakthroughs include nanorobotics and intelligent systems for environmental and nuclear waste management, nanofilters to separate isotopes in nuclear fuel processing, nanofluids for increased cooling efficiency of nuclear reactors, nanopowders for decontamination, and computer simulation at nanoscale for nuclear safety.

Biotechnology and Agriculture. Biosynthesis and bioprocessing offer fundamentally new ways to manufacture new chemicals and pharmaceutical products. Integration of biological building blocks into synthetic materials and devices will allow the combination of biological functions with other desirable materials properties. Imitation of biological systems provides a major area of research in several disciplines. Nanoscience will contribute directly to advancements in agriculture in a number of ways: (a) molecular-engineered biodegradable chemicals for nourishing plants and protecting against insects; (b) genetic improvement for animals and plants; (c) delivery of genes and drugs to animals; and (d) nanoarray-based technologies for DNA testing.

National Security. Critical defense applications include: (a) command/control/communications/intelligence systems; (b) more sophisticated virtual reality systems enabled by nanoelectronics; (c) enhanced automation and robotics to offset reductions in military manpower, reduce risks to troops, and improve vehicle performance; (d) higher performance (lighter weight, higher strength) military platforms with diminished failure rates and lower life-cycle costs; (e) chemical, biological, radiological, and explosives detection and protection; and (f) nano- and micromechanical devices for control of nuclear defense systems.

Other Potential Government Applications. Nanoscience and technology can benefit other government agency missions, including: (a) lighter and safer equipment in transportation systems (DOT); (b) measurement, control, and remediation of contaminants (EPA); (c) enhanced forensic research and ballistic protection (Department of Justice); and (d) printing and engraving of high quality, forgery-proof documents and currency (Bureau of Engraving and Printing).

Science and Education. Advances in nanoscale science, engineering, and technology will require and enable advances in many disciplines: physics, chemistry, biology, materials science, mathematics, and engineering. These interdisciplinary nanoscale research efforts will reinforce educational connections among disciplines and give birth to new fields that do not exist today. This will require changes in how students and professionals are educated and trained for careers in these fields.

Future U.S. Competitiveness. Technology is a major driving factor for growth at every level of the U.S. economy. Nanotechnology is expected to be pervasive in its applications across nearly all industries. Investment in nanotechnology research and development is necessary to maintain and improve our position in the world marketplace. The National Nanotechnology Initiative will continue to support the development of critical enabling technologies with broad commercial potential, such as nanoelectronics, nanostructured materials and nanoscale-based manufacturing processes, helping U.S. industry to take advantage of commercial opportunities.

5. Investment Opportunities

Need for Investment. Nanoscale scientific, engineering, and technical knowledge is exploding worldwide. This is being made possible by the availability of new investigative tools, synergies created through interdisciplinary approaches, and rapid dissemination of results; it is driven by emerging technologies and their applications. With sustained investment, the number of revolutionary discoveries reported in nanotechnology can be expected to accelerate in the next decade; these are likely to profoundly affect existing and emerging technologies in almost all industry sectors and application areas. Over the past few years, it has become evident that there is a clear need for Federal support to create a balanced infrastructure for nanoscale science, engineering, technology and human resources development, and to address critical areas of research. There were many more meritorious proposals than could be supported in the FY 2002 funding competitions.

International Perspective. The field is highly competitive and dynamic in the international arena. Even if the United States has taken an initial leadership role with the establishment of the NNI, there has been a strong international response, and now U.S. Federal investment accounts for about 30% of world government funding. There is a relative balance between U.S., Japan, and Western Europe in government funding, and there are significant increases in other countries as well (see the worldwide study *Nanostructure Science and Technology*, NSTC 1999, <http://www.ostp.gov/NSTC/html/iwgn/IWGN.Worldwide.Study/toc.htm>, and the update at <http://nano.gov/international>). Other regions, particularly Japan and Western Europe, are supporting work that is equal to the quality and breadth of the science done in the United States because there, too, scientists and national leaders have determined that nanotechnology has the potential to be a major economic factor during the next several decades. This situation is unlike the other post-war technological revolutions, where the United States enjoyed early leads. The international dimensions of nanotechnology research and the potential applications suggest that the United States must put in place a competitive and balanced research program and infrastructure. This emerging field also creates a unique opportunity for the United States to partner with other countries in ways that are mutually beneficial through information exchange, cooperative research and education activities, including leveraging cost of large facilities and personnel exchanges.

6. The First Year of the NNI

Fiscal year 2001 was the first year of the NNI. The program has emphasized long-term, fundamental research aimed at discovering novel phenomena, processes, and tools; addressed NNI grand challenges; supported new interdisciplinary centers and networks of excellence including shared user facilities; supported research infrastructure; and addressed societal implications of advances in nanoscience and nanotechnology. Funding was awarded on a competitive basis with other programs and within NNI. The budget identified in November 2000 was \$422 million. The actual expenditure at the end of fiscal year 2001 was \$464 million (Table 6.1).

Table 6.1
Actual Funding by NNI Research Portfolio in FY 2001 (all in \$ millions)

Agency	Fundamental Research	Grand Challenges	Centers and Networks of Excellence	Research Infrastructure	Societal Implications and Workforce	Total**
DOC/NIST		19		12.4	2	33.4
DOD	11	61	27	21	3	123
DOE	32	27	14	15		88
DOJ		1		0.4		1.4
EPA		5				5
NASA	5	12		5		22
NIH	8	19	1	10	2	40
NSF	95	7	29	13	6 /21/*	150
USDA	1.5					1.5
Total	152.5	151	71	76.8	13 /28/*	464.3 [+ 42.3]

* Includes the educational component for student support in research projects

** The difference as compared to the funds identified at the beginning of the FY 2001 is in brackets [..]

Several program solicitations were announced and correlated among the participating agencies in FY 2001 (listed at <http://nano.gov>). The main announcements were as follows:

- NSF: “Nanoscale Science and Engineering” – for interdisciplinary team research, centers and exploratory research
- DOD: “Defense University Research Initiatives on NanoTechnology” (DURINT) – for research projects and equipment requests; DARPA: “Simulation of Bio-Molecular Systems,” and “Molecular Electronics”
- DOE: “Nanoscale Science, Engineering, and Technology” – for materials, chemical and engineering sciences
- NASA: “University Research Emerging Technology Initiative” solicitation
- NIH: components of several solicitations
- EPA: “Exploratory Research”

The first year of NNI provided support to over 2,000 active university awards by the 15 participating departments and agencies, as well support for research in government and industrial laboratories. The NNI already has had broad impact through introducing the nanoscale as a key area in academic research, and increasing the interest of U.S. industry and business (as well as abroad). Most industrial countries have, or plan to establish, an R&D activity in nanotechnology at the national level.

Approximately 65% of the funds were allocated to academic researchers, 30% to government laboratories and 5% to industry (including SBIR, STTR, ATP). The distribution of funding among various research and education topics funded in FY 2001 is covered in Appendix C. Table 6.2 at the end of this chapter lists the top 50 projects with the corresponding publication references.

The remainder of this chapter highlights selected FY01 accomplishments in fundamental research (section A); grand challenges (section B); centers and networks of excellence

(section C); research infrastructure (section D); societal implications and workforce training (section E); and special cross-cutting national needs (section F). Selected examples of scientific, engineering, and technology breakthroughs are shown in section G. Section H includes examples of FY01 education and training activities.

A. Fundamental Research (\$152.5 million)

Significant scientific breakthroughs are moving research developments faster than expected. Key advancements are: engineering materials with atomic and molecular precision by using proteins, viruses and other biosystems as architects; creating circuits with the logic element a molecule wide; assembling DNA to build molecular devices and to detect anthrax with unprecedented speed; single molecule behavior and interaction; artificial genetic system; conducting polymers; and new concepts for large-scale production of nanotubes. Although many nanoscale science and engineering projects are interdisciplinary, we have delineated three major research areas: biosystems; novel structures, phenomena and tools; and nanoscale devices and systems. Selected highlights in the key fundamental science areas addressed by NNI in FY 2001 are as follows:

Focus on Biosystems (\$33.5 million)

Research with focus on biosystems supports the development of fundamental understanding of nanobiostructures, processes, and techniques. The goal is to stimulate rapid progress in the study of biological and biologically-inspired systems where nanostructures play an important role. Impact is expected across a broad range of applications in biomaterials, biosystem-based electronics, agriculture, energy, and health.

Contributions from: DOD, DOE, NASA, NIH, NSF

Biological assembly of nanostructures (NSF)

Building upon their earlier work demonstrating that peptides and proteins could guide the interconnection of semiconductor materials, researchers at the University of Texas at Austin are developing hybrid biological/semiconductor materials. Integrating quantum dot technology and complex nanoscale materials, the eventual products may impact biomedicine, advanced materials, sensors, and nanoscale electronics. *Principal Investigators: Angela Belcher, Brian Korgel, and Karen Browning, University of Texas, Austin.*

Using DNA molecules to construct nanoscale devices (NSF)

The unique properties of DNA molecules allow them to be crafted into intricate nanostructures. Researchers from New York University, the California Institute of Technology, and DOW Chemical are attempting to create operational DNA-based nanomachines. *Principal Investigators: Nadrian Seeman, Joey Storer, Erik Winfree, New York Univ. and William Goddard, Nagarajan Vaidehi, CIT.*

Artificial genetic system (NSF)

A new form of DNA has been created. The artificial genetic system behaves like natural DNA, but goes one step further, incorporating twelve letters into the genetic “alphabet” instead of the four found in natural DNA. This discovery can be used in clinical diagnostics tools today, and

possibly in personalized medicine tomorrow. This artificial nanoscale system can more quickly identify small changes in DNA that make individual humans different. *Principal Investigators: Steven A. Benner and Weihong Tan, University of Florida.*

Development of the biological force microscope (NSF)

The first biological force microscope that is capable of quantitatively measuring interfacial and adhesion forces between living bacteria and mineral surfaces, *in situ*, has been developed. Biological force microscopy has the potential to allow researchers, for the first time, to gain fundamental insights into the nanoscale and nanoforce world that exists at the interfaces between microorganisms and minerals in nature. Moreover, because the cells, substrate and fluid properties can be easily varied, this technique will be of interest to biologists, materials scientists, and medical researchers. Applications will be wide ranging, from understanding the mobility of pathogenic bacteria in a groundwater aquifer to determining the affinity of certain kinds of human lung cells to various mineral fibers. *Principal Investigator: Michael F. Hochella, VPI.*

Focus on Novel Structures, Phenomena and Tools (\$66 million)

Research in this area addresses techniques for synthesis and design of nanostructures, and explores the novel phenomena and properties that originate from the nanoscale. This research is critical to overcoming obstacles to miniaturization as device feature sizes reach the nanoscale.

Contributions from: DOD, DOE, NASA, NSF

Nanoscale film serves as molecular filter (NSF)

Researchers at Northwestern University have developed a thin-film material with nanoscale cavities that acts as a molecular gatekeeper. In solution, the film can also play a role in chemically transforming molecules. Potential applications include selective drug delivery, synthesis of specialized chemicals, and new types of semiconductors. *Principal Investigators: Joseph Hupp, SonBinh Nguyen, and Randall Snurr, NWU.*

“Magic” values for nanofilm thickness (DOE)

A key issue for nanotechnology is the structural stability of thin films and of devices made from nanostructures. It was recently demonstrated that nanofilms are significantly more stable at a few specific values of film thickness. The origin of this effect arises from the confinement of electrons within the film leading to electronic states with discrete energy values, much as atomic electrons are bound to the nucleus at discrete energy levels. Calculations have demonstrated that increased stability occurs when the number of electrons present in the film completely fill the set of available states, just as filled electronic shells make the noble gases very stable.

Artificial atoms (NSF)

At the extreme nanoscale limit, artificial atoms and molecules are being fabricated. These have quantized electronic energy levels, and it becomes possible to add and subtract electrons from among these levels. The fabricated structures include single electron transistors and quantum dots. Individual quantum states can be manipulated for sensor and memory applications. In magnetic cobalt nanoparticles, the individual energy levels shift and jump as a magnetic field rotates the direction of the particle’s magnetic moment, so that the energy of just one quantum

state could be used to measure the orientation of the particle in magnetic memory applications. *Principal Investigator: Dan Ralph, Cornell University.*

The world's smallest laser (DOE)

A team of materials scientists and chemists has built the world's smallest laser – a nanowire nanolaser 1,000 times thinner than a human hair. The device, one of the first to arise from the field of nanotechnology, can be tuned from blue to deep ultraviolet wavelengths. Zinc oxide wires only 20 to 150 nanometers in diameter and 10,000 nanometers long have been grown, each wire a single nanolaser. Discovering how to excite the nanowires with an external energy source has been critical to the success of the project. Ultimately, the goal is to integrate these nanolasers into electronic circuits for use in “lab-on-a-chip” devices that could contain small laser-analysis kits, or as a solid-state, ultraviolet laser to allow an increase in the amount of data that can be stored on high-density optical disks. *Principal Investigator: P. Yang, LBNL*

Investigating Earth processes on the nanoscale (NSF)

A variety of environmental contaminants, from mine wastes to industrial chemical spills, may interact differently with earthen materials on the nanoscale than they do at the macroscale. Researchers from the University of California at Berkeley will study the interactions of ions and metal oxide nanocrystals, revealing how some contaminants may become sequestered in the environment. *Principal Investigator: Jillian Banfield, UCB.*

Focus on Nanoscale Devices and Systems (\$37 million)

Research in this area focuses on creating nanostructures, assembling them into nanosystems, and integrating them into larger scale structures. New concepts and design methodologies are needed to synthesize nanosystems, create new nanoscale devices, and integrate them into architectures for various operational environments. This will require a profound understanding of the physical, chemical and biological interactions among nanoscale components. Research in this area includes development of new tools for manipulating, assembling, processing, and manufacturing across several length scales; testing nanostructures and devices; software specialized for nanosystem design and control; design automation tools for systems with large numbers of heterogeneous nanocomponents; and evaluation of the economic and environmental implications of manufacturing at the nanoscale.

Contributions from: DOD, NASA, NSF

Determining fluid properties within carbon nanotubes (NSF)

Carbon nanotubes have diameters that measure in nanometers. However, fluid processes are only known for tubes that are one thousand times wider. Researchers at Drexel University are attempting to uncover the fundamental properties of fluids as they interact with carbon nanotubes, aiding engineers as they develop the next generation of ink jets, biochips, and other nanotube devices. *Principal Investigators: Yuri Gogotsi and Constantine Megaridis, Drexel University.*

Micro lens for nano research (DOE)

A silicon lens that is 1/10 the diameter of a human hair has been fabricated and used to image microscopic structures with an efficiency 1,000 times better than existing probes. The combination of high optical efficiency and improved spatial resolution over a broad range of

wavelengths has enabled measurement of infrared light absorption in single biological cells. This spectroscopic technique can provide important information on cell chemical composition, structure, and biological activity. *Principal Investigators: G. Kino and K Goodson, Stanford University.*

Building semiconductor nanowires (NSF)

A multidisciplinary team is developing a method to synthesize nanowires comprised of a single crystal semiconductor sandwiched between metal contacts. In addition to engineering the devices, the study will explore how changes in nanowire dimensions affect fundamental electrical properties. The project also incorporates an extensive educational component, including the development of K-12 education and outreach activities. *Principal Investigators: Joan Redwing, Ari Mizel, Theresa Mayer, and Suzanne Mohney, Pennsylvania State Univ.*

Using nanowires to detect explosives (NSF)

Researchers have developed a silicon polymer nanowire that can identify trace amounts of explosives, such as TNT and picric acid, in both air and water. The fibers, which can be incorporated into materials ranging from paper to paints, reveal the presence of chemical residues when viewed in ultraviolet light. *Principal Investigators: Honglae Sohn (postdoctoral student), William Trogler, Michael Sailor, and Rebecca Calhoun, Univ. of Cal., San Diego.*

Focus on Multi-scale, Multi-phenomena Theory, Modeling, and Simulation (\$16 million)

The emergence of new behaviors and processes in nanostructures, nanodevices and nanosystems creates an urgent need for theory, modeling, large-scale computer simulation and new design tools in order to understand, control and accelerate development in new nanoscale regimes and systems. Research on theory, mathematical methods, modeling and simulation of physical, chemical and biological systems at the nanoscale will include techniques such as quantum mechanics and quantum chemistry, multi-particle simulation, molecular simulation, grain and continuum-based models, stochastic methods, and nanomechanics. Approaches that make use of more than one such technique and focus on their integration will play an important role in this effort. The interplay of coupled, time-dependent and multiscale phenomena and processes in large atomistic and molecular systems will be encouraged. A critical issue is the ability to make connection between structures, properties and functions.

Modeling and simulation of biological ion channels to cure illnesses (NSF)

Researchers from the Advanced Electronics Simulation (Descartes) Center at the University of Illinois at Urbana-Champaign and Stanford University, with collaborators from Rush Medical Center (Chicago), have used software components that were developed for the design of semiconductor devices and chip technology to simulate “biological ion channels” (BICs). BICs with nanometer dimensions in all directions are the nano-transistors of nature. They switch electrical currents and fulfill a multitude of functions. They can regulate the electricity of the heart; act as antibiotics, and even fight cancer. Their structure, facility for selective transport of ions, and switching mechanisms involve nanoscale physics, chemistry and mechanics. The simulations have successfully explained the magnitude of the electric currents in several BICs and the connection of these currents to macroscopic cell membrane potentials, thus connecting the nanoscale with macroscopic quantities and providing understanding for both. *Principal Investigator: K. Hess, University of Illinois at Urbana-Champaign.*

Multimillion-atom simulation of mechanical phenomena and engineering processes (NSF)

Multiscale atomistic simulations will combine quantum mechanics, molecular dynamics and continuum theories to yield realistic predictions of nanocomposites behavior. The multimillion-atom simulations will provide answers to both theoretical issues such bonding between dissimilar materials and engineering processes such as sintering of nanostructures. *Principal Investigator: Priya Vashishta, LSU.*

B. Grand Challenges (\$151 million)

The nine grand challenges, their level of funding in FY 2001, and selected accomplishments are listed below:

Nanomaterials “By Design” (\$35.5 million)

This topic involves the development of structural carbon and ceramic materials several times stronger than steel for use in industry, transportation, and construction; polymeric materials three times stronger than present “soft” materials, melting at 100°C or higher temperatures, for use in cars and appliances; and “smart” multifunctional materials.

Contributions from: DOD, DOE, NASA, NSF (lead)

Deformation, fatigue and fracture of interfacial nanomaterials (DOD)

First experimental simulation of the stress necessary to nucleate defects at grain boundaries in a nanocrystalline metal using the “bubble raft” model; this information is used as a guideline for molecular dynamics models of nanostructured metals to study the effects of nanoscale deformation at surfaces. *Principal Investigator: Subra Suresh, MIT.*

Nanostructured polymers by templating for terabit memory (one trillion bits per square inch) (NSF, DOE)

Novel block-copolymer nanostructural architectures have been obtained that allow creating magnetic nano-wire arrays from diblock copolymer templates (with NSF support). Through phase separation of these copolymers and field-effected orientation they obtain densely packed lattices of nanocylinders perpendicular to the substrate; these are then etched and filled with cobalt, thus generating arrays of nanowires 14 nm in diameter. The research included collaboration with IBM, which resulted in licensing of the nanowire arrays for magnetic storage to a new company named Paramount Capital. A 300-fold increase in magnetic storage density has been achieved using a patented technique for self-assembly of block copolymers under the influence of a small voltage (with DOE support). The new technique is simple, robust, and extremely versatile. The key to this discovery lay in directing the orientation of nanoscopic, cylindrical domains in thin films of block copolymers. By coupling this with routine lithographic processes, large area arrays of nanopores can be produced easily. Electrochemical deposition of metals, such as cobalt and iron, produces nanowires that exhibit excellent magnetic properties, key to ultrahigh density magnetic storage. The nanowires also are being used as field emission devices for displays. *Principal Investigators: Mark Tuominen and Thomas Russell, University of Mass., Amherst.*

Observations of atomic imperfections (DOE)

A new electron beam technique has been developed that has measured atomic displacements to a record accuracy of one-hundredth of the diameter of an atom. Such small imperfections in atomic packing often determine the properties and behavior of materials, particularly in nanostructured devices. This capability has been made possible by a new technique that couples electron diffraction with imaging technology. The result is a greatly enhanced capability to map imperfections and their resulting strain fields in materials ranging from superconductors to multi-layer semiconductor devices. *Principal Investigator: Y. Zhu, Brookhaven National Laboratory.*

High temperature nanotechnology (NASA)

High temperature nanotubes made of silicon carbide (SiC) have been fabricated by using both polymer-template synthesis and also a chemical vapor deposition (CVD)-template synthesis method. Polycrystalline SiCNTs as well as SiC nanorods (SiCNRs) with 200 nm diameters were produced via polymer/alumina-template synthesis. Additionally, highly uniform walled SiCNTs of 200 nanometer diameter have been produced in high yield via a CVD template approach. This work was accomplished through collaborations with Prof. L.V. Interrante of Rensselaer Polytechnic Institute. *Principal Investigator: David Larkin, Glenn Research Center.*

Nanoscale polymer yields extremely slick coating (NSF)

Chemical engineers at North Carolina State University have developed a technique to group molecules so tightly that they form a slick surface. The material may have a variety of applications, including non-stick cookware, computer disk drives, airplane surface coatings, and medical implants. *Principal Investigators: Jan Genzer and Kirill Efimenko, NC State.*

Silicate nanocomposites (DOD)

Polymer nanostructured materials represent a radical alternative to conventional filled polymers or polymer blends. Layered silicate nanoparticles have been shown to react *in situ* with aggressive environments to form a tough ceramic passivation layer on the surface of the polymer nanocomposite. Self-passivation and self-healing have been demonstrated during exposure to a solid rocket motor exhaust and plasma environments. *Principal Investigators: Richard Vaia and Jeffrey Sanders, AFRL/ML.*

Nanoelectronics, Optoelectronics and Magnetism (\$47.5 million)

Topics include nanometer structures for minuscule transistors and memory chips that will improve the computer speed and efficiency by factors of millions; expansion of mass storage electronics to multi-terabit memory capacity that will increase the memory storage per unit surface a thousand fold and make data available on a pinhead; and changes in communication paradigms by increasing bandwidth a hundred times, which will reduce business travel and commuting.

Contributions from: DOD (lead), DOE, NASA, NIST, NSF

Integrated cantilever micromagnetometry (DOD)

Semiconductor microprocessing has been used to fashion sub-micron micromechanical torsional magnetometers into which the nanostructure of interest was monolithically integrated. The

magnetometers have been combined with all-optical fiber-based interferometer detection techniques, and have achieved a sensitivity of better than 10^5 Bohr magneton in fields of 1 kG and higher, an improvement of more than four orders of magnitude upon any previous torsional sensor. The technique has been successfully tested over a broad range of magnetic fields (0-8T) and three orders of magnitude temperature (300mK – 300K). The results reveal an ability to detect ~200 magnetic atoms and the potential for single spin sensitivity. Potential applications include high-density magnetic storage solutions, characterization of buried integrated systems, magnetic field detection and robust frequency detection. *Principal Investigator: David Awschalom, UCSB.*

Ferromagnetic imprinting of nuclear spins in semiconductors (DOD)

Optically-generated electron spins in semiconductors show remarkable resilience against environmental decoherence, making it possible to envision a new class of magnetoelectronics based on the coherent superposition of quantum spin states. It has been shown that the presence of a ferromagnetic layer can cause nuclear spins in a GaAs layer to become hyperpolarized (~25%) and align with the magnetization. The polarized nuclei, in turn, generate large effective magnetic fields on the coherent electron spins through the hyperfine interaction. Ferromagnetic control of electron spin coherence can be achieved. These results demonstrate the possibility of imprinting ferromagnetic domains and patterned magnetic nanostructures onto the nuclear spin system of electronics for future high-density storage technology and quantum computation information processing. *Principal Investigator: David Awschalom, UCSB.*

Information retrieval (DOC)

This project developed a nanoscale recording system applicable to the retrieval of information from damaged or altered audio tapes. *Principal Investigator: Pappas, NIST.*

Superlattices for infrared detection (DOD)

Design and growth conditions for InAs/InGaSB superlattices have been developed and the first very long wavelength infrared (VLWIR) photodiode demonstrated. The samples were grown by Applied Optoelectronics Inc. under a Phase II SBIR and Northwestern University under an Air Force grant. *Principal Investigator: Gail Brown, Air Force Research Laboratory.*

Self-aligned quantum dot nanoswitches (DOD, NSF)

This project addresses the fabrication of quantum scale devices through the combined oxidation and etching of Si/SiGe/Si nanostructured pillars. The research spans issues of materials science, circuits, and device fabrication and characterization. The structures to be fabricated are closely integrated with resonant tunneling diodes, single electron transistors, and quantum level devices necessary for cellular automata circuits. Methods of high speed testing to characterize the devices as well as theoretical modeling to optimally design the structures are included. The project is highly collaborative among Ohio State, Illinois, Notre Dame, UC Riverside, the Naval Research Laboratory, and the Air Force Research Laboratory. *Principal investigators: Paul R. Berger, Ohio State U.; Roger Lake, UCR; Patrick J. Fay, ND; Gregory L. Snider, ND; Ilesanmi Adesida, U. Illinois.*

Nanoporous semiconductors – matrices, substrates and templates (DOD)

Porous SiC studied to date includes wafers from a commercial vendor as well as samples produced in-house. Structural characterization using electron microscopy and X-ray reflectivity reveals bulk porosity of typically 20%, with a particular tree-like morphology seen on most samples. A skin layer about 50 nm thick with porosity of only a few percent exists on the top of the wafers. This skin layer is believed to be detrimental for applications, and removal of it has been accomplished by both hydrogen-etching (at 1700°C) and reactive ion etching. Epitaxy of SiC and GaN on porous SiC has been performed and those films reveal a slight decrease in defect density relative to samples grown on nonporous materials. *Principal Investigator: Randall Feenstra, Carnegie Mellon.*

Silicon based infrared detection (DOD)

Ordinary silicon is transparent to wavelengths longer than 1.1 μm . This project has developed a surface treatment technique, which uses irradiation of the silicon surface by laser pulses, to produce a nanostructured surface. The processed silicon becomes opaque to the infrared and photo carrier generation is observed. This opens the door to silicon-based infrared detectors for use in telecommunications and remote sensing. *Principal Investigator: Eric Mazur, Harvard University.*

Quantum dot lasers (DOD)

The first continuous wave quantum dot (QD) laser has been demonstrated. This device could operate at room temperature, and enables the first quantum dot long-wavelength intersubband detectors in the far infrared. The work will impact high-speed optical communications, and the use of lasers for surveillance, imaging, and target identification. *Principal Investigator Pallab Bhattacharya, University of Michigan.*

Maskless lithography with scanning probes and carbon nanotubes (DOD)

Hundreds of nanotube atomic force microscopy tips have been grown from silicon tips using chemical vapor deposition, achieving mass production of nanotube tips for AFM and scanning probe lithography. Germanium nanowires with diameters on the order of 20 nm have been grown on the silicon pyramidal tips. Each wire has a gold nanoparticle at the end. These tips are potentially useful for imaging deep holes and trenches for metrology of microchips. Metal nanoparticles and dendrimer films have been made using this approach. *Principal Investigator: Hongjie Dai, Stanford Univ.*

Massively parallel dip-pen nanolithography (DOD, NSF)

Dip-pen probe arrays allow rapid generation of sub-100 nm features with applications in micro- and nanoelectronics and bio/nanotechnology. The probe consists of passive and active individually addressable dip-pen arrays interfaced with commercial scanning probe microscopy instruments. Candidate ink materials include biological structures of proteins and DNA. A 32-pen array is being evaluated in the context of patterning of metal and semiconductor substrates. Ultrahigh density gene chips and proteomic arrays on metal and oxide substrates can have densities of 10,000 to 1,000,000 times that of conventional microarrays. *Principal Investigators: Chad Mirkin, Northwestern University, and Chang Liu, U. of Illinois at Urbana-Champaign.*

Reconfigurable single molecule diode (DOD)

A rotaxane family molecule has been synthesized with groups at either end of the molecule designed to bond to electrode surfaces. The center of the molecule has two electron-donating (oxidizing) groups connected by a short spacer. They are surrounded by a ring that has a positive charge. This ring can move up and down the backbone of the molecule and has a sufficiently positive charge to change a donor group to a net acceptor (reducing group). This motion can be induced by oxidizing/reducing the molecule, which can be caused by raising the voltage across the ends of the molecule above a threshold (of a few volts). The net result is an I/V characteristic that looks like a diode but can reverse polarity by applying an over voltage across the molecule. This is an extremely interesting characteristic, and there is no equivalent two terminal device in the solid-state world. *Principal Investigators: Jim Heath, University of California Los Angeles, and Stan Williams, HP.*

Single molecule, negative differential resistor (DOD)

A single molecule with an I/V characteristic exhibiting negative differential resistance (NDR) has been synthesized. The switching mechanism has been correlated with the oxidation states of the molecule. In the off state, there is no molecular pronounced overlap. The results suggest a conformational change (a twisting of the central ringed group) is associated with this conductivity change. Experimental confirmation for the importance of this conformational change has recently been published by Penn State. The switching rate of the NDR molecule has been measured through some careful STM measurements of individual molecules in a background of an inert alkane SAM (self-assembling molecules). One of the main conclusions is that the local order (i.e., packing) is extremely important and the NDR molecule can effectively be frozen into one of its conduction states. *Principal Investigators: Jim Tour, Rice; Mark Reed, Yale; Paul Weiss, Penn State; and Jorge Seminario, Univ. S. Carolina.*

Quantum wires in semiconductor nanostructures (DOD)

Nanoelectronic devices based on transport in one dimensional quantum wire structures are being considered for future ultra-dense and ultra-low-power electronics. Such quantum wire devices have been fabricated using semiconductors, InAs and AlSb, and special fabrication technology. Transport measurements show that electrons are, indeed, confined to one dimension, and that quantum interference effects are prevalent. Such devices may provide the basis for quantum devices used in quantum computing schemes. *Principal Investigator: C.H. Yang, Univ. Maryland.*

Observation of Coulomb blockade in single-layer gold nanocluster films (DOD)

Single-layer films of gold nanoclusters have been shown to exhibit strongly nonlinear current-voltage characteristics. Electrical characterization of these films as a function of temperature, cluster size and other geometrical parameters has demonstrated that the nonlinear behavior results primarily from Coulomb blockade. Of particular importance is the demonstration that the threshold voltage decreases linearly with temperature and increases linearly with cluster core size. These conclusions have been verified and the differing roles of Coulomb blockade and disorder elucidated using extensive numerical simulations. As a further result, the thresholding behavior of the films was exploited to demonstrate ultra-sensitive, ultra-low-power chemical vapor sensors. *Principal Investigators: M.G. Ancona, W. Kruppa, R.W. Rendell, A.W. Snow, E.E. Foos, D. Park and J.B. Boos, Naval Research Laboratory.*

Ultra-low power Schottky junction transistor (DOD)

A gate current controlled transistor concept for silicon-on-insulator technology has been proposed, which has the potential to operate with 100 times less power than equivalent CMOS transistors. Device and circuit simulations predict that as gate lengths shrink, the power dissipation will continue to decrease and the cutoff frequency will rise, exceeding 100 gigahertz frequencies for gate lengths less than 100 nanometers. The first device has been demonstrated and its operation is in excellent agreement with the simulations. Ultra-low power electronic circuits are envisioned for applications in autonomous vehicles and other portable electronics, where battery lifetimes are critical factors. *Principal Investigator: Trevor Thornton, Arizona State Univ.*

Nanoscale fabrication technology (DOD)

Using the technique called “nanoimprint lithography” (NIL), nanometer scale structures in a variety of materials (magnetic, semiconductor, and polymers) have been produced. Most recently, arrays of rings were produced on a 4-inch wafer, in which the diameter is 250 nanometers and the wall thickness is 50 nanometers. This technology will be a major technology in developing future nanoelectronic, nanomagnetic and nanophotonic devices and circuits. *Principal Investigator: Stephen Chou, Princeton.*

Heterojunction bipolar transistors (NASA)

The Jet Propulsion Laboratory is working towards demonstrating the world’s fastest transistor using InP-based heterojunction bipolar transistors (HBTs). In 2001, JPL demonstrated an ultra-fast front-side HBT process, which has yielded excellent transistor performance, with betas of >60 and cutoff frequencies in excess of 120 GHz, even on large 2 μm emitter devices. Process development included precisely controlled RIE-etching and undercutting of the 40 nm InGaAs carbon-doped base, airbridge contacts, and passive monolithic millimeter-wave integrated circuit (MMIC) components such as capacitors and nichrome resistors. *Principal Investigators: Lorene Samoska, Andy Fung and Peter Siegel, Jet Propulsion Laboratory.*

Carbon nanotube field-effect inverters (NASA)

This project demonstrated the first successful carbon nanotube (CNT) based inverter logic circuit. The logic circuit comprised a p-type metal-oxide-semiconductor (PMOS) and complementary metal-oxide semiconductor (CMOS) inverters based on single-walled carbon nanotube field-effect transistors. The device structures consisted of a CNT grown via a chemical vapor deposition (CVD) method and contacted by two metallic source/drain electrodes. The circuit that uses both CMOS and PMOS platforms has been shown to work at room temperature, and this has huge implications for electronics applications. This innovation is paving the way for the development of carbon nanotube transistor based integrated circuits and for future computing systems. *Principal Investigators: Xialoei Liu, Chengulung Lee, Changwu Zhou and Jie Han, Ames Research Center.*

Healthcare (\$20 million)

Topics include effective and less expensive health care achieved through development of remote and in-vivo diagnostics and treatment devices; diagnostics and therapeutics based on rapid

genome sequencing and intracellular sensors; early detection of tumors by nanoengineered MRI contrast agents; biosensors that will allow earlier detection of diseases and infections; gene and drug delivery targeted to cancer cells and organs in the human body; longer-lasting and more effective artificial organs; and use of tiny medical devices that will minimize collateral damage to human tissues.

Contributions from: DOE, NIH (lead), NSF

Antibacterial agents from controlled self-assembly of amino acid analogues (NIH)

This project has demonstrated that nanotubes originally developed to serve as tiny test tubes (with an opening smaller than 1 nm across!) to study chemistry in molecularly-confined spaces, can also be used to punch holes in bacteria. With holes in their membranes, the bacteria become leaky and die quickly. The nanotubes are built of amino acid subunits very similar to those found in the proteins in our bodies, but with one important difference: alternating subunits have a structure that is the mirror image of the structure of our own amino acids (that is, naturally occurring L-amino acids alternate with D-amino acids). The strings of subunits (called peptides) therefore form small disks, which under the right conditions (such as are found in cell membranes) can stack to form tubes. By controlling the chains that stick out of the nanotubes walls, overall characteristics of the tubes can be fine tuned. This makes it possible for the nanotubes to perforate bacterial membranes without harming the cells of the animal (in this study, a mouse) that was infected by the bacteria. Studies continue to determine if these little tubes can be made specific for a wide variety of harmful bacteria, while sparing the cells of the host. *Principal Investigator: M. Reza Ghadiri, Scripps Research Institute.*

Nanoscale self-assembly for bone repair (NSF, DOE, DOD)

Researchers at Northwestern University have used nanoscale self-assembly to create a composite material that is very similar to bone. In addition to future medical applications, the material may have applications for nerve repair, nanoelectric wires, and high-strength materials. *Principal Investigator: Samuel Stupp, Northwestern University.*

Fluorescent imaging with quantum dots (NIH, DOD)

Quantum dots (QDs), semiconductor nanocrystals about 2 to 7 nm in diameter, offer advantages for fluorescent labeling in biomedical research over the traditional organic dyes, but have been difficult to use. A group at Indiana University has shown how to incorporate very specific ratios of different QDs, into 1 micron plastic beads to serve as “bar codes,” and to attach biological molecules to the surface of those beads. This offers a new way to do gene-chip experiments without the chip – in liquid samples that may be much faster and more flexible, while still allowing study of more than 10,000 different molecules in a single test. A second group demonstrated how to change the surface of the QDs themselves, so they could bind to short DNA strands for use in experiments to detect mutations inside cells. These basic experimental tools have many applications, including disease diagnosis, drug discovery, the study of basic disease mechanisms, and detection of infectious (including biothreat) agents. *Principal Investigators: Shuming Nie, Indiana University; Norman Arnheim and Mark Thompson, Univ. of Southern California.*

Nanopores distinguish subtle differences in DNA sequence (NIH, DOE, DOD)

Two independent research groups have made similar, important steps toward developing a nanopore-based DNA sequencing device. A group at the University of California, Santa Cruz, studied small DNA molecules bent into hairpin structures. When these molecules interacted with a protein pore that had been inserted into a membrane, and electrical measurements were made across the membrane, it was possible to distinguish between molecules that differed from each other by as little as one DNA base-pair in the length of the hairpin structure, or by one DNA base in the loop at the top of the hairpin. More strikingly, it was possible to distinguish between molecules in which the “stem” of the hairpin structure was perfectly base-paired (A with T and G with C), versus molecules in which the paired bases were mismatched (e.g., A with A). That is, by sensing differences in DNA structure, the investigators could distinguish differences in DNA sequence. Meanwhile, at Texas A&M University, a single-stranded DNA molecule was tethered within the pore itself. When a second single-stranded DNA molecule was introduced into the solution surrounding the pore, differences were detected in the electrical signals across the membrane, depending on whether the challenger DNA could base-pair exactly with the tethered DNA or if it contained a mismatch. Further, different mismatches (e.g., T with G versus T with C versus T with A) yielded different signals. Thus, both groups demonstrated the ability to sense DNA sequence-dependent signals using nanopore devices. *Principal Investigators: David Deamer, University of California Santa Cruz; Hagan Bayley, Texas A&M University.*

Nanoscale Processes in the Environment (\$6 million)

Nanotechnology has potential applications to monitor and remediate environmental problems, curb emissions from a wide variety of sources, and develop new, green processing technologies that minimize the generation of undesirable by-product effluents. Integration of biological building blocks into synthetic materials and devices will permit the combining of desirable materials properties with biological functions for materials released in the environment. The measurement, control, and remediation of contaminants in various media may also benefit from nanotechnological approaches.

Contributions from: DOE, EPA (lead), NSF

Nanoscale science and engineering center (NSF)

The NSEC on “Nanoscience in Biological and Environmental Engineering” at Rice University addresses societal implications of nanotechnology related to environment and biology. *Principal Investigators: Richard Smalley and Vicki Colvin, Rice University.*

Photocatalytic degradation of organic contaminants in water (DOE)

A “sense and shoot” approach has been developed for the photocatalytic degradation of organic contaminants from aqueous solutions. The feasibility of employing nanostructured ZnO films for simultaneous sensing and degradation of organic contaminants from aqueous solutions has been demonstrated. Detection sensitivity on the order of 1 ppm has been achieved for chlorinated phenols dissolved in water. *Principal Investigator: Prashant Kamat, University of Notre Dame.*

Greener synthesis of quantum dots (NSF)

This project involves development of green chemistry-based methods for the large-scale synthesis of nano-sized cadmium selenide crystals from the less toxic precursor cadmium oxide. These methods will be quite different from the presently used methods with precursor dimethyl cadmium, which is toxic, unstable and expensive. The award will help to develop new methods for the large-scale synthesis of semiconductor nanocrystals of uniform size and shape for applications in electrooptic devices. *Principal investigator: Xiaogang Peng, University of Arkansas.*

Energy (\$16 million)

Nanotechnology holds dramatic improvement in the efficiency of energy conversion and storage, and for doubling the efficiency of solar cells.

Contributions from: DOD, DOE (lead)

Nanofluids (Argonne National Laboratory, DOE)

Nanofluids (tiny, solid nanoparticles suspended in fluid) have been created that conduct heat ten times faster than previously thought possible, surpassing the fundamental limits of current heat conduction models for solid/liquid suspensions. These nanofluids are a new, innovative class of heat transfer fluids and represent a rapidly emerging field where nanoscale science and thermal engineering meet. This research could lead to a major breakthrough in making new composite (solid and liquid) materials with improved thermal properties for numerous engineering and medical applications to achieve greater energy efficiency, smaller size and lighter weight, lower operating costs, and a cleaner environment. *Principal Investigator: S.U.S. Choi, Argonne National Laboratory.*

Semiconductor nanocrystals as “artificial leaves” (DOE)

Recent experiments have demonstrated that carbon dioxide can be removed from the atmosphere with semiconductor nanocrystals. These “artificial leaves” could potentially convert carbon dioxide into useful organic molecules with major environmental benefits. However, to be practical, the efficiency must be substantially improved. New theoretical studies have unraveled the detailed mechanisms involved and identified the key factors limiting efficiency. Based on this new understanding, alternative means for improving efficiency were suggested that could lead to effective implementation of artificial leaves to alleviate global warming and the depletion of fossil fuels. *Principal Investigator: S. Pennycook, Oak Ridge National Laboratory.*

Microcraft and Robotics (\$5 million)

This topic involves continuous presence in space outside of the solar system with low-powered, autonomous spacecraft.

Contributions from: DOD, NASA (lead)

Nonvolatile memory based on silicon nanocrystals (NASA)

NASA requirements for computing and memory for microspacecraft emphasize high density, low power, small size, and radiation hardness. By using Si nanocrystal ensembles for the floating

gate of a flash memory, the distributed nature of a storage element leads to intrinsic radiation hardness. Researchers have demonstrated and measured charge injection into single Si nanocrystals (NC), and have developed a quantitative model of the charging process and of the amount of charge injected into a single nanocrystal. In addition, they have developed an aerosol fabrication process for Si nanocrystals that is compatible with the strict contamination standards of CMOS, and have completed the first generation of non-volatile memory devices incorporating aerosol-synthesized Si nanocrystals, in collaboration with Lucent Technologies. *Principal Investigators: L. Douglas Bell, Jet Propulsion Laboratory; Harry Atwater and Julie Casperson, CIT.*

Mechanical properties in CNT based nanocomposites (NASA)

Good dispersion of carbon nanotubes in a polymer matrix has been achieved by polymerization under sonication of the polymer resin (LaRC CP2) with carbon nanotubes. Nanocomposite films cast from the above resin were tested to determine mechanical properties. Dynamic mechanical data show that modulus increases with increasing nanotube concentration, with up to a 60% improvement at 1.0 vol% single wall nanotube loading level. Experimental results were found to be in good agreement with predicted theoretical models. The thermal stability of CP2 was also enhanced by the addition of SWNT. The uniformly dispersed nanotubes presumably provided thermo-oxidative stability to the polymers in the vicinity of the tube surfaces. *Principal Investigator: Tom Sutter, Langley Research Center.*

Functionalization of carbon nanotubes (NASA)

NASA/Ames researchers have demonstrated a clean, low-temperature process for the functionalization of single walled carbon nanotubes (SWNT) with atomic hydrogen. A cold plasma enhanced gas phase approach is used where a microwave discharge generates the atomic hydrogen. The approach of using a glow discharge provides a clean gas-phase process to functionalize SWNTs for further application development. The approach can be used to functionalize nanotubes with other chemical species. Gas phase functionalization techniques could prove extremely useful to fabricate sensors and devices based on SWNTs. Also, hydrogenated nanotubes may impart radiation shielding properties to composites for space applications. *Principal Investigator: Bishun Khare, M. Meyyappan, Alaln Casell, Cattien Nguyen, and Jie Han, Ames Research Center.*

Quantum dot based laser (NASA)

Most atmospheric and planetary gases have strong absorption bands in the 2 to 5 micron wavelength range. Therefore, semiconductor laser diodes and detectors in this range are enabling technologies for NASA missions. Quantum dot (QD) lasers are expected to have superior lasing properties, such as lower threshold current density and higher temperature stability compared to quantum well lasers, and radiation tolerance. Hence, the goal is to develop quantum dot based lasers and detectors that operate at 2-5 microns. As a first step toward this goal, researchers have demonstrated high performance spatial single mode quantum dot narrow ridge wave guide F-P lasers at 1.3 μm using four stacks of InAs QDs embedded within strained InGaAs quantum wells. *Principal Investigators: Yeuming Qui, Pawan Gongga, R. Muller, P. Maker, and Siamak Forouhar, Jet Propulsion Laboratory; and Andreas Stintz and Luke Lester, University of New Mexico.*

Bio-nanodevices for Detection and Mitigation of Threats to Humans (\$10 million)

This topic involves efficient and rapid biochemical detection and mitigation *in situ* for chemical- and bio-warfare, HIV, and tuberculosis. Miniaturized electrical/mechanical/chemical devices will extend human performance, protect health, and repair cellular and tissue damage. In FY 2002 this grand challenge has been redefined and broadened into chemical, biological, radiological, and explosive detection and protection. The highlights presented below have been selected to be consistent with this broader definition.

Contributions from: DOD, NASA, NIH, NSF

Efficient and ultrafast light-harvesting dendrimers (DOD)

Dendrimers are tree-like structures growing from a central point. Researchers at U. of Missouri have demonstrated the efficient and ultra-fast energy transfer properties of a new type of light-harvesting dendrimer based on phenylacetylenes. Such dendrimers exhibit broad absorption windows and possess an intrinsic energy gradient towards the core. With an energy trap (such as perylene) at the dendritic core, energy transfer quantum yields of over 90% and subpicosecond timescale excited state dynamics were obtained. Such dendrimers are being used as efficient fluorescence-based ion sensors and nonlinear optical materials. *Principal Investigator: Zhonghua Peng, University of Missouri, Kansas City.*

Development of sensors for detecting TNT in seawater (DOD)

The objective of this research is to re-design the specificity of *E. coli* periplasmic binding proteins to bind TNT instead of their natural ligands, and to incorporate a reporter fluorophore or electrochemical redox group as a readout for TNT occupancy of the re-designed binding site. Initial calculations have been completed, and 21 candidate designs, spanning four different protein scaffolds within the periplasmic family, have been identified. Nanomolar binding and reporting of TNT was observed within the very first set of engineered receptors. Directed evolution of these is expected to appreciably refine their binding and readout properties. *Principal Investigator: Homme W. Hellinga, Duke University Medical Center.*

Development of an icosahedral plant virus as a display system and reaction platform (DOD)

A successful derivitization of the native virus and the crystal structure of a derivitized CPMV particle was reported recently, as well as the preparation of the site-specific mutations that allow the attachment of fluorescent dyes and gold clusters through maleimide linkers. Derivitized CPMV particles generally display 60 copies of the attached molecule, and these high local concentrations of attached chemical agents may result in novel chemical and/or biological properties. These dramatic results are the first demonstration that virus particles can be exploited as addressable nanoblocks imbued with a variety of chemical and physical properties. *Principal Investigator: John E. Johnson, Scripps Research Institute.*

Chip-based technologies for forensic applications of DNA analysis (DOJ)

The first chip, created at the Whitehead Institute, uses a capillary based system similar to that employed in existing forensic DNA laboratories, but on a chip format that will ultimately lead to greater speed of processing and improved efficiency in the use of forensic DNA labs. This project has a working prototype chip that allows for simultaneous analysis of 16 DNA samples for all of the 13 short tandem repeat (STR) genetic markers required to search the National DNA

Index System (NDIS) containing convicted offender and unsolved casework DNA. The Whitehead DNA chip is entering its evaluation phase by the forensic DNA community. The second chip, under development by Nanogen Corp., is a hybridization chip that has the potential for higher resolution power than a capillary system. With three of the 13 STR genetic markers already embedded in this format, the developers are looking at the addition of new markers, called, “single nucleotide polymorphisms” (SNPs), for future use as investigative aids at the crime scene. These DNA analysis chips will provide portability, smaller instrument footprints, and higher DNA analysis throughput to effectively and efficiently address the expected increased use of DNA analysis in the criminal justice system. *Principal Investigators: Dr. Daniel Erlich, Whitehead Institute; and Dr. Ronald Sosnowski, Nanogen.*

New broadband stochastic biosensors with digital readout (DOD)

The objective is to create stochastic sensor elements from *single* genetically engineered channels (e.g., alpha-hemolysin) and incorporate these into rugged, portable devices for real-time classification and quantification of trace levels of DOD-relevant analytes in complex backgrounds: divalent metal ions, organics (e.g., explosives), proteins (e.g., bacterial toxins), nucleic acids (e.g., gene fragments, antisense therapeutics), and microorganisms (e.g., pathogenic viruses). Using α -hemolysin variants with engineered binding sites, it was shown that practically any divalent metal cation (e.g., Zn, Ni, Cd, Co) could be analyzed at nanometer scale, individually or in mixtures. A very large number and variety of organics (e.g., drugs, contaminants) can be combinatorially processed, using molecular adaptors such as cyclodextrins. Targets that cannot enter the channel (e.g., protein toxins) are transiently captured externally via chemical tethers. Single strand nucleic acid sequencing has also been demonstrated, as has the use of the plugged channel as a nanoreactor. *Principal Investigator: Hagan Bayley, Texas A&M.*

Gold cluster nanosensors and nanodevices (DOD)

Researchers at North Carolina State University have been characterizing fundamental electron transport behaviors in individual gold nanoclusters and have demonstrated that single electron tunneling behaviors can be accessed in fluid media. (Single electron tunneling is manifested as a step-like current vs. voltage curve commonly known as the Coulomb staircase. These behaviors are a unique property of nanometer-sized particles.) They further demonstrated that Coulomb staircase behaviors could be programmed to respond to certain analytes in solution. Ultimately, the goal of this work is development of low power, portable sensor arrays capable of detecting single analyte molecules. *Principal Investigators: Daniel Feldheim, Christopher Gorman, N. Carolina State Univ.*

Nanotube and nanowire mechanical resonance for sensing applications (DOD)

Researchers at Northwestern University are developing fundamental understanding of the mechanical resonance of nanotubes and nanowires, and are developing mechanically resonating structures into real sensor architectures. One example is the integration of individual nanotubes or nanowires into a functional mechanical resonator sensor, e.g., in sensor arrays having hundreds to thousands of individual nanostructure sensors. The goal is to develop sensors for multiple environments including gas phase, liquid and biological environments. *Principal Investigators: Rodney Ruoff, Wing Kam Liu, and Junghoon Lee, Northwestern Univ.*

Nanoscience of microwave-based integrated biological sensors (DOD)

Researchers at the University of Wisconsin and NRL are developing new methods for directly detecting biomolecules in solution by measuring the changes in electrical properties that accompany binding to chemically-modified surfaces of silicon and/or diamond. The method is based upon the fabrication of small resonant surface structures that exhibit electrical resonances at microwave frequencies; by measuring the shift in frequency of the resonators, biomolecular binding events can be detected directly. The program aims to develop devices that integrate detection of biological agents with a direct interface to electronic signal transduction. *Principal Investigators: Robert Hamers, Lloyd Smith, and Daniel Van der Weide, University of Wisconsin; and John Russell and James Butler, NRL.*

Combinatorial processing and characterization of nano-scaled photovoltaic/photo sensing devices using contact electrostatic self-assembly (DOD)

This project has exploited electrostatic self-assembly (ESA) processing – localized and continuous – to examine new materials and multilayer structures for flexible solar cells. Processing and characterization of PPV(donor)/C₆₀(acceptor) multilayer structures has revealed optimum thicknesses of both “block” thicknesses for photovoltaic performance. Localized (<100 μm) multilayer growth through the use of hydrogel-pen contact assembly of electroactive polymers has been demonstrated and extensively characterized. This is now enabling the rapid screening of acceptor/donor combinations on the basis of short-circuit current and open-circuit voltage. Finally, continuously graded multilayer “libraries” have been processed by imposing in-plane temperature gradients on electroactive multilayer structures and characterized discretely using fine ITO lines patterned with acid-etching in microfluidic channels. These new photovoltaic structures and characterization methods will enable the realization of flexible, polymer-based solar cells through rapid optimization of both material combination and multilayer structuring. *Principal Investigators: P.T. Mather, University of Connecticut, and M. Durstock, AFRL/ML.*

Miniaturized sample concentrators and real-time chemical agent sensors using nanobio- and nanobiomimetic materials (DOD)

A miniaturized intelligent sensor (MIS) consisting of a nanocapsule-based sample concentrator, a nanobiomimetic materials-based capture/target recognition probe, and a real-time optical signal transduction platform was developed. The sensor is capable of concentrating analytes with enzyme (e.g., OPAA) containing nanocapsules while performing real-time detection at parts per trillion (ppt) levels. Nanobiomimetic materials employed in this research are the best known for nerve agent and pesticide detection. Hydrolyzed and non-hydrolyzed organophosphate compounds, a major class of compounds that cover both nerve agents and pesticides, can be readily detected with molecularly imprinted polymer (MIP) based fiber-optic sensors at low or sub parts per trillion level without using fluorescent tags. *Principal Investigators: Ray Yin and Amanda Jenkins, ARL.*

Nanoscale Instrumentation and Metrology (\$11 million)

Development of highly capable, low-cost, standardized, and efficient tools and instruments for the measurement of nanoscale phenomena and for the manipulation of nanostructures. New calibrated instruments with nanoscale resolution will accelerate scientific discovery, provide

quality control in the fabrication and assembly of manufactured nanostructures, and stimulate new approaches to miniaturized sensors and actuators. This grand challenge topic has been formally established in FY02; however, anticipating its importance, projects were already initiated in FY01.

Contributions from: NIST (lead), NSF

Linewidth metrology instruments (DOC)

Developed prototype critical dimension reference materials for calibrating line width metrology instruments used in manufacturing semiconductor devices. *Principal Investigators: M. Cresswell, NIST*

Nanometrology standards (DOC)

Developed SPM oxidation method for lithographic patterning with capability for producing 10 nm to 40 nm line widths on silicon for application to nanometrology standards, nanoelectronic device structures and templates. *Principal Investigators: J. Dagata, NIST*

Deposition of multilayer GMR films (DOC)

Demonstrated the importance of measuring and controlling oxygen partial pressure during the deposition of multilayer GMR read/write heads; the process is used by all major hard-disk drive manufacturers. *Principal Investigators: W. Egelhoff, NIST*

C. Centers and Networks of Excellence (\$71 million)

Fourteen new centers have been established or competed: 6 NSF, 3 DOE, 3 NASA, 1 DOD. The new centers will enable activities that cannot be done in the traditional mode of single investigators and small groups or with the current research infrastructure. In addition, support has been provided to existing activities as those at the National Nanotechnology User Network (five universities), the Science and Technology Center on Biotechnology (Cornell University), the Materials Research Science and Engineering Centers, and the Engineering Research Centers.

NSF Nanoscale Science and Engineering Centers (NSEC)

The National Science Foundation (NSF) has made awards of \$65 million over five years to fund six major centers in nanoscale science and engineering. The six centers will be located at Columbia and Cornell Universities and Rensselaer Polytechnic Institute in New York, Harvard University in Massachusetts, Northwestern University in Illinois, and Rice University in Texas. Each of the six centers has a bold vision for research at the frontiers of science and technology. Together they will provide coherence and a longer-term outlook to U.S. nanotechnology research and education. The centers are expected to significantly advance the information, medical, manufacturing and environmental technologies, while other NSF grants will fund small, interdisciplinary research teams and individuals doing exploratory research in a wide range of areas. The centers involve key partnerships with industry, national laboratories and other sectors. They will support education programs from the graduate to the pre-college level designed to develop a highly skilled workforce, advance pre-college training, and to advance the public understanding of science and engineering.

DOE Centers

The Department of Energy's Nanoscale Science Research Centers (NSRC) are an important companion to the activities that support individual investigators and small groups of investigators in the BES and in research programs of other agencies. NSRCs have two main goals: (1) the advancement of science at the nanoscale and (2) making available to the scientific community state-of-the-art instrumentation and facilities. NSRCs will provide advanced instrumentation and access to facilities for investigators and groups working together on problems of a scope, complexity, and disciplinary breadth not possible working separately. They will provide a mechanism for short- and long-term collaborations and partnerships among DOE laboratory, academic, and industrial researchers. NSRCs must actively reach out to local and national universities and to industrial research facilities through a variety of formal mechanisms including, for example, joint appointments, resident scholar programs, student training, and broadly based advisory boards. NSRCs are intended to serve the Nation's needs and complement existing university and industrial capabilities in the tradition of the BES user facilities and collaborative research centers. As with all BES facilities and collaborative research centers, the NSRCs will operate with no fees for users who intend to make the results of their research widely available. NSRCs will be sited at laboratories already hosting BES facilities and will build on the existing research and facility strengths of the host institution in areas of materials science, chemistry, and x-ray and neutron scattering. When possible, NSRCs will be sited adjacent to or appended to an existing BES major user facility. Based on peer review, three centers (Molecular Foundry at Lawrence Berkeley National Laboratory, Center for Nanophase Materials Sciences at Oak Ridge National Laboratory, and Center for Integrated Nanotechnologies at Sandia National Laboratories and Los Alamos National Laboratory) were authorized to proceed with Conceptual Design.

NASA University Research Engineering and Technology Institute (URETI) Program

The URETI Program seeks to start five Institutes in R&D areas critical to NASA missions. Of these, three of the Institutes will focus on Bio/Nano Technology: Bio/Nano/Information Technology Fusion; Bio/Nano Technology Material and Structures for Aerospace Vehicles; and Nano Electronics and Computing. The Institutes will be funded for a possible 10 years at up to \$3 million per year, and will emphasize interdisciplinary and synergistic research groups as well as educational opportunities. Proposals were submitted in December 2001. Evaluation Teams have completed their recommendations and awards will be announced in May 2002.

Army University Affiliated Research Center

In March 2002 MIT was awarded the five-year, \$50 million center entitled "Institute for Soldier Nanotechnology" (ISN). Industry will contribute an additional \$40 million in funds and equipment. The ISN will be staffed by up to 150 people, including 35 MIT professors from nine departments in the schools of engineering, science, and architecture and planning. In addition to MIT faculty, 80 graduate students, and 20 postdoctoral associates, the ISN will also include specialists from the Army; E.I. du Pont de Nemours and Co., Wilmington, Del.; Raytheon Co., Lexington, Mass.; and physicians from Massachusetts General Hospital and Brigham and Women's Hospital. The ISN will focus on six key soldier capabilities: threat detection, threat

neutralization (such as bullet-proof clothing), concealment, enhanced human performance, real-time automated medical treatment, and reduced logistical footprint (i.e., lightening the considerable weight load of the fully equipped soldier).

D. Research Infrastructure (\$76.8 million)

This topic includes: modeling and simulation infrastructure, user facilities, tools and equipment. This is supported by a variety of facilities and networks. Examples include the following:

NSF Modeling and Simulation Network

This is focused on multiphenomena at the nanoscale and integration of scales. A network of universities, in collaboration with industry and government laboratories, will develop advanced nanoscale simulation software and a user facility.

National Nanofabrication Users Network (NNUN)

NNUN provides the nation's researchers with access to advanced nanofabrication equipment and expertise to enable research in nanotechnology across all disciplines. Goals include expanding the applications of nanotechnology and supporting a broad spectrum of activities to develop the scientists, engineers, and nanotechnology workers of the future.

Naval Research Laboratory Nanoscience Building

This new building was funded with \$12 million of Military Construction money. The Nanoscience Building has been specially designed to minimize sources of noise (vibration, acoustic, electromagnetic, temperature and humidity fluctuations) that would inhibit measurement and manipulation at the nanoscale. There will be 5000 sq. ft. of Class 100 clean room, 4000 sq. ft. of quiet space (<35 dB acoustic, <0.3 mG EMI, ± 0.5 °C), and 1000 sq. ft. of ultra-quiet space (<25 dB acoustic, ± 0.1 °C). In addition ONR and NRL are providing about \$5 million for special purpose equipment, including a high resolution TEM, an Omicron nanomanipulator, an e-beam writer and a dual beam FIB. This special facility will be available to researchers throughout DOD and universities.

FY02 Defense University Research Instrumentation Program (DURIP)

This funded \$5 million in equipment purchases to university professors engaged in nanoscience research.

NIST Advance Measurement Laboratory

NIST continues construction of \$200 million facility that will provide a building with state-of-the-art control over potential noise sources.

E. Societal Implications and Workforce Education and Training (\$13 million)

Several activities have been initiated concerning societal implications of nanoscience and nanotechnology: (a) support for social and economic research studies has been made a high priority (new theme in the NSF program solicitations – several centers include societal implications in their programs); (b) a workshop on “Societal Implications of Nanoscience and Nanotechnology” was cosponsored by NSF and the results distributed to all agencies and NSTC; (c) a study on converging technologies for improving human performance was initiated; (d) collaboration with European Union in this area has been initiated; and (e) James Batterson, a Fellow at NNCO, prepared a report on reforming undergraduate education in nanoscience and engineering.

The budget is primarily directed to education and training is 13 million. The total education budget including education contributions to research assistantships and fellowships is estimated at \$28 million. At NSF, this component for 5,000 (students, teachers and scientists) in fiscal year 2001 is \$17.5 million (assuming the average education contribution is about \$3,500 for each student, teacher and scientist trained per year).

The Defense University Research Initiative in NanoTechnology (DURINT) program awarded 45 3-year Fellowships in FY01 to support the education of U.S. graduate students in nano-science, -engineering and -technology. Fellows could select the school of their choice. The DURINT fellowships are contributing \$2 million a year toward education and training.

Specific education and training activities are supported by NSF, NIH, and DOD (see list of examples in Tables 6.3-6.9).

F. Special Cross-Cutting National Needs

National Security

National security draws on essentially all of the grand challenges, but with special emphasis in Nanomaterials by Design; Nanoelectronics, Optoelectronics, and Magnetics; and Chemical, Biological, Radiological and Explosive Detection and Protection. DOD is the lead organization. In addition to those DOD-funded examples of research conducted under the fundamental research component of the NNI and the grand challenges that support national security, other agency projects include: (1) mechanical properties in CNT based nanocomposites (NASA, Microcraft and Robotics G.C.); (2) antibacterial agents from controlled self-assembly of amino acid analogues (NIH, Healthcare G.C.); (3) photocatalytic degradation of organic contaminants in water (DOE, Nanoscale Processes in Environment G.C.), and (4) nanofluids (DOE, Energy G.C.).

Transportation

Transportation draws on many of the grand challenges, but with special emphasis on Nanomaterials by Design; Energy; Nanoscale Processes and Environment, and Chemical, Biological, Radiological and Explosive Detection and Protection. Examples of research

conducted under other grand challenges that support Transportation include: (1) NSF-supported research on nanoscale polymer coatings and DOD research on silicate nanocomposites (Nanomaterials by Design G.C.); (2) DOD research on gold cluster nanosensors/nanodevices, microwave-based biological sensors, and Miniaturized Intelligent Sensors (Bio-nanodevices G.C.); and (3) DOE research on nanofluids (Energy G.C.). DOT is the lead organization.

G. Examples of Scientific, Engineering and Technology Breakthroughs in FY2001

Selected examples of scientific, engineering and technological breakthroughs itemized in Chapter 6 are also listed in Table 6.2, along with appropriate references. Those examples (bold in table) with greater expected impact are elaborated in Appendix B.

Table 6.2
Selected Breakthroughs

Breakthrough (recognized in 2001)	Principal(s)	Organization(s)	Supporting agency	Reference
Biological assembly of nanostructures	Belcher	UT-Austin	NSF	<i>Abstr Pap Am Chem S</i> 221: 415-INOR Part 1 Apr 1 2001; <i>Abstr Pap Am Chem S</i> 222: 53-POLY Part 2, Aug 2001.
Using DNA molecules to construct nanoscale devices	Seeman Goddard	New York Univ CIT	NSF	<i>Biophys J</i> 82, 1659 Part 2 (2002); <i>Nature</i> 415 (6867), 62-5 (2002)
Simulation of biological ion channels	Hess	U. of Ill-Urbana	NSF	VLSI Des 13(1-4), 179-87 Sp. Iss. SI (2001)
Artificial genetic system	Benner	University of Florida	NSF, NIH	<i>Abstr Pap Am Chem S</i> 221, 245-ORGN Part 2 Apr 1 2001
Nanocircuits	Heath Avouris	UCLA, IBM	DOD, NSF, NIST	<i>Science</i> 294, 2442 (2001)
Nanoscale film serves as molecular filter	Hupp	NWU	NSF	<i>Adv Mater</i> 13(24), 1895 (2001)
Artificial atoms and molecules	Ralph	Cornell	NSF	<i>Phys Rep</i> 345(2-3), 62-173 Apr 2001
UV laser from ZnO nanorods	Yang	LBNL	DOE	<i>Science</i> 292(5523), 1897-9 (2001)
Flow within carbon nanotubes	Gogotsi	Drexel U	NSF	<i>Appl Phys Lett</i> 79(7), 1021-1023 (2001)
MicroLens for nano research	Kino	Stanford	DOE	<i>J. Microelectromech. Sys</i> 10, 450-459 (2001)
Building semiconductor nanowires	Redwing	Penn State	NSF	<i>Adv Mater</i> 13(19), 1489 (2001); JVST B20(1), 389-92 (2002)
Multimillion atom simulation of mechanical phenomena	Vashishta	LSU	NSF	<i>Appl Surf Sci</i> 182 (3-4): 258-264 Sp. Iss. SI (2001)
First biological force microscope in geochemistry	Hochella	VPI	NSF	<i>Geomicrobiol J</i> 18(1), 63-76 (2001)
Predicting deformation, fatigue and fracture of interfacial nanomaterials	Suresh	MIT	DOD	<i>Nature</i> 411(6838), 656-6 (2001)
Templating polymers for terabit arrays	Tuominen	U Mass	NSF, DOE	<i>Langmuir</i> 17, 6396-8 (2001)

Breakthrough (recognized in 2001)	Principal(s)	Organization(s)	Supporting agency	Reference
Observations of atomic imperfections	Zhu	Brookhaven NL	DOE	<i>PRL</i> 85, 5126-5129 (2000)
Silicate nanocomposites for self-healing coatings	Vaia	AFRL/ML	DOD	<i>Chem Mater</i> 13(11), 4123-9 (2001)
Ultra-low power Schottky Junction Transistor	Thornton	Arizona State Univ	DOD	<i>IEEE T Electron Dev</i> 48(10), 2421-2427 (2001)
Silicon based Infrared Detection	Mazur	Harvard	DOD	<i>Appl Phys Lett</i> 78(13), 1850-1852 (2001)
Maskless Lithography with Scanned Probes	Dai	Stanford	DOD	<i>Adv Mater</i> 14(3), 191 (2002)
Quantum Dot Lasers	Bhattacharya	Univ Michigan	DOD	<i>IEEE Circuits Device</i> 18(1), 14-24 (2002)
Single Molecule Negative Differential Resistance	Tour	Rice	DOD	<i>Chem Eur J</i> 7(23), 518-34 (2001)
Massively Parallel Dip-Pen Nanolithography	Mirkin	NWU	DOD	<i>J Am Chem Soc</i> 123(32), 7887-7889 (2001); <i>MRS Bull</i> 26(7), 535-538 (2001)
Coulomb blockade in single-layer Au nanocluster films	Ancona	NRL	DOD	<i>Phys Rev B</i> 64(3), art. No. 033408 Jul 15 2001
Nanoscale fabrication Technology	Chou	Princeton	DOD	<i>Appl Phys Lett</i> 79(6), 845-847 (2001)
Carbon nanotube field-effect inverters	Liu	Ames Research Center	NASA	<i>Appl Phys Lett</i> 79, 3329 (2001)
Nanoscale recording system	Pappas	NIST	DOC	<i>Proc SPIE</i> 4232, 11-18 (2001)
Ferromagnetic Imprinting of Nuclear Spins in Semiconductors	Awschalom	UCSB	DOD	<i>Science</i> 294(5540), 131-4 (2001)
Defect Tolerant Moletronics	Williams	HP	DOD	Patent application
Molecular memory devices	Heath	UCLA	DOD, NSF	<i>J. Am. Chem. Soc</i> 123, 12632-41 (2001)
Superlattices for infrared detection	Brown	AFRL/ML	DOD	<i>IEEE Photonic Tech L</i> 14(3), 372-4 (2002)
Self-Aligned quantum dot nanoswitches	Berger	Ohio State U.	NSF	<i>Electron Lett</i> 37(23), 1412-1414 (2001)
Peptide nanotubes as antibacterial drugs	Ghadiri	Scripps Research Institute	NIH	<i>Nature</i> 412, 52-455 (2001)
Nanoscale self assembly for bone repair	Stupp	NWU	NSF, DOE, DOD	<i>Abstr Pap Am Chem S</i> 222: 171-Inor Part 1 AUG 2001; <i>Science</i> 294(5547), 1684-88 (2001)
Fluorescent visualization with quantum dots	Nie Arnheim	Indiana Univ U So Cal	NIH	<i>J. Am. Chem. Soc.</i> 123, 4103-4104 (2001); <i>Nature Biotech.</i> 19, 631-635 (2001)
Nanopores Distinguish Subtle Differences in DNA Sequence	Deamer Bayley	UCSC Texas A&M	NIH	<i>Nature Biotech.</i> 19, 248-252 (2001); <i>Nature Biotech.</i> 19, 636-639 (2001)

Breakthrough (recognized in 2001)	Principal(s)	Organization(s)	Supporting agency	Reference
Photocatalytic Degradation of Organic Contaminants in water	Kamat	Univ Notre Dame	DOE	<i>J Phys. Chem.</i> B106, 788-794 (2002)
Greener Synthesis of Quantum Dots	Peng	Univ. of Arkansas	NSF	<i>JACS</i> 124 (13), 3343-3353 (2002)
Nanofluids	Choi	Argonne National Lab	DOE	<i>Appl. Phys. Lett.</i> 78, 718-729 (2001)
Nonvolatile memory based on silicon nanocrystals	Bell	JPL	NASA	<i>Appl Phys Lett</i> 78, 3133 (2001)
Functionalization of carbon nanotubes	Khare	Ames Research Center	NASA	<i>Nanoletters</i> 2, 73 (2002)
Quantum dot based laser	Qui Stintz	JPL Univ New Mexico	NASA	<i>Appl Phys Lett</i> 79, 3570 (2001)
Explosive Detection by Nano-Thermo-Mechanical Signatures	Thundat	Oak Ridge National Laboratory	DOT, DOE	<i>Abstr Pap Am Chem S</i> 221: 324-IEC Part 1, Apr 1 2001
Nanostructures for Chemical/ Biological Agent Detection	Mirkin Snow	NWU NRL	DOD, NSF	<i>J. Am. Chem. Soc.</i> 122 (15), 3795-3796 (2000); <i>Abstr Pap Am Chem S</i> 221: 324-IEC Part 1, Apr 1 2001
Nanoparticles for Chemical/ Biological Agent Decontamination	Klabunde Baker	KSU U Michigan	DOD, NSF, NIH	<i>J. Am. Chem. Soc.</i> 123, 1636-1644 (2001); <i>Microbiological Research</i> 156, 1-7 (2001)
Detect TNT in Seawater	Hellinga	Duke	DOD	<i>Science</i> 293 (5535): 1641-1644 (2001)
Icosahedral Plant Virus as a Display System and Reaction Platform	Johnson	Scripps Res Inst	DOD	<i>Angew. Chem. Int. Ed.</i> 41(3), 459-462 (2002)
Stochastic Biosensors	Bayley	Texas A&M	DOD	<i>Nature</i> 413(6852), 226-230 (2001)
Linewidth Metrology Standards	Cresswell	NIST	DOC	<i>IEEE Trans. on Semiconductor Manuf.</i> 14(4), 9 (2001)
SPM Oxidation for Lithography	Dagata	NIST	DOC	<i>Appl. Surf. Sci.</i> 158(3-4), 205-216 (2000)
Multilayer GMR Materials	Egelhoff	NIST	DOC	<i>J. Appl. Phys.</i> 89(9), 5209-5214 (2001)

H. Examples of Education and Training Activities in Fiscal Year 2001

Examples of education and training activities supported directly by education and training programs, or indirectly by research awards, are shown in Tables 6.3 through 6.10. NSF has a key role in funding those activities, in collaboration with DOD, NIST, NIH and other agencies. Table 6.3 shows examples of nanoscale science and engineering courses offered in U.S. universities.

Table 6.3
Examples of Courses on Nanoscale Science and Engineering Offered in U.S. Universities

Topic	University
Nano-course (for undergraduate, summer course)	Cornell Nanofabrication Facility (A. Clark, M. Isaacson)
“Capstone” course on nanotechnology “hands-on” (for undergraduates and two-year colleges)	Nanofabrication Facility, Pennsylvania State University (S.J. Fonash)
Semiconductor manufacturing and nanofabrication (laboratory for undergraduates)	University of California at Los Angeles (J.P. Chang)
Advanced quantum devices (for graduate students)	University of Notre Dame (EE 666)
Nanotechnology	Virginia Commonwealth University (M. El-Shall)
New technologies	University of Wisconsin, Madison (R. Hamers)
Nanostructured materials (for graduate students)	Rensselaer Polytechnic Institute (R. Siegel)
Colloid chemical approach to construction of nanoparticles and nanostructured materials	Clarkson University (J.N. Fendler)
Nanoparticle processes (for graduate students)	Yale University (D. Rosner)
Nanorobotics (for graduate students)	South California University (A. Requicha)
Chemistry and physics of nanomaterials	University of Washington (Y. Xia)
(a) Scanning probes and nanostructure characterization; (b) Nanoscale physics	Clemson University (D. Correll)
Nanomanufacturing processes, using Distributed Interactive Studio House (DISH), a multimedia classroom integrated laboratory	University of Arkansas, in partnership with states Arkansas, Oklahoma and Nebraska (A.P. Malshe)
Nanoscale science and engineering	Purdue University (R. Reifengerger)

Graduate Education, Research and Training (IGERT) Projects

Table 6.4 shows examples of Integrative Graduate Education, Research and Training (IGERT) projects sponsored by NSF with focus on nanoscale science and engineering. Graduate students receive fellowships for interdisciplinary topics and move under the guidance of several professors with various expertise. The awards are made for five years.

Table 6.4
IGERT Projects

Topic	University (lead investigator)	Starting Year
Nanophases in the Environment, Agriculture and Technology (NEAT)	University of California – Davis (A. Navrotsky)	1999
Nanostructured Materials and Devices	City University of New York (D.L. Akins)	2000
Nanobiotechnology	University of Washington (V. Vogel)	2000
New materials for electronics and optics through control of nanoscale structure	University of Oregon (D. Johnson)	2001
Nanoparticle science and engineering	U. of Minnesota (U. Kortshagen)	2001
Multidisciplinary graduate materials creation training program	University of California, Los Angeles (F. Wudl)	2001
Macromolecular science and infrastructure engineering	Virginia Polytechnic Institute and SU (J. Riffle)	2001
Biophotonics materials and applications	SUNY-Buffalo (A. Cartwright)	2001

Centers and Networks

Large research groups, centers and networks offer special interdisciplinary/multi-relevance opportunities for both R&D and education and training. NSF has established six Nanoscale Science and Engineering Centers (NSEC) in September 2001 under the NNI. Those centers are funded for five years, and are renewable after review in 2006 for other five years. Their educational and outreach activities in addition to diversifying graduate education are summarized in Table 6.5. This is an extension of the tradition of significant education and outreach activities at the National Nanotechnology User Network (NNUN), Dechartes nanoscale simulation network, and Science and Technology Center on Nanobiotechnology at Cornell University, as well as at several Materials Research and Engineering Centers (MRSEC) and Engineering Research Centers (ERC). For example, the NSEC education activities at Cornell University will include the K-12 Teacher Institute, freshman Introduction to Nanotechnology course, Nanotechnology Equipment Lending Library with nanoscience experiments for use by teachers with high-school students, Montessori K-4 curriculum development, and a modular traveling exhibition for the family Ithaca Science Center. Social scientists were involved from the first year of the new NSEC awards. A special focus on societal implication is at the NSEC on Biological and Environmental Engineering (Rice University). Other models are the Research Experience for Undergraduate (REU) and Research Experience for Teachers (RET) sites funded by NSF. Examples are the REU site for nanotechnology at Cornell University, and the RET on nanoscale copolymer at University of Massachusetts, Amherst. Table 6.5 shows key educational activities of the Nanoscale Science and Engineering Centers (NSEC) funded in September 2001.

Table 6.5
Education and Training in Centers and Networks

NSEC (2001-2006)	Key Educational Activities (in addition to graduate education)
Electronic Transport in Molecular Nanostructures (Columbia University)	Engaging high school students in collaboration with the City University of New York; and mentor undergraduates and graduates through specialized summer and academic year programs.
Nanoscale Systems in Information Technologies (Cornell University)	Partnering with industry to support a K - 12 Teachers Institute and a nanotechnology teaching laboratory; freshman Introduction to Nanotechnology; collaboration with Ithaca Sciencecenter (traveling exhibition)
Science of Nanoscale Systems and their Device Applications (Harvard University)	Outreach to middle school students and teachers; and fostering public education in partnership with the Boston Museum of Science.
Integrated Nanopatterning and Detection Technologies (Northwestern University)	Web-based outreach to high school science teachers and the development of curriculum material for middle and high schools; Initiating a small business entrepreneurs program; Partnering with the Museum of Science and Industry in Chicago; summer research programs for minority undergraduates.
Directed Assembly of Nanostructures (Rensselaer Polytechnic University)	Partnerships with industry and several colleges (Morehouse, Mount Holyoke, Smith, Spelman and Williams) to enhance research opportunities for groups that are underrepresented in science; K - 12 teaching program in collaboration with the Junior Museum of Troy.
Nanoscience in Biological and Environmental Engineering (Rice University)	Identify, recruit, and train a nanoscience workforce, particularly among groups currently underrepresented in the science workforce; a partnership with the Jones Graduate School of Management for an entrepreneurial education program.

Combined Research Curriculum Development (CRCDD) Projects

Table 6.6 shows examples of Combined Research Curriculum Development (CRCDD) projects focused on nanoscale science and engineering. The program offers a special opportunity for integration of research and education in the field of nanotechnology

Table 6.6
CRCDD Projects Focused on Nanoscale Science and Engineering

Topic	University (lead investigator)
Computer simulation of materials from atomistic to the continuum level	Virginia Polytechnic Institute and State University (R. Krill)
World wide web – based textbook on molecular simulation	University of Tennessee – Knoxville (P. Cummings)
Computational materials science and nanoscale science and engineering	University of Illinois at Urbana (D.M. Ceperley)

Local and Long-distance Outreach Education

Outreach activities are focused on K-12 (Kindergarten through 12th grade), academic institutions without strong infrastructure, and the public at large. Several illustrations are given in Table 6.7. Table 6.8 shows two leading examples of technological education.

Table 6.7
Educational Outreach Activities

University	Activity
University of Wisconsin	Education for schools and public at large
University of North Carolina	“The nanoManipulator”
Rensselaer Polytechnic Institute	Long distance undergraduate laboratory experience in nanoscience
Rice University	“Introduction to Nanoscience”
University of Tennessee	“Molecular Modeling and Simulation” network on the Internet
Arizona State University	“Interactive Nano-Visualization in Science and Engineering Education”
University of Illinois at Chicago	Course on “Micro and nano-electronic processes”

Table 6.8
Technological Education: Two Leading Examples

University	Activity
The Pennsylvania State University (S. Fonash)	“Regional center for nanofabrication manufacturing education” with the state and NSF grant support for 2001-2004. A partnership between the states, 14 universities, all state community colleges, vocational technical school, and industry has been established to enhance the state of Pennsylvania’s workforce preparation in nanotechnology. It targets degrees and outreach in “Nanofabrication Manufacturing Technology” via new curricula at community colleges and universities, training the teachers and community college educators, promote awareness of career opportunities.
University of Texas at Arlington, College of Engineering	The Nanotechnology Research and Teaching Facility has been established in 2001. This facility will provide laboratory “hands-on” training for technical, undergraduate and graduate education.

Public Education (non-technical audiences)

The public is the ultimate user and sponsor of the new technology. The importance of this activity has been underlined in a recent study on societal implications of nanoscience and nanotechnology. For example, the NSEC at Harvard University has outreach activities with the Boston Museum of Science. Examples of NSF sponsored projects focused specifically on public science education are given in Table 6.9 below. Examples of outreach to the public were listed earlier in Table 6.5.

Table 6.9
NSF-sponsored Projects for Public Science Education

Organizers	Activity
The University of Wisconsin and Discovery World science museum in Milwaukee	“Making nanoworld comprehensible”
The Arizona Science Center internships for undergraduate students and schoolteachers for programs with emphasis on nanotechnology for public and school outreach	“Internships for Creating Presentations on Nanotechnology Topics at a Science Center”
NSF	“Small Wonders: Exploring the Vast Potential of Nanoscience,” manifestation for the public and non-specialists at large in a public place (Washington, D.C. World Trade Center)
Industry group, with participation from NNI agencies	“National Nanotechnology Initiative: From Vision Towards Commercialization,” a status report and outlook for NNI research and education

International Dimension

International educational interactions are accelerating. Exchange of information, leveraging the research efforts, and education of younger generation are the main drivers. Examples are shown in Table 6.10.

Table 6.10
International Educational Interactions

Organizers	Activity
NSF and other agencies	Groups of young researchers travel to Japan, EU and other areas to present their work and visit centers of excellence in the field
NSF and other agencies	Bilateral and international activities have been under way since 2000 with European Union, Japan, Korea, India, Switzerland, Germany, Latin America, and APEC to name the most important.
NSF	Four joint workshops in 2002, one each on manufacturing, societal implications and education, tools, and materials.

7. Proposed Federal Contribution to the National Nanotechnology Initiative

A. Fiscal Year 2003

Government's Role in Nanoscience and Technology

While nanotechnology research is in an early stage, it already has produced several promising results. It is clear that it can have a substantial impact on industry and on our standard of living by improving healthcare, the environment and the economy. But investments must be made in science and engineering that will enable scientists and engineers to invent totally new technologies and enable industry to produce cost-competitive products. Since many of the findings on nanostructures and nanoprocesses are not yet fully measurable, replicable, or understood, it will take many years to develop corresponding technologies. Industry needs to know what the principles of operation are and how to economically fabricate, operate, and integrate nanostructured materials and devices. Private industry is unable in the usual 3-5 year industrial product time frame to effectively develop cost-competitive products based on current knowledge. Furthermore, the necessary fundamental nanotechnology research and development is too broad, complex, expensive, long-term, and risky for industry to undertake. Thus, industry is not able to fund, or is significantly under-funding, critical areas of long-term fundamental research and development that help to build R&D infrastructure. A coordinated national effort focuses resources on stimulating cooperation, avoiding unproductive duplication of efforts, capturing the imagination of young people, and supporting basic sciences. Government support provides for expansion of university and government laboratory facilities, helps to build the workforce skills necessary to staff future industries based on nanotechnology and future academic institutions, encourages cross-disciplinary networks and partnerships, ensures the dissemination of information, and encourages small businesses to exploit the nanotechnology opportunities.

Budget Summaries for Participating Departments and Agencies

Table 7.1 shows the Federal agency investments planned for the current fiscal year and requested for 2003. Activities that would be enabled by the proposed budget increase in FY 2003 include the following:

- New grand challenges on: Nanoscale Instrumentation and Metrology, Manufacturing at Nanoscale, and Chemical/Biological/Radiological/Explosive Protection and Detection
- Continue the development of the NNUN and the Modeling and Simulation Network (NSF), the NSF-sponsored Nanoscale Science and Engineering Centers, facilities at the DOE national laboratories; the University Aerospace Research Centers (NASA), and the University Affiliated Research Center (DOD)
- Promote educational programs involving teachers and K-12 activities
- Increase international components of various activities, including training and mobility of researchers
- Augment applied research funding to explore possible applications of the nanoscience discoveries

Table 7.1
National Nanotechnology Initiative R&D Funding (\$ millions)

	FY 2002	Proposed Augmentation	FY 2003	Percent Increase
Department of Defense	180	21	201	12
Department of Energy	91.1	48.2	139.3	53
Department of Justice	1.4	0	1.4	-
Department of Transportation	2	0	2	-
Environmental Protection Agency	5	0	5	-
NASA	46	5	51	11
National Institutes of Health	40.8	2.4	43.2	6
NIST	37.6	6.2	43.8	16
National Science Foundation	199	22	221	11
US Department of Agriculture	1.5	1	2.5	67
TOTAL	604.4	105.8	710.2	17

Funding Themes and Modes of Research Proposed for Funding Agencies in FY 2003

Below is an outline of the funding mechanisms (for more details on agency plans for each theme please see Appendix C).

1. *Fundamental research (total FY 2003 is \$227.5 million, \$14 million above FY 2002). This investment provides sustained support to individual investigators and small groups conducting fundamental, innovative research.*
2. *Grand challenges (total FY 2003 is \$266.7 million, \$32.2 million above FY 2002). Fund interdisciplinary research and education programs, which aim to achieve major, long-term objectives. The use of applied research monies, beginning in FY02 and growing in FY03, fuels the growth in grand challenge funding.*

Grand challenges initiated in FY 2001 (see NNI, Supplement to the President's FY 2001 Budget for details). Seven of the grand challenges initiated in FY01 continue to address the goals set out last year:

- Nanomaterials “by design”
- Nano-electronics
- Optoelectronics and Magnetism
- Healthcare
- Nanoscale Processes and Environment
- Energy
- Microcraft and Robotics

Grand challenges initiated in FY 2002 (see Chapter 10 for details). Reflecting new requirements and research opportunities, the NSET has decided to initiate three new grand challenges in FY03:

- Chemical, Biological, Radiological, and Explosive – Protection and Detection (CBRE)
 - Nanoscale Instrumentation and Metrology
 - Manufacturing at the Nanoscale
3. *Centers and networks of excellence (total FY 2003 is \$108 million, \$17 million above FY 2002).* Fund new centers at about \$3 million each per year for five years with opportunity of one renewal. Encourage research networking and shared academic users' facilities. Establish nanotechnology research centers, similar to supercomputer centers, that will play an important role in reaching other initiative priorities (fundamental research, grand challenges and education), in developing and utilizing the specific tools, and in promoting partnerships in the next decade. The NSF NSECs will develop partnerships with other universities and with national laboratories. The DOE national laboratory centers will be further refined with input from the potential user communities. The new NASA centers will be fleshed out and inaugurate their research programs. The new DOD Center for Soldier Nanotechnologies will begin its research program and augment its applied research efforts.
 4. *Research infrastructure (total FY 2003 is \$92 million, \$41 million above FY 2002).* Encourage university-industry-national laboratory and international collaborations as well as knowledge and technology transfer between universities and industry. Develop a flexible enabling infrastructure so that new discoveries and innovations can be rapidly commercialized by U.S. industry. The DOE program is to be substantially augmented, accounting for most of the \$41 million increase, to begin construction of its new center facilities. Construction of the NIST and Naval Research Laboratory nanoscience facilities will continue. Complementing the Federal investments, the number of facilities at universities will continue to grow with state and local funding providing most of the capital.
 5. *Societal implications and workforce education and training (total FY 2003 is \$16 million, \$1.6 million over FY 2002).* Fund student fellowships/traineeships and curriculum development on nanotechnology; and change general teaching paradigms with new teaching tools. Focused research on societal implications of nanotechnology, including social, ethical, legal, economic and workforce implications, will be undertaken. Educational programs involving teachers and K-12 activities will be developed.
 6. *Special cross-cutting national needs.* National security, and economical and safe transportation were listed as grand challenges in prior years. To adequately address their needs, these two topics must draw on the progress from many of the grand challenges. A more accurate representation of the relationship between the NNI and these two critical topics is as follows:
 - a. Economical and safe transportation: Transportation draws on many of the grand challenges, but with special emphasis on Nanomaterials by Design; Energy; Nanoscale Processes and Environment; and CBRE.
 - b. National security: National security draws on essentially all of the grand challenges, but with special emphasis in Nanomaterials by Design; Nanoelectronics, Optoelectronics and Magnetics; and CBRE.

Table 7.2 illustrates the NNI research portfolio by themes in FY 2003, as well as the FY 2003 increment above FY 2002 by each agency.

Table 7.2
National Nanotechnology Initiative Research Portfolio in FY 2003* (\$ million)

Agency	Fundamental Research	Grand Challenges	Centers and Networks of Excellence	Research Infrastructure	Societal Implications and Workforce	Total
DOD	20	136	38	5	2	201
DOE	35	31.3	23	50	-	139.3
DOJ	-	1.4	-	-	-	1.4
DOT	-	2	-	-	-	2
EPA	-	5	-	-	-	5
NASA	15	27	9	-	-	51
NIH	15	21.2	-	5	2	43.2
NIST	-	31.8	-	10	2	43.8
NSF	140	11	38	22	10	221
USDA	2.5	-	-	-	-	2.5
Total	227.5	266.7	108	92	16	710.2

* Estimations for individual themes may change depending on the merit review process.

Collaborative Activities in the FY 2003 National Nanotechnology Initiative

The NSET will coordinate joint activities that create synergies between the individual agencies in a variety of topics and modes of collaboration. The coordination will: identify the most promising research directions; fund complementary/synergistic fields of research critical to the advancement of the nanoscience and engineering field; develop a balanced infrastructure (portfolio of programs, development of new specific tools, instrumentation, simulation infrastructure, nanoscale standards); correlate funding activities for centers and networks of excellence; cost-share high-cost R&D activities; develop a broad workforce trained in the many aspects of nanotechnology; study the diverse, complex implications on society (e.g., effects of nanomaterial manufacturing on environment, effects of nanodevices on health); and avoid unnecessary duplication of efforts. The coordination also will address NNI management issues.

Improved internal coordination in large agencies, concurrently with interagency collaboration, has also been noteworthy in the planning process. The coordination addresses issues relate to research, infrastructure, societal implications, and education and training. The main collaborative activities planned for FY 2003 are listed below:

- Coordinated research and education activities in all five priority areas. Agency participation in the different priority topics is shown in Table 7.2 above.
- Focused joint programs on grand challenges and related topics: bioengineering (NIH, NSF, DOD and DOE); unmanned missions (NASA and DOD); lab-on-a chip (NIH, DOE, DOD, NIST, and NSF); quantum computing (DOD, DOE, NASA, NIST and NSF); and environmental monitoring (DOE and NASA).
- University-based centers on modeling and simulation at nanoscale, integration of components and devices at nanoscale, nanoscale systems and architectures, nanofabrication, nanotechnology and bio-robotics, and nano-biomedicine (Participants: NSF with STC,

MRSEC, ERC, NNUN and other centers; DOD with MURI; NIH and NASA; state and private organizations).

- Government laboratory-based user facilities and research networks. (Participants: All agencies, state and private organizations).
- An education and training network for nanoscience and engineering (Participants: all agencies).
- National facility at NIST for calibration and standards at the nanoscale (Participants: all agencies).
- NNI/NNCO information center for nanotechnology (Participants: all agencies).
- Societal implications of nanotechnology (Participants: DOD, NIH, NIST, NSF and other agencies).

Examples of major collaborative NNI activities crossing the participating agencies are shown in Table 7.3.

The NSET is reaching out to the nanoscience and nanoengineering efforts of other nations in order to take best advantage of knowledge developed by their S&T investments and collaboration opportunities. The NSET will continue the worldwide survey; the DOD international field offices will continue to assess the nanoscience investment strategies and commercial interests in their geographies of responsibility.

Table 7.3
Examples of Proposed NNI Interagency Collaborative Activities*

Topic/Agency	DOD	DOE	DOJ	DOT	DTr	EPA	NASA	NIH	NIST	NSF	USDA
Fundamental research	x	x			x		x	x		x	x
Nanostructured materials	x	x		x	x	x	x	x	x	x	x
Molecular electronics	x						x		x	x	
Spin electronics	x						x			x	
Lab-on-a-chip (nanocomponents)	x	x	x	x	x		x	x	x	x	x
Biosensors, bioinformatics			x	x			x	x		x	x
Bioengineering	x	x						x		x	x
Quantum computing	x	x					x		x	x	
Measurements and standards for tools	x	x		x		x		x	x	x	x
Nanoscale theory, modeling, simulation	x	x					x			x	x
Environmental monitoring and remediation		x				x	x			x	x
Nanorobotics		x					x			x	
Unmanned missions	x						x				
International collaboration	x	x	x	x	x	x	x	x	x	x	x
Nanofabrication user facilities	x	x		x		x	x	x	x	x	x

* (DOS is contributing to international aspects on all topics) (subject to funding approval)

Partnerships will be encouraged among the following:

- Disciplines (small group research)
- Institutions and types of institutions (e.g., universities, industry, government labs)
- U.S. Federal government and state funding agencies (support for complementary activities)
- Expensive equipment users (joint funding and use of facilities in centers)
- Countries (international collaborations to promote access to centers of excellence abroad, visits by young researchers abroad, and bilateral and multilateral agreements)

B. Outlook for the Future

Research Opportunities and Priorities

The proposed budget increase of \$106 million in FY 2003 (see Table 7.2) will focus primarily on fundamental research including biomimetics; augmenting the three new grand challenge programs (manufacturing at the nanoscale, nanoscale instrumentation and metrology, and chemical/biological/radiological/explosive detection and protection); and the development of a more balanced infrastructure. If additional funding were available beyond this proposed level, the following additional activities could be undertaken: increased support in fundamental research areas (important for relieving some of the NNI proposal pressure), augmented acquisition of instrumentation (important since instruments capable of measuring/manipulating at the nanoscale are evolving rapidly and must be constantly upgraded), eight new centers based either in universities or national laboratories (important to establishing focussed, multidisciplinary approaches on a greater variety of topics), a testing and training facility for academic institutions, nanotechnology training at all levels including teachers, and societal implications studies.

Program Priorities

The key priorities in the next five years are education and training; infrastructure, partnership with universities, private sector and states; and synergy with other national initiatives and priorities.

Education and training at all levels

The educational foundation in science and engineering will move from the microscopic to the molecular level. Education of K-12, undergraduate and graduate students, as well as continuing education activities for retraining, are envisioned. An important corollary activity is the retraining of teachers.

It will be necessary to fund training of students and support of postdocs under fellowships that will attract the best students available. This is extremely important, considering the rapid changes in the knowledge base. Students should receive multidisciplinary training in various nanotechnology fields. Both organizational attention and funding should also be devoted to ensuring the open exchange of information in multidisciplinary meetings and to rapid publication of results, through, for example, workshops and widely disseminated summaries of research.

Infrastructure needs for nanotechnology

Centers involving multiple grantees or laboratories where these tools would be available should be established at a level of several million dollars annually. These centers should also have diverse research teams that will be effective in different scientific disciplines. Means should be investigated to achieve remote use of these facilities. Funding mechanisms should be emphasized that encourage collaboration between centers, university, laboratories, and industry, as well as single investigators who are tied into these networks. A major potential barrier to cooperative efforts is the issue of intellectual property rights, which must be addressed in a national framework.

Partnership with universities, private sector and states

Joint investments from universities, industry, and states are already evident and will play an essential role in the advancement of the field of nanotechnology.

Synergy with other national initiatives and priorities

Complimentary, synergistic efforts will proceed in the areas of revolutionary computing (with ITR) and molecular biology (with modern biology). The nano-bio-digital triad is expected to play a determinant role in the science and engineering of the next decades.

- Information Technology Research and Development (ITR&D) Program. Over the last forty years, the rapid progress in information technology owes much to new, cost-effective, electronic, electrooptic, and magnetic devices. The miniaturization and cost reduction of those devices has been characterized by an empirical relationship called “Moore’s Law.” According to the International Technology Roadmap for Semiconductors (<http://public.itrs.net>), this continued miniaturization of semiconductor devices may end around 2010. Moore’s Law will eventually fail – unless nanotechnology or other advances successfully remove known roadblocks. One way the ITR&D Program can exploit continuing hardware improvements into the next decade is for the NNI to provide the science base necessary to continue the miniaturization of electronics components from micron into nanometer size scales.

Advances in nanotechnology will impact both computing and networking hardware. In the nearer term, technologies such as nanocrystals and carbon nanotubes could allow the fabrication of devices such as single-electron transistors, field-effect transistors, and non-volatile memories. These devices, of conventional function but nanoscale size, could deliver increased speed and density, reduced size and power/heat limitations, and even radiation hardness. In the longer term, nanotechnologies could make possible more complex devices that are difficult or expensive to fabricate using current-scale technologies, such as multi-state logic devices or high-connectivity devices like single-chip crossbar switches. Simultaneously with the NNI developing new nanoscale devices, the ITR&D Program is investigating alternative approaches to computation and networking. The NNI and the ITR&D Program will coordinate these activities to best exploit future opportunities.

Continued improvements in computing systems and software will have important consequences for nanotechnology. Understanding the properties of nanostructures depends critically on modeling and simulation. Nanostructures are small enough, and simple enough,

that the long-term materials science goal of reliable property predictions becomes possible. In selected cases, such as carbon nanotubes, the theory/modeling of nanostructures has predicted effects long before experimental confirmation. Present computational capability permits first-principal calculation of nanostructure properties, but only for small nanostructures and for limited dynamical time frames (nano- to pico-seconds). Progress in computing will reduce those limitations and is important to the rapid advance of nanoscience and nanotechnology. The NNI must communicate its specific computational needs to the ITR&D Program and work to exploit rapidly any ITR&D breakthroughs in computational hardware and software.

It is clear that close coordination of these two national initiatives is useful. The collocation of the National Coordination Office (NCO) for ITR&D the National Nanotechnology Coordination Office (NNCO) for the NNI facilitates the synergies.

- Modern biology and healthcare. Biomolecular reactions occur at the same length scale that forms the focus of the NNI. The potential for conceptual and technical crossover between modern biology and nanotechnology is therefore outstanding.

The synergy between the NNI and healthcare is clear. Medicine will benefit because nano-based technologies will replace time-intensive laboratory methods and permit point-of-care diagnosis. Based on the tremendous impact that DNA microarrays have already had on basic and clinical research, it is clear that expansion of micro- and nanotechnology for measuring a broader range of biomolecules will revolutionize disease research and diagnosis. Based on knowledge of molecular biology, concepts and components from biological systems will form the basis of classes of nanoengineered systems.

The impact of this knowledge of biological nanosystems has impact far beyond biology. Engineered systems whose design is based on biology’s design concepts, or that are hybrids of biological and non-biological materials, should have utility in, for example, bottom-up materials manufacturing processes. Nanoscience research therefore can leverage the long-standing investment in modern biology research.

Time Line Summary

Table 7.4 lists NNI key deliverables in the next five years (fiscal years 2003-2007). Out-year deliverables depend on regular increases in funding for this initiative.

Table 7.4
Deliverables

Outcomes Of The Investment	Target Date
<u>Provide augmented research and development</u> in fundamental research, grand challenges, infrastructure, education and nanotechnology’s societal impacts in response to open competitive solicitations and regular program reviews	FY 2003 -
Establish ten <u>new centers and networks</u> with full range of nanoscale measurement and fabrication facilities	FY 2003 -
Focused research on nanoscale <u>metrology and manufacturing</u>	FY 2003 -

Outcomes Of The Investment	Target Date
Develop new <u>standard reference materials</u> for semiconductor nanostructures, lab-on-a-chip technologies, nanomagnetics, and calibration and quality assurance analysis for nanosystems	FY 2003 -
<u>Leverage NNI funds</u> by at least 25% by working with states, universities and private sector to increase funding and synergism in R&D	FY 2003 -
Develop standardized, reproducible, microfabricated approaches to nanocharacterization, nanomanipulation and <u>nanodevices</u>	FY 2004 -
Develop <u>quantitative measurement methods</u> for nanodevices, nanomanipulation, nanocharacterization and nanomagnetics; Develop 3-D measurement methods for the analysis of physical and chemical properties at or near atomic spatial resolution	FY 2004 -
Ensure that 50% of research institutions' faculty and students have <u>access to full range of nanoscale research facilities</u>	FY 2005 -
Enable access to <u>nanoscience and engineering education for students</u> in at least 25% of research universities	FY 2005 -
Develop <u>three-dimensional modeling of nanostructures</u> with increased speed/accuracy that allows practical system and architecture design	FY 2005 -
Content <u>standards for nanotechnology education</u> for K-12	FY 2005 -
Nanoelectronics: first <u>terabit per square inch memory chip</u> demonstrated in the laboratory	FY 2006 -
<u>Manufacturing at nanoscale</u> for three new technologies	FY 2006 -
Monitoring contaminants in air, water, soils with increased accuracy for <u>improving environmental quality</u> and reducing emissions.	FY 2006 -
Integrate <u>facilities for nanoscale and microscale testing and manufacturing</u> at ten R&D centers	FY 2006 -
Develop <u>methods, tools and computational tools for structure analysis</u> for the extraction of information from Nature's nanoscale materials and machines	After 2006
Catalyze creation of several <u>new commercial markets</u> that depend on <u>three-dimensional nanostructures</u>	After 2007
" <u>Biomimetic thinking</u> ," probably the derivation of artificial neural networks as an outgrowth of studying the cellular organization of the brain	After 2007
The incorporation of <u>biological molecules into</u> otherwise <u>electronic devices</u> , mimicking biological structures in fabricated devices, and the incorporation of lessons learned from biological signal processing into the logic of electronic systems	After 2007
<u>Nanoscale measurements on microsecond time scales</u> to provide a blueprint for the development of nanomachines and synthetic molecular processors that carry out complex functions	After 2007
<u>Photovoltaic proteins in plants</u> that extract electronic energy from light energy, or insect hearing organs 1 mm apart that have highly directional sound source localization sensitivity, as <u>models for, or components of, nanosystems</u> that accomplish other functions	After 2007
Introduction of <u>revolutionary technology options</u> to enable International Technology Roadmap for Semiconductors (ITRS) goals	After 2007

IMPLEMENTATION PLAN

8. Management Plan

Funding of the recommended R&D priorities outlined in this document will be conducted by the participating agencies as a function of their missions and contingent on available resources. A coherent approach will be developed for funding the critical areas of nanoscience and engineering, establishing a balanced and flexible infrastructure, educating and training the necessary workforce, and promoting partnerships to ensure that these collective research activities provide a sound and balanced national research portfolio. By facilitating coordination and collaboration among agencies, the NNI will maximize the Federal Government's investment in nanotechnology and avoid unnecessary duplication of efforts.

A. NNI Interagency Management Objectives

NNI will enable agencies collectively to meet the primary objective of the initiative: to achieve the maximum National benefit of long term fundamental nanoscale science, engineering and technology research while meeting the mission-oriented technology goals of participating government agencies. Two overriding management principles will be as follows:

1. Open competition and/or peer review will ensure that:
 - The best ideas for research in nanoscale science, engineering and technology are identified and pursued
 - The best individuals and teams are selected to carry out the research
 - The best providers of physical and computational infrastructure resources are selected
 - Academic, national laboratory, and private sectors – including institutions from all geographic areas, historically minority institutions, and small colleges and universities – have equal opportunities to compete for access to available research and infrastructural resources

2. Interagency coordination will ensure that:
 - Participating agencies work together to address issues that meet, but also transcend mission objectives
 - Resources are leveraged to maximize benefit to NNI, related ongoing research, and agency missions
 - The nanotechnology infrastructure is optimized to meet NNI and agency objectives

B. Nanoscale Science Engineering and Technology Subcommittee (NSET)

The NNI has been managed within the framework of the National Science and Technology Council's (NSTC) Committee on Technology (CT). The Committee, composed of senior-level representatives from the Federal Government's research and development departments and agencies, provides policy leadership and budget guidance for this and other multiagency technology programs.

The CT's Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) will continue to coordinate the Federal Government's multiagency nanoscale R&D programs, including the NNI. The NSET Subcommittee will coordinate planning, budgeting, implementing, and reviewing the NNI to ensure a broad and balanced initiative. The Subcommittee is composed of representatives from agencies with plans to participate in the NNI and White House officials. The NSET Subcommittee is chaired by a representative from an agency participating in the NNI, designated by the CT.

Under the NNI, each agency will invest in those R&D projects that support its own mission as well as NNI goals. While each agency will consult with the NSET Subcommittee, the agency retains control over how it will allocate resources against its proposed NNI plan based on the availability of funding. Each agency will use its own methods for inviting and evaluating proposals. Each agency will evaluate its own NNI research activities according to its own GPRA policies and procedures.

C. National Nanotechnology Coordinating Office (NNCO)

The National Nanotechnology Coordinating Office (NNCO) serves as the secretariat to the NSET Subcommittee, providing day-to-day technical and administrative support. The NNCO supports the NSET Subcommittee in the preparation of multiagency planning, budget, and assessment documents. The NNCO is the point of contact on Federal nanotechnology activities for government organizations, academia, industry, professional societies, foreign organizations, and others to exchange technical and programmatic information. In addition, the NNCO develops and makes available printed and other material as directed by the NSET Subcommittee, and maintains the NNI Web Site (<http://www.nano.gov>).

The NNCO Director is an NSTC agency representative appointed by the Associate Director for Technology at the White House Office of Science and Technology Policy, in consultation with the Chair of the NSET Subcommittee. The NNCO Director reports to the Associate Director, but works in close collaboration with the Subcommittee Chair to establish goals and priorities for NNCO support.

Initially the NNCO Director is a part-time position. As the duties and workload of the NNCO expand, the NSET Subcommittee may recommend to the OSTP Associate Director the appointment of a full-time NNCO Director. The full time NNCO Director must be a Federal employee, but recruitment is not limited to NNCO sponsoring organizations. The term of appointment will be established by the OSTP Associate Director, and is not to exceed two years. The NNCO will have a small initial staff (2.5 to 3 FTEs), which will increase only as workload warrants. The NNCO Director works with the NSET Subcommittee and OSTP in meeting the staffing needs for the NNCO office.

The NNCO budget includes the cost of contracting with an outside organization to review NNI progress towards meeting its goals. Beginning in FY 2002 and annually thereafter, the NNCO must submit an annual budget to the NSET Subcommittee for approval. If the NNCO's proposed budget exceeds the previous year's budget by 15 percent or greater than the previous year, approval by the Executive Committee of the Committee on Technology is required.

Based on an approved budget, the NNCO's annual funding will be derived from cash and in-kind contributions of agencies participating in the NNI based on a percentage of each agency's total (enacted) investment in nanoscale R&D. The percentage may vary slightly from year to year. Agencies can contribute in excess of the amount they have agreed to provide. However, agencies cannot count these extra contributions in one year towards their financial obligations for the following year.

D. Establish Grand Challenge and Cross-Cut Champions

It is important for the NSET to manage actively the NNI's "grand challenges" and to demonstrate progress towards its goals. Each grand challenge will have an agency "champion" to serve as the chief advocate for that grand challenge within the Federal Government, as shown in Table 8.1.

Table 8.1
Agencies Participating in Grand Challenges and Cross-Cutting Areas

Grand Challenge and Cross-Cut Needs	Lead and Associated Agencies/Departments
Nanostructured materials “by design”	NSF with DOD, DOE, DOT, and NASA
Nanoelectronics, optoelectronics, magnetics	DOD with NSF, NASA
Advanced healthcare	NIH
Nanoscale processes for the environment	EPA with NSF and DOT
Efficient energy conversion and storage	DOE with NASA, DOD, and DOT
Microcraft and Robotics for space and industry	NASA with DOD
CBRE Protection and Detection	DOD with all others
Nanoscale Instrumentation and Metrology	NIST
Manufacturing at the Nanoscale	NSF with NIST
Economical and Safe Transportation	DOT
National Security	DOD

The exact strategy for doing this will vary depending on the grand challenge, but might include:

- Definition of the grand challenge, with possible intermediate milestones
- Identification of the relevant research that is being sponsored by the Federal Government
- Yearly report on progress that is being made (or special “bulletin” if there is a very significant breakthrough)
- Reporting to the NSET on adequacy of current level of investment to support the grand challenge
- Encouragement of inter-agency cooperation, as appropriate (e.g., sharing of information between agencies about current activities and future plans, participation in each others’ review panels, joint solicitations, agreements on division of labor)
- Encouragement of cooperation within the research community (joint principal investigator meetings, internet-based collaborations)
- Promoting partnerships and leverage additional resources from the private sector
- Identifying other government policies and agencies that could support the grand challenge
- Identifying education/training needs for commercial applications

E. Planning (Roadmaps) for R&D Areas

Specific medium-term plans are needed for each of the grand challenges, including transition into the development phase. Such plans will be formulated in collaboration with academe, government laboratories and private groups. The Nanoelectronics, Optoelectronics and Magnetics Grand Challenge has been selected for the development of a comprehensive investment strategy, since the International Technological Roadmap for Semiconductors (ITRS, showing that in 10-15 years most of the basic features in microelectronics will be at nanoscale), a Semiconductor Research Corporation (SRC) study of research needs, and an SRC study of manpower deficiencies have already been developed. Based on that experience, investment strategies for other grand challenges will be developed.

F. Outside Review

In its letter to the President, the PCAST recommended that a non-government advisory committee review the NNI to assess progress towards its goals. A report would be provided to the Committee on Technology. The Committee on Technology would work with the NSET Subcommittee to address issues raised by the outside advisory committee and to implement changes to the NNI strategy. The National Research Council will publish the first of these reports in June 2002.

9. Fundamental Research

(total investment proposed for FY 2003 is \$227.5 million, \$14 million above FY 2002)

Vision and Strategy

The National Nanotechnology Initiative maintains five “high priority” research areas for funding in FY2003. The first and largest of these is “long-term science and engineering research leading to new fundamental understanding and discoveries of phenomena, processes, and tools for nanotechnology.” The investment will provide sustained support to individual investigators and small-groups, with a typical award of \$200K to \$500K. Sustained and larger funding for fundamental research in the early years of the initiative is critical for its success.

Vision

The NNI will develop the capacity to create affordable products with dramatically improved performance through gaining a *basic understanding of ways to control and manipulate matter at the ultimate frontier – the nanometer* – and through the incorporation of nanostructures and nanoprocesses into technological innovations. In addition to producing new technologies, the study of nanoscale systems also promises to lead to fundamentally new advances in our understanding of biological, environmental, and planetary systems.

The reasons for emphasizing fundamental research at this stage in the development of nanotechnology, and the long-term promise of the initiative, were outlined in detail in the FY 2001 NNI Implementation Plan (see <http://www.nano.gov/nni2.pdf>).

Nanoscience offers one of the most exciting opportunities for innovation in technology. It will be a center of fierce international competition when it lives up to its promise as a generator of technology.

Long-term, basic research opportunities

- Discovering and eventually tailoring the novel chemical, physical, and biological properties and phenomena associated with individual and ensembled nanostructures being anticipated.
- Linking biology, chemistry, materials science, physics and information science from the nanoscale to accelerate progress in understanding the fundamental principles behind living systems and the environment.
- Developing scaling laws, and threshold length and time scales for the properties and phenomena manifested in nanostructures.

- Creating new instruments with the sensitivity and spatial localization to measure, manipulate, and able to *in-situ* monitor processing of nanostructures; utilizing the new ability to measure and manipulate supramolecules to complement and extend prior measurements derived from ensemble averages.
- Addressing the synthesis and processing of engineered, nanometer-scale building blocks for materials and system components, including the potential for self-organization and self-assembly.
- Exploiting the potential for both modeling/simulation and experiment to understand, create and test nanostructures quantitatively.
- Developing new device concepts and system architecture appropriate to the unique features and demands of nanoscale engineering.

Priorities and modes of support

Long-term nanoscale research should focus on understanding basic processes for the new ranges of length and time scales, on developing new measurement and manipulation tools, and on developing processes necessary to fabricate quality nanostructures. Areas of focus include the following: (a) biosystems at the nanoscale; (b) novel phenomena and nanoscale structures, including quantum control; (c) device and system architecture; (d) multiphenomena and multiscale theory, modeling, and simulation, as well as other topics such as nanoscale processes in the environment, including geosciences aspects and other areas of engineering and science.

Nanoscale science and engineering is inherently interdisciplinary. A focus on interdisciplinary teams of researchers and on exploratory research projects is recommended. Active collaboration between academic and industrial scientists and engineers, and integration of research and education will be encouraged. Interagency partnerships will play a synergistic role in these activities.

Agency Participation and Partnerships

NSF will contribute the largest investment to this generic fundamental research topic (\$140 million, \$13 million over FY 2002). While DOD (\$20 million), DOE (\$35 million), NASA (\$15 million), and NIH (\$15 million) will maintain their FY 2002 investment in fundamental research. Both academic institutions and government research laboratories will conduct fundamental research.

10. New Grand Challenges in Fiscal Year 2003
(total FY 2003 is \$266.7 million, \$32.2 million above FY 2002)

The following grand challenges were identified as essential for the advancement of the field in FY 2002 and they will continue in FY 2003: nanostructured materials “by design;” nanoelectronics, optoelectronics and magnetics; advanced healthcare, therapeutics and diagnostics; nanoscale processes for environmental improvement; efficient energy conversion and storage; and microcraft and robotics. Both national security and economical and safe transportation (listed in earlier documents as grand challenges) are now identified as national priorities that benefit from several of the grand challenges.

Two new challenges have been proposed for FY 2003: Nanoscale Instrumentation and Metrology, and Manufacturing at the Nanoscale. The Grand Challenge on Bio-Nanosensors for Communicable Disease and Biological Threat Detection has been refocused as Nanostructures for Chemical, Biological, Radiological, and Explosive (CBRE) Detection and Protection for Homeland Defense. The two new topics and the refocused CBRE topic are presented below in detail.

A. Manufacturing at the Nanoscale

Vision and Strategy

Vision

Manufacturing of nanostructures, devices and systems will be realized with a high degree of control at the nanoscale to achieve prescribed performances, and with hierarchical integration to incorporate nanostructures into macroscale products. This may combine directed molecular assembling techniques with top-down, macroscopic fabrication techniques. Highly efficient manufacturing processes are envisioned – minimizing materials, energy and waste, and enabling high-rate, cost-effective production of new products.

Special research opportunities

Nanotechnology will fundamentally change the way both basic types of manufacturing – continuous and discrete – are conducted in the future. Continuous manufacturing refers to the production of substances or materials through continuously operating processes, e.g., chemicals or rolls of sheet metal. Discrete manufacturing is the production of individual parts, e.g., bolts or devices such as integrated circuits or assembled systems such as computers. Atoms, molecules and clusters are the “raw materials” for manufacturing at the nanoscale. As a result the processes and equipment for manufacturing at the nanoscale are expected to be significantly different even from those currently used for microfabrication. Special research opportunities include the following:

- Basic understanding of the phenomena and processes influencing manipulation of matter at the nanoscale.
- Synthesis and fabrication methods for nanostructure building blocks in the 1-100 nanometer range with tailored properties and functions. Such structures include quantum dots (0-D), tubes and wires (1-D), surfaces (2-D), and clusters and other three-dimensional molecular assemblies.
- Control of the size, shape, and polydispersity of nanostructure building blocks.
- Modification and control of building block surface composition and structure to ensure stability and to enable subsequent directed assembly.
- Measuring, understanding and controlling the role of interfacial and interface properties in nanocomposite processing.
- Sustainable, user-friendly, affordable, high-throughput patterning technologies.
- Directed, hierarchical self-assembly of building blocks into functional devices and systems. This includes processes that mimic biological systems.
- Developing and applying replication methods for nanostructures.

- Developing equipment and processes to achieve directed molecular assembly into functional nanostructures and devices, including highly parallel processing and robotics.
- Accounting for the broad complexity of problems involved in the production of systems containing structure and function across many length scales.
- Integration of bottom-up and top-down fabrication techniques into the most cost-effective manufacturing approaches.
- Analytical capability for real-time processing quality control.
- Techniques for the cost effective removal, repair, and trimming of nanofabricated structures and properties.
- Tools for modeling and simulating the broad range of manufacturing processes involving nanostructures, allowing the processes to be understood and optimized.
- Scale-up of manufacturing techniques.
- Nanofluidics.

Relevance

Manufacturing techniques at the nanoscale have equal relevance as components of traditional industries and as engines for revolutionary technologies. These techniques will allow increases in the efficiency of existing technologies and in the establishment of industries that would have not been possible otherwise.

Nanoscale manufacturing encompasses all processes aimed toward building nanoscale structures, features, devices, and systems in one, two and three dimensions. It will meld both bottom-up assembling of nanostructure building blocks with top-down processes for economical devices and systems. Advances in manufacturing at the nanoscale are anticipated to result in rapid commercialization of: nanostructured materials with novel and improved properties; information technology nanodevices including advanced silicon semiconductors, molecular electronics, and spintronics; measuring devices and tools for manufacturing; nanobiotechnology – diagnostics, implants, and therapeutic delivery; higher performance safety and security technology including sensors, adsorbents, filters, and decontamination techniques; and nanoelectromechanical systems (NEMS).

Priorities and modes of support

- Systematic methods for synthesis and fabrication of a broad spectrum of products through manufacturing at the nanoscale.
- Centers large enough to integrate the various expected critical components of nanoscale manufacturing such as bottom-up assembly of nanostructure building blocks, top-down fabrication techniques, fabrication of hierarchical multiscale structures with atomic precision, nanolithographic patterning, and biomimetics.
- Nanoscale metrology endorsed by national and international organizations.
- Development of know-how and data permitting an informed evaluation of the economic, safety, and environmental implications of nanoscale manufacturing processes.
- Certified education and training programs integrated with nanomanufacturing research.

- SBIR, STTR, and MANTECH projects, and/or company/university/national laboratory partnerships to accelerate transition of science discovery into manufacturing technology.
- Workshops and conferences to share new nanotechnology opportunities among research, manufacturing, and financial interests with a goal of promoting partnerships, synergism and realistic expectations.

Infrastructure

- Geographically distributed nanofabrication user facilities, including adequate characterization capabilities, are needed for both research and education/training.
- Infrastructure for development of measurement and manufacturing tools and standards.
- Models and simulation software for nanomaterials processing, with the required attention to boundary conditions, such as in nanofluidics.
- Marketplace-neutral resources to facilitate people, software, and science-based understanding integration across the entire manufacturing enterprise.

Agency Participation and Partnerships

All agencies will be involved. The National Science Foundation will focus on fundamental research for manufacturing processes, new theoretical models/simulations, and instrumentation for characterization/quality control. The Nanoscale Instrumentation and Metrology grand challenge will develop new approaches to accurate measurement and standards, providing assistance to industry and other agencies in this area. Other agencies will incorporate this grand challenge into the realization of their mission-specific programs.

B. Nanoscale Instrumentation and Metrology

Vision and Strategy

Vision

This grand challenge topic seeks to encourage the development of highly capable, low-cost, standardized, and efficient tools and instruments for the measurement of nanoscale phenomena and for the manipulation of nanostructures. New calibrated instruments with nanoscale resolution will accelerate scientific discovery, provide quality control in the fabrication and assembly of manufactured nanostructures, and stimulate new approaches to miniaturized sensors and actuators.

Special research opportunities

The development of the scanning tunneling microscope and force microscope initiated the nanoscience revolution; the continued improvement in measurement and manipulation capabilities is a speed limiter on the rate of progress of the National Nanotechnology Initiative. The complexity and breadth of nanotechnology provide a wealth of research opportunities for instrumentation and metrological advancements. Some key opportunities are as follows:

- The analysis of single molecule, supramolecules, biomolecules and polymers. Current proximal probe instruments such as scanning tunneling microscopy and spectroscopy are optimized for hard, electrically conducting materials. New analytical tools are needed to characterize soft materials, and approaches must be developed for interpreting measurements

on molecular materials. Since biology, medicine, and health issues primarily involve molecules, progress in this is a rate limiter for biotechnology.

- The ability to perform depth-dependent measurements. Current instruments probe near-surface features and properties; new metrology is required to obtain information as a function of depth.
- The chemical identification of an unknown material at the nanoscale. Present techniques for quantitative nanoscale compositional analysis utilize expensive, highly specialized equipment. Lower cost, simpler instruments must be developed for routine analysis.
- The ability to measure multiple features and properties of a nanostructure with a single platform tool. Currently, multiple tools are required to fully characterize the composition, structure and properties of a nanostructure. A single tool with multiple, integrated proximal probes and other instruments such as high-energy electron microscopes would greatly accelerate the pace of nanoscale R&D.
- Measurements of nanostructure arrays or of large domains, as compared to the characteristic nanoscale feature. Measurements on a single nanostructure are often difficult and time-consuming; as multiple nanostructures are incorporated into commercial devices, the demand for simpler, faster measurements will escalate. The ability to measure many nanostructures in parallel using an array of proximal probes will be critical.
- The ability to locate and maintain a position with nanometer accuracy and precision. Instrumentation for precise position control across samples of centimeter dimensions will be required to realize commercial nanodevice fabrication.
- The ability to precisely manipulate nanostructures. Three-dimensional manipulation of chemical moieties must be accomplished to build molecules or clusters and then assemble them into larger devices. The extension of microelectromechanical systems (MEMS) into the nanometer regime will facilitate the development of hybrid machines for fabricating such devices.
- Metrology. Measurements at the nanoscale have little metrology underpinning and few standards to ensure reliability and repeatability. Standard reference materials need to be developed and calibrated in order to evaluate the reproducibility of a given nanoscale measurement technique (analytical tool). This would create a nanoscale “ruler.”
- Uniform-size particles. Standardization and calibration of nanoscale measuring instruments will require uniform-size nanoparticles of known size and composition.
- Definition of fundamental standards. The creation of atomically controlled and measured structures may lead to the establishment of fundamental standards. For example, quantized electron devices may provide electrical current standards.

Relevance

The recent exponential growth in nanoscience and nanotechnology was stimulated by the development of a broad class of new analytical tools that provide the “eyes” to measure and characterize specific nanostructures and the “fingers” to manipulate them. However, the rate of progress is still limited by inadequacies in the spatial and temporal resolution of these tools. The rate of progress in all of nanoscience and nanotechnology is dependent on the successes in this grand challenge. It can be expected that the new analytical tools will first find their usefulness in laboratory research projects, but then evolve to quality control tools for industrial manufacturing. As a spin-off, analytical tools capable of dealing with the small size and constituency of nanostructures are likely to lead to innovations in high sensitivity sensors and detectors.

Priorities and modes of support

- The development of new instrumentation and standards for nanoscale measurements, especially proximal probes, depends critically on synergistic work between university and government researchers (innovations) and industrial developers (commercial realization). The investment strategy must encourage and reward multidisciplinary collaborations among these communities.
- Priority research areas are three-dimensional measurements with high spatial and temporal resolution, simultaneous measurements of several properties, new instrumentation for properties that are not yet measurable at the nanoscale (especially chemical composition and local physico-chemical properties), and the development of standards to assure quality measurements.
- SBIR, STTR and ATP programs should play a large role in this grand challenge as a mechanism to incorporate novel ideas and concepts into commercial products. The investment strategy must also revive lagging interest in instrument development in the United States compared to Europe. Scholarships and fellowships focused on nanoscale metrology should be instituted to attract high-caliber students and post-doctoral researchers to the field.

Infrastructure

The development of novel nanostructure analytical tools will likely come primarily from single investigator research programs; frequently the tool innovation is an outgrowth of efforts to improve the sensitivity and accuracy of a measurement. However, the integration of proximal probes of differing functions with other instruments will require a coordinated, multidisciplinary effort. Further, the proximal probes will need to be compatible with specialized user facilities such as synchrotron (photon) and neutron beam sources. Appropriate NSF, NIST, DOE, DOD and NIH sponsored facilities – such as the National Nanofabrication Users Network (NNUN) – should be created and supported for this purpose. Centers, especially in conjunction with microfabrication capabilities, will be critical for these interdisciplinary efforts.

Agency Participation and Partnerships

High performance equipment is a central need for all of the participating NNI agencies. Since NSF has the largest fraction of university research funding in NNI, its programs will be a primary source of new instrumentation concepts. NIST will support effective applications of nanoscale characterization equipment through scientific development (metrology), standards, and calibration sources. The NIH BECON symposium on nanobiotechnology identified improved measuring capability as an important topic for attention; NIH, NSF and USDA collaboration will ensure rapid progress. Measurements on nanostructures require improvements in signal-to-noise ratios that the DOD, DOE, EPA, FAA and NASA should exploit for higher sensitivity sensing and detection.

C. Chemical, Biological, Radiological, and Explosive – Detection and Protection for Homeland Defense

Vision and Strategy

Vision

Nanostructures, with their small size, light weight, and high surface-to-volume ratio, will dramatically improve our capability to detect chemical, biological, radiological, and explosive (CBRE) agents with sensitivity (potentially a single threat moiety) and selectivity (through microfabricated sensor suites); to protect through filtration, adsorption, or neutralization of agents (nanoporosity and high surface-to-volume nanomaterials); and to provide site-specific prophylaxis.

Relevance

a. Detection. The use of nanoscale sensors for CBRE can critically impact national security programs, by providing sensitive, selective, and inexpensive sensors that can be deployed for advance security to transportation modes (security protection for air, bus, train/subway, etc.); the environment (public water supplies, waste treatment plants, natural resource areas, reservoirs, etc.); food supplies (production, processing, storage, and distribution); military (for protection of facilities and equipment); Federal buildings (White House, U.S. embassies, and all other Federal buildings); Customs (for border crossings, international travel, etc.); civilian businesses (in large and small cities); and schools (to prevent weapons, explosives, etc.).

The potential impact is vast and critical. Small amounts of chemical, biological, or radiological agents can potentially inflict much larger scale damage to people than can an equivalent amount of explosive (see Table 10.1). Micrograms of anthrax and milligrams of nerve agent are sufficient to kill a person, as compared to many grams of high explosive. However, while larger amounts of explosive are necessary for deleterious consequences, their detection in the air is made difficult by low vapor pressures (particularly in the case of military explosives). As a practical consequence, it is necessary to find technology that will detect very small amounts of all CBRE material.

What role might nanotechnology play in the drive toward better detection against CBRE threats? The nanoscale offers the potential for orders of magnitude improvements in sensitivity, selectivity, response time, and affordability. For the instruments being developed to measure and manipulate individual atoms with sub-nanometer precision, one pathogen or even one chemical molecule is huge. The detection of a single CBRE moiety becomes possible. You can't get any better sensitivity – however there is still the nontrivial problem of getting that single moiety to the location where it can be detected.

Table 10.1
Comparative Lethality of Selected Toxins, Chemical Agents, Biological Agents
and Radiological Hazards

Agent	LD50 (µg/kg body weight)	Source
Botulinum Toxin	0.001	Bacterium
Shiga Toxin	0.002	Bacterium
Diphtheria Toxin	0.10	Bacterium
Ricin	3.0	Castor Bean
VX	15.0	Chem Agent
GB	100.0	Chem Agent
Anthrax	0.004-0.02*	Bacterium
Plutonium	1	Nuclear Fuel

*Anthrax calculations based on a spore volume of 5.0E-10 µl, an assumed spore density of 1.0 g/mL, and the LD50 estimated from the Sverdlovsk Model of 8,000 to 45,000 spores. Spores from the recent attacks measured 1.0 µm x 1.0 µm x 0.5 µm (W x H x L). Since theoretically one organism is capable of causing infection under the right conditions, body weight of the subject is not necessarily relevant. Thus, the value for anthrax is not a true LD50, but could be considered as the weight of spores that would kill 50% of individuals in a statistically normal distribution.

The collection of airborne or surface-attached samples of chem/bio/explosive is a key part of a total detection system. Nanostructures can be sufficiently small and light to avoid gravitational settling. There is the possibility for maneuverable (magnetic, electric coupling) nanostructures that would circulate through large volumes of air/water and then be proactively drawn to the sensor. A front-end collection system must match the flow impedance of the nano-detection sensor for the system to be fully functional. The most efficient collection systems would employ some type of preconcentration media, which requires research and development on nanoscale coatings (e.g., development of monolayer polymer coatings for chemically selective absorption/desorption of agent molecules).

Selectivity is no less important than sensitivity. A detection system with frequent false positives (false alarms) is quickly ignored (more likely discarded), while false negatives lead to death. In contrast to sensitivity, the nanoscale doesn't automatically lead to the expectation of greater selectivity. The nanoscale enables the potential for deploying sensor suites, where multiplicity in the tens to thousands may compensate for the loss of performance of any single measurement. Further, analytical tools used in nanoscience make possible the measurement of molecular properties – such as size, shape, and mechanics – not accessible by conventional analytical chemistry tools.

Diagnostic speed is a real issue for chemical, biological, and radiological exposures. For instance, ten seconds may be all the time one has to respond to threat level quantities of nerve agent. With the slower incapacitation rates for biological and radiological agents, detection times of seconds to minutes could limit the amount inhaled and simplify subsequent prophylactic action. If one can solve the problem of rapidly bringing sufficient quantity of agent into the detection volume, nanostructures do minimize the time to diffuse into and out of that volume. The nanoscale may also enable inexpensive sensor suites so that one can afford to distribute them prolifically and minimize the distance from a threat to a sensor.

b. Protection. Gas mask filters used in nuclear, biological, and chemical (NBC) applications remove toxic chemicals by a process that remains essentially a WWII technology. The material

responsible for chemical vapor/gas removal is an activated carbon impregnated using a Whetlerite method that impregnates metal oxides, such as, copper, zinc, molybdenum, and silver, into the larger pores of the carbon. In a very real sense activated carbon is replete with nanopores ranging from about 0.5 nm to 500 nm. Nanoscience can provide new opportunities for high surface area adsorbents and can further provide new molecular templating techniques that can augment the bonding strength. Optimized in another way, nanoporous materials can assist in the separation technologies necessary to geometrically block the migration of agents through use of a membrane.

Collective protection systems and protective clothing frequently utilize fibrous filters to remove agents. High-efficiency particulate arresting (HEPA) filters can be effective against particulates; even the biological toxins that might be dispersed as aerosols could be filtered out by HEPA. The use of nanotubes, nanofilaments, and nanoporous membranes might make these filters even more effective, and might include catalytic degraders as well.

Decontamination and neutralization of harmful moieties can also benefit from nanoscale materials. To ensure their general effectiveness and to simplify logistics, military decontamination solutions traditionally have involved the use of highly aggressive chemicals. Unfortunately, while effective against agents, these chemicals also attack incidental materials, including humans. Catalytic nanostructures, both inorganic and organic, should improve this situation as nanoscience provides clearer understanding of composition/structure versus function relationships. Further, as the role of nanostructures in cellular activity is better understood, new mechanisms to disrupt and neutralize harmful pathogens are being discovered.

Nanotechnologies also hold the promise of less toxic chemical processing. Hence, hazardous materials and wastes may be eliminated or minimized and their potential for use in terrorist attacks reduced. New catalysts and smaller chemical processing plants are preventative means for eliminating the materials of potential terrorism, such as chlorine storage at wastewater treatment facilities or hazardous solvents at chemical manufacturing plants.

Special research opportunities

a. Nanoscience basis for detection: miniaturized, intelligent sensors (MIS). The objective is to develop nanoscience and nanostructures that more effectively collect and deliver samples to sensitive, selective sensors (chemical, biological, radiological, electromagnetic, acoustic, magnetic, etc.) with information processing electronics and communication for miniaturized, intelligent sensor suites that can actively respond to homeland defense requirements.

Homeland defense impact: Miniaturized, intelligent sensors will enable important new capabilities to counter CBRE threats to civilian and military populations:

- Detection and communication support for individuals participating in prevention/remediation of CBRE incidents. Lighter, smaller, and highly functional systems to provide rapid detection of threats, and communication systems with greater versatility and bandwidth will affect the performance and safety of the individual participant.
- With sensing, detection, and signal processing at nanometer scales, surveillance “platforms” can be miniaturized to sizes that are inconspicuous and produced at costs low enough to enable prolific coverage of enclosed spaces such as office buildings, transportation hubs, etc.

- Uninhabited vehicles for surveillance to reduce the risk to human lives.
- Personnel monitors for detection of CBRE threats or fatigue, or for other medical applications, require the linkage of biological function and nanostructured semiconductor devices. Small sizes will be required for functional systems embedded in the body where they can detect the small changes in body chemistry incipient to more severe problems, and can initiate corrective action.

Why nanoscience to best achieve MIS? Enclosed spaces (office buildings, transportation hubs, airplanes, etc.) and CBRE response individuals/teams require continued improvement in the ability to detect with better sensitivity; more discrimination against noise sources; lower power consumption; and faster, lighter, smaller, and cheaper systems. Miniaturization in electronics, and more recently the miniaturization of mechanical devices (microelectromechanical systems, MEMS), have already provided improvements in all of these capabilities. Continued miniaturization into the nanometer size scale holds the promise of still more dramatic improvements: sensor suites with 1000 times smaller size/power; processors with 100 times faster speed, 100 times higher density and 1000 times less power per function; non-volatile, radiation-resistant static memory with 100 times higher density and 50 times faster access speed; low cost fabrication; and biotic/abiotic integration.

Nanotechnology promises to enable the incorporation of sophisticated electronics signal processing with innovative mechanical actuators and communication components. This will be more than a simple extrapolation of capability from the microscale; nanostructures will provide capabilities not realizable from larger structures. For instance:

- At the nanometer length scale quantum mechanics becomes the dominant physics controlling the function of electronic devices and sensors. From a science perspective, the physics of coherent quantum devices and coherently coupled systems need to be better understood. From a technology perspective, the high speed, small size and low power consumption provided by quantum devices and quantum information processing will be required in order to realize intelligent, autonomous remote sensing systems.
- The proof of concept for selective, trace biological and chemical species detection by nanotechnology has already been demonstrated by several groups (see Table 10.2). The science opportunities include the ability to probe the mechanical properties of single molecules, providing a revolutionary approach to understanding the structure and dynamics of polymers, proteins and other macromolecules. From a technology perspective, new approaches to sensor selectivity (e.g., force differentiation) and several orders-of-magnitude improvements in sensitivity are highly likely.
- Nanostructured devices can potentially exploit power scavenged from the ambient. For instance, molecular motors embedded in an in-situ monitoring system might utilize body chemistry as their power source. Scientifically, the ability to individually manipulate and monitor those molecular motors will accelerate our understanding of muscle mechanisms. Additionally, biological energetics is inherently electrochemical; natural biological processes may be exploited to create electrochemical energy conversion. Nanostructured thermoelectric devices also are being developed that might allow one to harness energy from the environment.
- At the nanoscale, molecules may provide alternative approaches to inorganic semiconductors for signal processing. From a science perspective, we will learn the electronic, magnetic, and

optical properties of single macromolecules. From a technology perspective, the incorporation of molecular function with semiconductor materials provides an opportunity to link biotic and abiotic systems.

MIS program: To best exploit the opportunities, MIS requires an interdisciplinary approach to the development of sensing, information processing, decision, and actuation functions. MIS will address the following issues:

- Sample collection and concentration
- Sensing, actuation, and transduction
 - Transduction properties of individual nanostructures, polymers and proteins
 - Transduction properties of nanostructure arrays
 - Molecular machine/nanomachine concepts
 - Tethered nanodots/nanowires with magnetic or electric field actuation
 - Magnetic, electric, optical, and chemical signaling
 - Artificial cells
- Molecule–Semiconductor/Metal Interface
 - The balance of bond stress and bond energy in surface reconstruction
 - Electron/hole transfer between molecule/biomolecule and semiconductor
 - Novel bonding chemistry
- Biotic/Abiotic Interface
 - Surface compatibility of semiconductors in aqueous/physiological environment
 - Linkers with retention of biological function such as molecular recognition
 - Membrane gating
 - Development of functional interconnects between nanoscale building blocks
- Fabrication with a focus on assembly of building blocks (i.e., nanodots, nanowires, etc.)
 - Techniques for patterning and fabrication of circuits with nanostructures
 - Hierarchical assembly of functional arrays
 - Directed assembly utilizing designated chemical/molecular recognition eventsNanodevices: shape, size, defects, and impurities
- Methods to model and design nanostructure properties and nanodevice performance
- Power sources
 - New methods, materials and devices to harvest energy from the environment
 - Ability to interconnect power sources with nanostructures and complex architectures
 - Molecular motors

b. Nanoscience basis for protection, neutralization, and prevention (PN&P). The objective is to develop nanoscience and nanostructures which enable revolutionary advances in adsorbent materials (personal and collective protection), separation technologies (protective clothing and filters), decontamination and neutralization of agents, and prophylactic measures.

Homeland defense impact: Empirically derived nanoscale materials have been a mainstay in CBRE protection and neutralization. Attention to the underlying nanoscience base should lead to dramatic improvements, especially as that knowledge enables the development of more sophisticated systems:

- Decontamination via aggressive chemical systems, damaging to human and equipment as well as chemical and biological agents, can be replaced by treatments as effective at decontamination but benign to human and environment.
- Decontamination of sensitive equipment (where water is not allowed).
- Protective clothing that incorporates decontamination activity rather than simple adsorption, and permits water vapor migration for cooling.
- Masks and filters with adsorbents having greater selectivity and capacity for harmful agents, incorporating miniaturized sensing to alert for breakthrough, and potentially with the capability of neutralizing the agents.
- Innovative approaches to the deactivation of biological agents, especially spores.
- Manufacturing and processing industries free of hazardous materials and wastes.

Why nanoscience to best achieve protection/neutralization/prevention? Nanoscience offers the following unique advantages for achieving these goals:

- Nanostructured surfaces contain larger amounts of more reactive edges and defect sites yielding high reactivity and capacity.
- Small molecule adsorption sites tailored for recognition.
- Small molecule filtration through controlled nanoporosity.
- Clothing that breathes – nanofibers have far more surface area, also smaller voids; designer nanostructured membranes.
- Catalytic action – small for rapid access and reactivity; incorporation in creams for skin protection and into coatings and fabrics.
- Biochemistry of cells depends critically on nanostructures – as those are discovered and understood, there will be new insights on defeating spore/bacterial/viral activity.

Protection/neutralization/prevention program: To best exploit the opportunities, PN&P requires an interdisciplinary approach to the development of nanostructures that selectively interact with CBRE molecules. The PN&P will address the following:

- High-surface area, selective adsorbents
 - Non-carbon adsorbents
 - Templated surfaces for more selective adsorption
 - Hierarchical control of porosity for low-pressure drop
 - Incorporation of catalytic decomposition for agent destruction
 - Biomolecular adsorbent/filtration materials
- Catalytic materials
 - Proteins as biological enzymes
 - Tailored nanoclusters for selective catalysis and benign products
 - Tunable photocatalysts
 - Environmentally benign catalysts
- Nanostructures for clothing/separators
 - Fabrication of polymer nanofilaments
 - Incorporation of catalytic centers in fibers
 - Fiber surface modification
 - Nanoporous materials
 - Designed nanostructured membranes

- Nanostructures disruptive of biological agent function
 - Nanoemulsions
 - Protein nanotubes for membrane disruption
- Prophylactic nanostructures
 - MEMS/NEMS for drug delivery
 - Nanostructured reactors in skin creams
 - Nanostructured materials for wound cleaning and treatment

Transition opportunities

The National Nanotechnology Initiative has its prime focus on science. However, the NNI builds on two decades of Federal funding at the nanoscale. There are a range of opportunities for commercial products, some with near-term reach (1-5 years), others likely in the mid-term (5-10 years), and yet others where complexity or lack of present understanding will require long-term science attention (10-20 years).

a. Short-Term (1-5 years) transition opportunities. For success, these opportunities must already have: (a) demonstrated proof-of-principle and (b) commercial interest. Specific examples are shown in Table 10.2.

Table 10.2
Examples of Opportunities for Transitioning to Applications

Investigator	Institute	Technology	Company
Mirkin	Northwestern	NanoAu biological sensing	Nanosphere
Lieber	Harvard	nanotube sensors	Nanosys
Snow	NRL	NanoAu chemical sensing	MicroSensor Systems
Klabunde	Kansas State	Nanocluster agent catalysis	Nanoscale Materials
Thundat	ORNL	cantilever sensing	Protiveris
Smalley	Rice	CNT for adsorbents	CNI
Doshi	–	polymer nanofibers	eSpin
Tatarchuck	Auburn	CNT adsorbent media	IntraMicron
Baker	Michigan	Nanostructured bio decon	NanoBio Corp.

Funding for the acceleration of these opportunities might come from the mission-oriented agencies such as DOD where 6.2-6.4 monies are available for the development of new technology; DOT Transportation Security Administration; and the Office of Homeland Security. Agencies will also continue to exploit the SBIR/STTR programs to accelerate commercial transitions.

b. Mid-term (5-10 years) transition opportunities. These are areas where an investment in nanoscience holds the promise for paradigm-breaking approaches to detection and protection with commercial product transition in the 5-10 year time frame.

- Sensing
 - Transduction/actuation mechanisms for greater sensitivity/selectivity
 - Biotic/abiotic interfaces to marry semiconductors with in-vivo biology
 - Environmental energy sources to minimize battery requirements
 - Incorporate separation and detection technologies at micron scales with lab-on-a-chip

- Protection
 - High surface area materials with templated structure for selective adsorption
 - Controlled porosity for selective migration and separation
 - Nanofibers for clothing with improve adsorption/neutralization of agent
 - Designer materials for control of diffusion and active mass transport
- Neutralization/Decontamination
 - Nanostructures to disrupt biological function
 - Catalytic nanostructures (e.g., metal oxides, zeolites)
- Prevention
 - Nanostructures to reduce/replace hazardous substances in manufacturing
- Therapeutics
 - Encapsulated drugs for targeted release
 - MEMS “capsules” for controlled drug release
 - Bioscavengers

c. Long-term (10-20 years) transition opportunities. Invest in the science base believed to be important for ultimate integration of many components into a complex system (e.g., sensor suites) or for providing sufficient insights into a complex system (e.g., cell physiology) to enable innovative technologies.

- Multifunctional surfaces – surfaces that provide all the signature control needed and contain sensing and/or reactive moieties for protection.
- Cell-based sensing – sensing technology that responds to unknown new threats by measuring the response of living systems that can mimic human biochemistry.
- NEMS – extension of MEMS technologies another three orders of magnitude smaller in order to incorporate significantly more capability.
- Hierarchical self-assembly – the incorporation of greater complexity into detection/protection systems will exacerbate fabrication costs unless innovative approaches to directed self-assembly in multiple dimensions is made viable.

Priorities and modes of support

- Integrate the biology, chemistry, engineering, materials and physics research communities to establish the interdisciplinary nanoscience knowledge and expertise needed to exploit nanostructures in the development of the following:
 - Miniaturized, real-time, intelligent, redundant sensor systems with revolutionary CBRE performance
 - New high-surface area, templated adsorbents for personnel/collective protection systems, potentially incorporating catalytic reactive systems
 - Nanofibers/nanoporous membranes for effective protective clothing without undue heat loading, potentially incorporating catalytic materials to neutralize agents while relatively benign to humans and environment
 - Mechanisms to disrupt biological agent viability
 - Multifunctional materials that recognize and generate a response to a threat agent
 - Nanoscale processes that reduce/eliminate the use or production of hazardous substances
- Strengthen the linkages between the University research communities and the Federal laboratories where CBRE test and evaluation has traditionally proceeded.

- Achieve critical mass in nanoscience toward the aggressive CBRE goals by leveraging the other NNI research programs (and other nanoscale R&D), especially NASA programs in microsattellites; DOE programs in environmental sensing; NIH programs in for medical sensors; NSF programs in simulation/modeling; EPA programs in improved sensors; treatment/remediation, and hazardous substance reduction/elimination; DOT programs in trace explosives detection; and DOD programs in nanoelectronics, molecular electronics and chemical and biological defense.
- Accelerate the incorporation of the excellent and extensive European and Pacific Theater nanoscience research into CBRE detection/protection.
- Couple closely with existing programs addressing the CBRE threat, especially the DOD Joint Service Chemical and Biological Defense Program¹, the Interagency Technical Support Working Group (TSWG, <http://www.bids.tswg.gov>), the DOE radiological and environmental protection program, and the DOT Weapons and Explosives Detection Program (aviation).

Infrastructure

MEMS/NEMS fabrication facilities will be necessary to implement the sensing goals. Nano-powder and nano-filament production scale-up will be necessary to implement the protection goals. Since any new technology must ultimately be tested against real agents, access to surety test and evaluation facilities in the Joint Chemical and Biological Defense Program must be included in this grand challenge. Once the nanoscience basis for improved technology is validated, the work should be transitioned to one of the Federal funding agencies – DARPA, TSWG, DTRA, DOE CBNP – already participating in the coordinated response to this problem

Agency Participation and Partnerships

To maximize the rates of scientific discovery and its commercial transition, this grand challenge will exploit the traditional strengths of the NNI participating agencies/departments, as follows:

DOD	chem/bio agent – sense/protect; landmine sense
DOE	radiological/explosive; system integration – lab on a chip
DOJ	chem/bio agent – sense/protect
DOT	explosive detection; advanced transportation security systems
EPA	chem/bio detection; decon/neutralization; hazardous substance reduction
NASA	system integration, miniaturization, robotic systems
NIH	therapeutic treatment for chem/bio/radio; sensors
NIST	chemical microsensors, single molecule measurement
NSF	fundamental science underpinning
State/Intel	detection for treaty verification and non-proliferation
USDA	chem/bio agents – sensing, prevention, and neutralization; securing food and other agricultural production

¹ Department of Defense, Chemical and Biological Defense Program, Annual Report to Congress, March 2000; DTIC ATTN: DTIC-E (Electronic Document Project Officer), 8725 John J. Kingman Road, Suite 0944, Fort Belvoir, VA 22060-6218

Coordination amongst many of these agencies at the technology level is already implemented through the Technical Support Working Group (TSWG).

11. Centers and Networks of Excellence

(total FY 2003 is \$108 million, \$17 million above FY 2002)

Vision and Strategy

Fund 15 new nanoscience and technology centers and networks, each at about \$3 million/year for approximately five years, with the opportunity for one renewal after an interim review. A focus on research networking and shared academic user facilities will continue. The establishment of these new Nanoscience and Technology Centers (NTCs) will play a critical role in attaining other NNI priorities (e.g., fundamental research, grand challenges, and education), in development and use of tools, and in promoting partnerships. Collaboration with academic networks (such as NNUN for nanotechnology equipment and NSF modeling and simulation network), and with national users facilities (such as synchrotron radiation facilities and neutron sources at national laboratories) is envisioned.

The long-term opportunities, priorities and modes of support outlined in the FY 2001 Supplement Budget Request remain the same.

Agency Participation and Partnerships

All agencies participating in NNI will contribute.

12. Research Infrastructure

(total FY 2003 is \$92 million, \$41 million above FY 2002)

Vision and Strategy

A balanced, strong, but flexible infrastructure will be developed to stimulate new discoveries and innovations that can be rapidly commercialized by U.S. industry. The focus will be on developing measurements and standards, research instrumentation, modeling and simulation capabilities, and R&D user facilities.

One of the NSET “high priority” themes for additional funding beginning in FY 2003 continues to be “research infrastructure” that includes metrology (\$9 million), instrumentation (\$33 million), modeling and simulation (\$18 million), and user facilities (\$32 million).

The potential is great for universities and government to transition this science and technology, bringing forth fundamental changes. There are great demands in industry to attract new ideas, protect intellectual property, and develop high performance products. The transition will require a sustained and timely investment. If the issues associated with research infrastructure and transition from knowledge-driven to product-driven efforts are not satisfactorily addressed, the

United States will not remain internationally competitive and, therefore, have difficulty maintaining the economy and quality of life and security that exist today.

Instrumentation and metrology

The long-term challenges and opportunities in this topic were presented in the FY 2001 Supplement Budget Request. A new grand challenge for FY 2003 will specifically address these issues. Priorities in this area include the following:

- Fund the purchase of instrumentation enhancing the capabilities of the existing research centers, networks and consortiums. This includes funding of industry/university/government collaboration to develop the tools and technology. The major R&D instrumentation and facilities will be made available to users not only from the institution that houses the facilities, but also for users from other institutions, industries and government.
- Provide computer network capabilities and a nanotechnology database for the management and dissemination of information to the nanotechnology science and engineering community in order to promote collaborations.

Modeling and simulation infrastructure

The long-term challenges and opportunities were presented in the FY 2001 Supplement Budget Request. Priorities in this area include the following:

- Develop computational facilities and human resources to facilitate development of interdisciplinary centers and network to serve nanotechnology R&D activities. Collaboration among groups working in different disciplines and areas of relevance (chemistry, thermodynamics, mechanics, electronics, biological processes, others) will be encouraged.
- Multiscale and coupled phenomena modeling and simulation of nanostructures at the atomic and molecular level in order to further fundamental understanding, explore new phenomena, and improve design predictions, will be supported with priority.
- Develop new simulation and design software to systematically create new materials and systems for given properties and functions. Computational thrusts could focus on the modern advances of quantum chemistry, molecular mechanics, molecular dynamics and device modeling and prediction applied to the chemical, energy, environmental, and advanced materials technologies. The methods may include Quantum Mechanics (QM), Force Fields (FF), Molecular Dynamics (MD), Coarse Graining (CG), Statistical Mechanics (SM), and Continuum Parameters (CP). Simulations that incorporate multiscale/multiphenomena descriptions need to be developed.
- Development of software, computational approaches, and simulation tools for process control and molecular manufacturing. This area is a very timely topic as it focuses on the regime between atomistic simulations (quantum theory, molecular dynamics) and physicochemical engineering practice (process simulation and design). The idea here is to use the results of atomistic calculations to supplement experimental data in determining the parameters of the coarse grain, phenomenological models required for process simulation and design. The use of new data on structural correlations from the atomistic simulations should provide more detailed information not available from experiment and would lead too much more detailed and accurate predictions.
- Develop a network for sharing software development in the academic community.

User facilities

The long-term opportunities were presented in the FY 2001 Supplement Budget Request. Priorities in this area include the following:

- Multiple-user national centers and networks equipped with nanotechnology-specific equipment (type of measurement, industry, etc.) need to be funded and staffed; the centers may be based in universities or at national laboratories.
- Vertical integration of fundamental and technological research within the multiple-user centers will be encouraged for synergistic purposes. Multi-technology engineering demonstration facilities funded by mission-oriented agencies and industry should be included in the centers.
- Development and use of regional university-national laboratory-industry facilities will be encouraged.
- The issue of *information sharing* is paramount; an agency and specific funding might be identified to foster communication of ideas and results among the various subfields within nanotechnology. One approach would be for an agency such as NIST to sponsor a nanotechnology-specific information facility agreed by participating agencies.

Agency Participation and Partnerships

All agencies participating in NNI will contribute.

13. Societal Implications of Nanotechnology and Workforce Education and Training

(FY 2003: \$16 million, \$1.6 million above FY 2002 for projects focused only on this topic; \$35 million, \$4 million above FY 2002 including also the educational component in research fellowships and traineeships in other projects)

Vision and Strategy

When radically new technologies are developed, social, economical, ethical, legal, environmental and workforce development issues can arise. Those issues would require specific research activities and measures to take advantage of opportunities or reduce potential risks. NNI will address these issues in a program that will establish research into ethical, social, economic, and workforce impacts of information technology, including transformation of individuals and social institutions, impact of legislation and regulation, barriers to nanotechnology diffusion, and effective use of technology in education, ensuring that all Americans have the education to take advantage of high-wage jobs created in the new economy.

The science, engineering, and technology of nanostructures will require and enable advances across a number of interrelated disciplines: physics, chemistry, biology, materials, mathematics, engineering and education. The dynamics of interdisciplinary nanostructure efforts will reinforce educational connections between disciplines and give birth to new fields that are only envisioned at this moment. Rapid development of nanotechnology will require changes in the laboratory and human resource infrastructure in universities, and in the education of nanotechnology professionals including lifelong learning.

A key objective of the national initiative is to provide new types of education and training that lead to a new generation of skilled workers in the multidisciplinary perspectives necessary for rapid progress in nanotechnology. The proposed initiative will leverage the existing strong foundation of nanoscience and engineering in the U.S., and will address the formidable challenges that remain.

The long-term educational opportunities and relevance were outlined in the FY 2001 Supplement Budget Request.

Several workshops and reports were prepared to guide future activities. These include:

- NSF Workshop on Societal Impact of Nanotechnology. Report published in 2001. The National Science and Technology Council (NSTC), Committee on Technology (CT), Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) — the Federal interagency group coordinating the NNI — sponsored a workshop on “Societal Implications of Nanoscience and Nanotechnology.” Held September 28–29, 2000, at the National Science Foundation, this workshop brought together nanotechnology researchers, social scientists, and policy makers representing academia, government, and the private sector. Their charge was to: (1) survey current studies on the societal implications of nanotechnology (educational, technological, economic, medical, environmental, ethical, legal, etc.); (2) identify investigative and assessment methods for future studies of societal implications; (3) propose a vision for accomplishing the nanotechnology goals, while minimizing undesirable consequences. The workshop participants offered recommendations to: (a) accelerate the beneficial use of nanotechnology while diminishing the risks, (b) improve research and education, and (c) guide the contributions of key organizations. These recommendations made to the NSTC are summarized below:
 - Make support for social and economic research studies on nanotechnology a high priority. Include social science research on the societal implications in the nanotechnology research centers, and consider creation of a distributed research center for social and economic research. Build openness, disclosure, and public participation into the process of developing nanotechnology research and development program direction.
 - The National Nanotechnology Coordination Office should establish a mechanism to inform, educate, and involve the public regarding potential impacts of nanotechnology. The mechanism should receive feedback from the nanotechnology community, social scientists, the private sector, and the public with the goals of: (a) continuously monitoring the potential societal opportunities and challenges; and (b) providing timely input to responsible organizations.
 - Create the knowledge base and institutional infrastructure to evaluate nanotechnology’s scientific, technological, and societal impacts and implications from short-term (3 to 5 years), medium-term (5 to 20 years), and long-term (over 20 years) perspectives. This must include interdisciplinary research that incorporates a systems approach (research-technology development-societal impacts), life cycle analysis, and real time monitoring and assessment.
 - Educate and train a new generation of scientists and workers skilled in nanoscience and nanotechnology at all levels. Develop specific curricula and programs designed to:

- (a) introduce nanoscale concepts into mathematics, science, engineering, and technological education;
 - (b) include societal implications and ethical sensitivity in the training of nanotechnologists;
 - (c) produce a sufficient number and variety of well-trained social and economic scientists prepared to work in the nanotechnology area;
 - (d) develop effective means for giving nanotechnology students an interdisciplinary perspective while strengthening the disciplinary expertise they will need to make maximum professional contributions; and
 - (e) establish fruitful partnerships between industry and educational institutions to provide nanotechnology students adequate experience with nano-fabrication, -manipulation, and -characterization techniques.
- Encourage professional societies to develop forums and continuing education activities to inform, educate, and involve professionals in nanoscience and nanotechnology.
 - James Batterson, an NNCO Fellow on detail from NASA/Langley, prepared a report for NSET on reforming education in nanoscience and engineering.
 - NSF held a workshop and is preparing a report on “Converging Technologies (Nano, bio, information and cognition) to Improve Human Performance.”

Priorities and modes of support

To most effectively respond to the opportunities discussed above, several specific priorities are:

- Introduce nano-science and engineering in existing and new courses.
- Nanotechnology centers and networks, with facilities and interdisciplinary research teams that will enable educating a new generation of young scientists.
- Create “regional coalitions” that involve industry-tech generation that include educational and training programs.
- Support student and post-doctoral fellowships for interdisciplinary work.
- Support student and young scientist internships at centers of excellence abroad.

Agency Participation and Partnerships

NSF in collaboration with NIH, NIST and DOD and other agencies will establish an education and training program for the critical areas in nanoscience and engineering. An education and training network with the participation of all interested agencies is envisioned. University based centers will be co-funded by various agencies. DOD, DOE, NASA and NIST will offer opportunities for research work with university research centers to arrange for student and postdocs participation in research. NIH has in place several programs to support an additional prong of the NNI strategy, namely training and workplace issues that will be used for nanotechnology education and training. One specific example is the Mentored Quantitative Research Career Development Award program, initiated last year through the efforts of BECON and with cooperation from most of the NIH ICs. The Food and Drug Administration (FDA) will have an important role to play, in reviewing and approving nanotechnology-based products affecting public health.

14. Transition of Scientific Discovery into Innovative Technology

It is fair to say that nanotechnology has been contributing to commercial products for over one hundred years. Nanometer-sized carbon (carbon black) improves the mechanical properties of tires, nanometer silver particles initiate photographic film development, and nanometer particles are the basis of catalysts critical to the petrochemical industry. These nanotechnologies were developed through empiricism; the structure and composition of nanostructures was very difficult, if not impossible, to ascertain. More recently, in the late 1960s, the discovery of surface analytical tools enabled the first revolution in nanoscience – surface science where one dimension is constrained at the nanometer scale. In turn, the scientific understanding of surfaces and surface processes has led to many important technologies, including the microelectronic devices, integrated circuits, and superlattice devices presently driving the remarkable advances in information technology. The discovery and development of scanned probes in the 1980s has led to a second revolution in nanoscience. One can now measure and manipulate not only surfaces, but also structures with 2 dimensions (lines, wires) and 3 dimensions (dots, clusters, proteins, viruses) at the nanoscale. The National Nanotechnology Initiative (NNI) was initiated in 2001 to exploit fully this revolution.

While the NNI is only one year old, and has fundamental research as its primary focus, its ancestral programs have already made enormous impact in commercial markets. High electron mobility transistors, vertical surface emitting lasers, and giant magnetoresistance read heads (all examples of one-dimensional nanotechnology) provide evidence that buttresses the expectation for similar impact from the NNI investment. Nevertheless, it is important for the NNI to proactively work toward technology transitions. It must address two questions: what actions are likely to accelerate the rate of transition, and what metrics can be used to measure progress toward the transition goals? The NNI is addressing this transition challenge on several fronts:

- Grand challenge investment strategies to ensure a range of technology options buttressed by scientific understanding, infrastructure to provide capability for nanoscience measurement, manipulation, and metrology
- SBIR and STTR programs to foster innovation in companies
- Outreach efforts to encourage business involvement
- Education and training to develop a skilled industrial/technical workforce

The urgency of the U.S. taking steps to move nanoscale science, engineering and technology into manufacturing cannot be overly emphasized. Consider the International Technology Roadmap for Semiconductors (ITRS) as being representative of the ever-increasing speed of technology development and implementation in manufacturing. In the 1999 ITRS projections, the period of time projected to advance to a sub-100 nm half-pitch in minimum feature size was accelerated with a “two-year pull-in” from the earlier projections. In nanotechnology the acceleration of transition from science and engineering into manufactured products is striking. A new form of carbon – the nanotube – was discovered in 1991. Subsequently, it was discovered in 1995 that these new nanotubes were excellent sources of field-emitted electrons. Then in 2000 a nanotube-based light source – the “jumbotron lamp” – using these field-emitted electrons to bombard a phosphor – was made available as a commercial product. By contrast, the semiconducting property of germanium was known and modeled in 1931, 17 years before the invention of the

transistor, and 23 years before a commercial product, a transistor radio, was made available in 1954.

A. Grand Challenge Programs

Within the NNI, grand challenges have been established for areas with high likelihood of nanotechnology impact. Figure 14.1 shows a notional strategy that illustrates the expectation of fundamental (undirected) research feeding new, unexpected discoveries into the grand challenge programs, and the grand challenge research feeding scientific understanding and options into industrial development programs.

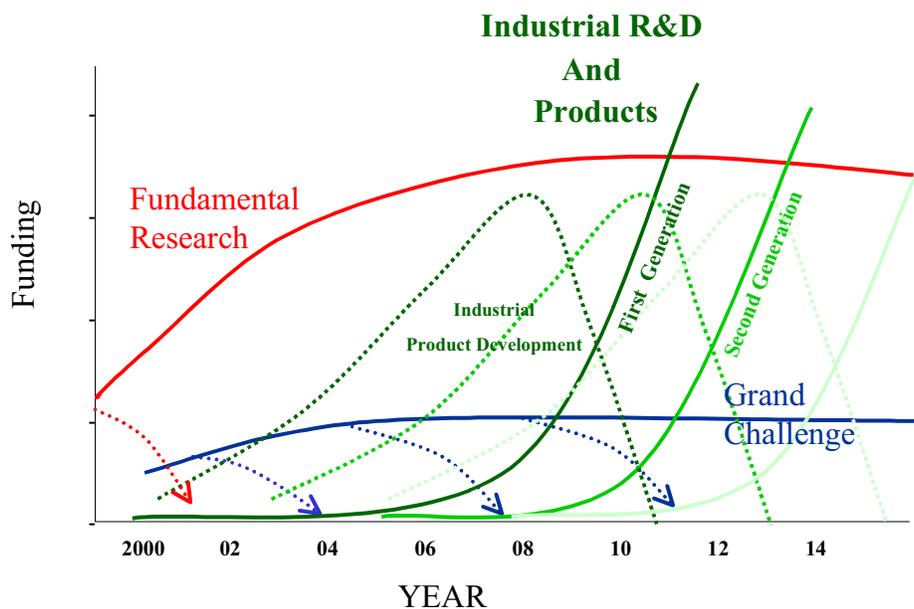


Figure 14.1. Notional investment planning for a grand challenge.

High-density memory provides an example of the notion illustrated by Figure 14.1; the National Storage Industry Consortia (NSIC) has a goal of demonstrating terabit/in² storage density by the year 2006. For terabit/in², each bit of memory must occupy an area about 25 nm on a side – clearly nanotechnology. Industry begins serious development programs 3-5 years prior to product introduction, so the science base for terabit data storage must already be largely in place. While not exhaustive, Table 14.1 lists a number of new approaches, spawned from nanoscience projects over the last ten years, which provide options for terabit/in² data storage. It is far from clear what the winning technology will be, but the proliferation of options promises not only success at that scale, but for an even greater packing density.

Each of the NNI grand challenges has a designated lead agency with the responsibility for ascertaining the present investment, identifying under-funded topics, developing an investment strategy, and working with industrial partners to accelerate technology transition. The Nano-Electronics, Optoelectronics, and Magnetics grand challenge will be the subject of a Special Technology Area Review by the DOD Advisory Group on Electron Devices in 2002. The Semiconductor Research Corporation (SRC) and the Electrical and Computer Engineering

Department Heads Association (ECEDHA) will assist in the review. This grand challenge was chosen for the first extensive NNI assessment because electronics is a major economic driver and the Semiconductor Industries Association (SIA) projects microelectronics to evolve fully into nanoelectronics in 10-15 years. The 2001 ITRS identifies many technology areas without adequate options available. This is the right time for basic nanoscience research programs to focus on providing the scientific understanding and discovery for technology decisions some ten years away.

Table 14.1
Innovative Nanodevice Concepts

Principal	Institution	Technology
Chou	Princeton	magnetic rods
Sun	IBM Almaden	magnetic nanocrystal
Tiwari	Cornell	nanocrystal floating gate
Vettiger	IBM Zurich	plastic deformation
Heath	UCLA	molecular switch
Lieber	Harvard	carbon nanotube switch
Aono	Osaka	Ag ₂ S switch
Prinz	NRL	giant magnetoresistance
Quate	Stanford	quantum dot charge storage

Evaluation of the NNI program during FY01 exposed two critical weaknesses important to the transition of science discovery into technology – the problems of scaling up laboratory efforts into full industrial production, and the limited capability to measure and manipulate nanoscale objects. Two new grand challenges have been introduced in FY02 – Manufacturing at the Nanoscale (NSF lead), and Nanoscale Instrumentation and Metrology (NIST lead). The details of these two new efforts are provided in Chapter 10. A joint NSF/European Commission workshop on nanomanufacturing was held 5-7 January 2002 to identify the critical issues needing attention and to find opportunities for joint programs. Since the U.S. share of nanoscience research is only one-third of the world total, it is important to find ways to leverage and complement the other investments.

The mission-oriented agencies participating in the NNI have funds available for applied research and exploratory development. As nanoscience discoveries grow, one might expect to see growing commitment of these funds toward nanotechnology. Since the DOD clearly parses its S&T funds into basic research (6.1), applied research (6.2) and exploratory development (6.3), the NNI has begun to track the DOD S&T investment. There is clear evidence (see Table 14.2) for the transition of science discovery into more applied funding programs.

Table 14.2
DOD S&T Funding of Nanoscience/Nanotechnology

Year	6.1	6.2/6.3
1998	73	
2000	90	
2001	107	16
2002 (est)	82	98
2003 (est)	96	105

From past experience, the time between scientific discovery and commercial product is 10-20 years. There is a need for metrics that are capable of reflecting progress toward the grand challenge goals in shorter time intervals. Those metrics might include: growing use of applied research and exploratory development funding; patents that cite nanoscience papers; SBIR/STTR programs and evidence for transition into commercial product; University professors directly associated with companies commercializing new products; and the growth of new technologies utilizing ever more sophisticated nanostructured systems.

B. Infrastructure

Nanostructures are very small. This makes their measurement and manipulation very difficult; control of noise sources in the environment is essential. NIST is in the construction phase of its Advanced Measurements Laboratory (<http://aml.nist.gov>), a building that has been designed to minimize noise sources. Many universities, national laboratories and companies are planning to construct new buildings for nanoscale research, development and manufacturing efforts. All of the new nanotechnology buildings must be carefully designed and constructed. As part of the new Nanoscale Instrumentation and Metrology Grand Challenge, NIST is organizing a topical conference/workshop to explore two critical questions: what are the building requirements to enable nanoscience research to proceed successfully, and what are the cost effective options one might use for these new designs? To get a complete perspective, the workshop will include research scientists/engineers, commercial instrument designers, and building architects. The report from this effort will provide invaluable guidance to the many new builders and architects designing buildings for nanoscience and nanotechnology.

The high cost of a properly designed nanotechnology building, added to the high cost of many nanoscale measurement and manipulation tools, could limit progress in nanotechnology. The NNI is working to provide centers (see Table 14.3) where individuals might gain access to special purpose capabilities that are too expensive for their local institutions. The National Nanofabrication Users Network predates the NNI and continues under its aegis. Three new DOE centers are being set up explicitly as nanotechnology user facilities. Each DOE center has hosted a workshop at which potential users had the opportunity to identify equipment and capabilities important to them. The NASA centers are presently under competition.

Metrics that are capable of reflecting progress toward the NNI infrastructure goals for shorter time intervals might include: adequately equipped, well used centers for measurement and manipulation; standards and techniques for measurement and quality control; and new commercial tools providing improved measurement and manipulation.

Table 14.3
NNI Centers

Center Title	Investigator	Institution
NSF		
Nanoscale Systems in Information Technologies	Buhrman	Cornell
Ctr. for Nanoscience in Biological & Environmental Engineering	Smalley	Rice
Nanoscale S&E Ctr. for Integrated Nanopatterning & Detection	Mirkin	Northwestern
Ctr. for Electronic Transport in Molecular Nanostructures	Yardley	Columbia
Nanoscale Systems and their Device Applications	Westervelt	Harvard
Ctr. for Directed Assembly of Nanostructures	Siegel	RPI
National Nanofabrication Users Network	Tiwari	Cornell
	Harris	Howard
	Plummer	Stanford
	Fonash	Penn State
	Hu	UCSB
DOE		
Integrated NanoSystems	Michalske	Sandia/Los Alamos
Nanostructured Materials	Lowndes	Oak Ridge
Molecular Foundry	Alivisatos	Lawrence Berkeley
DOD		
Institute for Soldier Nanotechnologies	Thomas	MIT
NASA		
Bio/Nano/Information Technology Fusion	TBD in 02	
Bio-Nanotechnology Materials and Structures for Aerospace Vehicles	TBD in 02	
Nanoelectronics and Computing	TBD in 02	

C. SBIR/STTR

Small businesses are frequently at the forefront in the development of new high technology products, particularly in the United States. There are many budding examples in nanotechnology. Table 14.4 lists a number of small companies that are selling nanomaterials; note that many (denoted by *) have utilized SBIR programs to establish their products.

The SBIR and STTR programs provide a mechanism to accelerate the development of nanotechnology through small companies. Table 14.5 shows the number of SBIR phase 2 nanotechnology programs initiated prior to the NNI by NASA and DOD through 1999. Data for more NNI agencies and more recent years is being collected now for future reports. With the growing NNI investment, one might expect to see growth in the number of these programs.

Table 14.4
 Sampling of Companies with Commercially Available Nanotechnology Building Blocks

Name	URL	Products
Nanopowders		
Altair	www.altairtechnologies.com	TiO ₂
AP Materials*	www.apmaterials.com	non-oxides
Argonide Nanomaterials*	www.argonide.com	aluminum
BuckyUSA	www.flash.net/~buckyusa/	fullerenes
Inframat Corporation*	www.inframat.com	YSZ, FeS, n-WC/Co, Co/SiO ₂ ,..
NanoEnergy Corp*	www.nanoproducts.com	metal oxides
Nanophase Technologies†	www.nanophase.com	oxides
Nanopowder Enterprises	www.nanopowderenterprises.com	oxides, metals
NanoPowder Industries	www.nanopowders.com	precious/base metals
Nanoscale Materials, Inc.*	www.nanmatinc.com	metal oxides
NanoSonic, Inc.*	www.nanosonic.com	ferrites, self assembly
Nanox	www.nanox-online.com	ZnO
NexTech Materials	www.nextechmaterials.com	oxides
Powdermet	www.powdermetinc.com	metals, ceramics
US Nanocorp, Inc.	www.usnanocorp.com	n-MnO ₂ , n-Ni(OH) ₂ , n-FeS ₂
Nanowires/nanotubes		
Carbolex	carbolex.com	Single Wall Nanotubes (SWNT)
Carbon Nanotechnology	cnanotech.com	SWNT
ESpin	www.nanospin.com	polymer nanofibers
Hyperion Catalysis*	www.fibrils.com	Multi Wall Nanotubes (MWNT)
Materials & Electrochem Res.*	www.mercorp.com	SWNT, MWNT
NanoLab	www.nano-lab.com	CNT and arrays
Nanopores/filters		
Argonide Nanomaterials	www.argonide.com	filters with bioactive nanofibers
NanoPore, Inc.	www.nanopore.com	silica xerogel
Nanocomposites		
Triton Systems*	www.tritonsys.com	coatings, packing
Nanocor	www.nanocor.com	nanoclay in plastics
Nanogate	www.nanogate.de	scratch resistant coating

* companies that have utilized SBIR programs to help establish their products.

† company that has utilized NIST/ATP program to help establish itself.

Table 14.5
 Number of New SBIR Phase 2 (DOD and NASA) Nanotechnology Projects

Year	SBIR
1995	6
1996	16
1997	21
1998	10
1999	14

A metric that could reflect progress toward the SBIR and STTR goals for time intervals shorter than 20 years might be the number of Phase 2 programs (useful initially), but this must be followed quickly by the number of commercialized products emanating from the SBIR/STTR programs

D. Outreach Programs

Nanotechnology has huge economic potential but is relatively early in its development. State and regional authorities are recognizing the opportunity to create an analog to Silicon Valley, sometimes referred to as “Nano-Valley.” A number of states have instituted their own funded programs to exploit this opportunity; a partial listing of these efforts is shown in Table 14.6. States – Virginia, Maryland, and Texas among others – have also sponsored workshops and NSET committee members are contributing to these workshops.

Table 14.6
State and Local Funded Nanotechnology Programs

State	Item	Financial Commitment
CA	California Nanosystems Institute	\$100 million over 4 yrs
NY	Center of Excellence in Nanoelectronics	\$50 million
IL	Nanoscience Center	\$36 million
IN	Nanotechnology Center	\$5 million
PA	Nanotechnology Center	\$10.5 million over 3 yrs
TX	Nanotechnology Center	\$0.5 million over 2 yrs
VA	CIT, UVA, and CTRF reported funding	\$3.3 million
SC	NanoCenter	\$1 million

Some states are supporting the development of technology parks at their universities. The Indiana contribution of \$5 million in Table 14.6, added to \$40 million from private contributions and other funds, will fund the Birck Nanotechnology Center as the first building in the Purdue University Discovery Park. Kansas State University has proudly announced that Nanoscale Materials, Inc. has the first building in its K-State Research Park. There is opportunity for other states to foster new industrial cooperative opportunities.

NSET members have utilized EPSCoR forums to preach this gospel; Oklahoma has created the NanoNet, a network of Oklahoma scientists, engineers and students, enhanced by EPSCoR support for research infrastructure for three key types of systems: epitaxial nanostructures, colloidal particles, and connectors. State nomination of nanoscience projects to the EPSCoR programs could grow.

Nanotechnology is a relatively new “buzz word” and is essentially meaningless to many people outside of the university science and engineering departments. Of the NSET agencies, DOC and DOE are leading the efforts to help industry understand and exploit the opportunities. The DOE Office of Industrial Technologies hosted a nanoscience symposium at the 4th Industrial Energy Efficiency Symposium & Exposition, February 19-22, 2001 in Washington, DC. Under the NNI mantle, the DOC Office of International Technology Policy and Programs is organizing a series of regional workshops with the following goals: (a) making industry better aware of pending nanotechnology developments, and (b) making the NNI better aware of science deficiencies limiting industrial commercialization of nanotechnology. The first workshop (western region) was held on Sept 10, 2001 at UCLA; it was run by the California NanoSystems Institute and the UCLA School of Public Policy and Social Research. The second (southern region) is planned for Houston, Texas in May 2002. Minneapolis (midwest) and Boston (eastern) will complete the presently planned suite of four workshops.

The financial and business community is not totally ignorant of nanotechnology opportunities. Several private initiatives are seeking to accelerate the introduction of nanotechnology into the market. The NNI contributes to these efforts as an information resource. For instance, the NanoBusiness Alliance is actively fostering nanoscience and nanotechnology by compiling three nanotechnology directories – venture capital, industry, and nanotechnology service and support. The Texas Nanotechnology Initiative hosted Nanoventures 2002 in March 2002. The Los Angeles Regional Technology Alliance (LARTA) hosted a meeting on February 21, 2002, “Japan Meets the Nano Republic of California,” a focused half-day event that brought together leading business and research leaders from Japan and California for a practical discussion on current research and potential future business opportunities in nanotechnology. LARTA also has created the Nanotechnology Yellow Pages, an industry report and directory, presently focused on Southern California.

Metrics that could reflect progress toward the outreach goals for time intervals shorter than 20 years might include: number of NNI/NNCO outreach events; investment at state and local levels; and industrial investment in nanoscience and nanotechnology to complement the Federal programs.

E. Education and Training

Education and training are important for technology transition in at least two ways. First, a citizenry knowledgeable in science is necessary for informed judgment on all new technology, nanotechnology included. Second, industry must have an adequate supply of trained people for its workforce. Education in nanoscience must begin in the primary and secondary schools – K-12. Not only will this education result in an informed citizenry, but it will also supply youth interested in science and engineering careers. One might hope that nanoscience, as a new highly interesting area of science, might also excite a new generation of students toward science as a profession. Dr. James Batterson, a NASA employee detailed to the NNCO, has prepared a paper entitled, “Extending Outreach Success for the National Nanoscale Science and Engineering Centers – A Handbook for Universities,” providing guidance for impacting the curricula development process. The NSF Nanoscale Science and Engineering Centers have funds specifically to address K-12 education.

It is reasonable to expect, especially in the early years of its development, that nanotechnology will require a highly educated and trained workforce. The workforce demands of the microelectronics industry certainly support that expectation. Many of the more exciting prospects for nanotechnology are highly multidisciplinary; the traditional university department structures and degrees may not be best suited for nanotechnology expertise. The NNI must promote the evolution of university programs specifically focused on nanotechnology. The University of Washington (Washington State) and the University at Albany (New York) are currently exploring graduate degrees in nanoscience. Pennsylvania State University offers both an associate degree and a certificate option in its Nanofabrication Manufacturing Technology Program.

Metrics that are capable of reflecting progress toward the outreach goals for time intervals shorter than 20 years might include: multidisciplinary nanotechnology centers at universities;

masters and doctoral degrees focused on nanoscience; curricula adaptations to incorporate nanoscience; and increased multi-disciplinary research groups and programs at universities and colleges.

NATIONAL NANOTECHNOLOGY INITIATIVE **PUBLICATIONS**

Below is a list of nanotechnology publications that have been prepared by the Interagency Working Group on Nanoscience, Engineering and Technology (IWGN) and respectively Nanoscale Science, Engineering and Technology (NSET) Subcommittee of the National Science and Technology Council's Committee on Technology.

Nanotechnology: Shaping the World Atom by Atom

(<http://www.nano.gov> or
<http://www.ostp.gov/NSTC/html/iwgn/IWGN.Public.Brochure/welcome.htm>)

National Nanotechnology Initiative – Leading to the Next Industrial Revolution

(<http://www.nano.gov> or
<http://www.ostp.gov/NSTC/html/iwgn/IWGN.FY01BudSuppl/toc.htm>)

Nanostructure Science and Technology: A Worldwide Study

(<http://www.nano.gov/> or
<http://www.ostp.gov/NSTC/html/iwgn/IWGN.Worldwide.Study/toc.htm>)

IWGN Workshop Report: Nanotechnology Research Directions

(<http://www.nano.gov/> or
<http://www.ostp.gov/NSTC/html/iwgn/IWGN.Research.Directions/toc.htm>)

Societal Implications of Nanoscience and Nanotechnology

(<http://www.nano.gov/>, click on “Reports”)

Examples of Research Accomplishments in the First Year of the National Nanotechnology Initiative (FY 2001)

Although the National Nanotechnology Initiative (NNI) began officially just over a year ago (in fiscal year 2001), there are already some important examples of where NNI-related research supported by the Federal Government in FY 2001 and earlier years has shown great promise for addressing pressing national needs. This appendix includes a sampling of such evolving “success stories.”

B.1. Nature’s Tools to Assemble Materials with Atomic Precision

The basic assembly processes at the nanoscale used in nature are self-assembly, molecular recognition, self-correction and nano-structural regularity. The University of Texas at Austin has developed techniques for specific biomolecular recognition to control the assembly of non-biological electronic and magnetic materials, for example semiconductors. They are working to control crystal growth, and placement and assembly of nanoparticles using the tools from nature. Synthetic bifunctional peptides are synthesized to selectively bind different nanoparticles through molecular recognition. The peptides assemble semiconductor/magnetic heterostructures to obtain new materials in multiple length scales. In another example, the same group used viruses as the assembling biosystems with molecular precision.

In Figure B.1, we are reminded that nature makes a very strong version of CaCO_3 , the abalone shell (with CaCO_3 and proteins), 3000 times stronger than amorphous CaCO_3 . The structure in the figure is micron scale, but the underlying natural assembly process is nanoscale. The challenge, then, is how to use the tools of the natural biological process to control crystal growth and placement and assembly of non-biological electronic and magnetic materials. The idea, shown in Figure B.2, illustrates, symbolically, two bifunctional peptides, one that binds (on respective ends) to gallium arsenide and iron oxide and the other that binds to iron oxide and zinc sulfide. So far, a peptide for gallium arsenide has been isolated, and the investigators work now to produce bifunctional peptides “by design.”

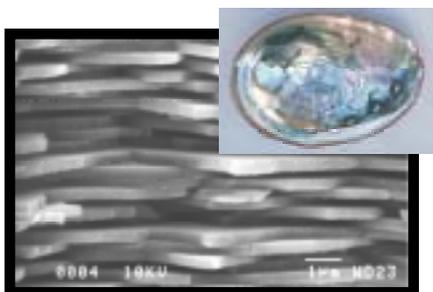


Figure B.1. Picture and schematic showing the structure of naturally made abalone shell.

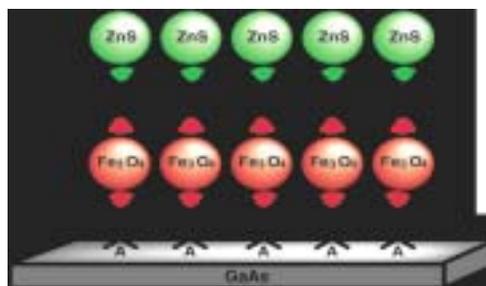


Figure B.2. Illustration of protein-assisted magneto-electronic heterogeneous structure. Nanoparticles are arranged in layers using bifunctional peptides to bind them to surfaces.

This is an example of the synergism of using nanoscience with bio-tools to obtain ultrafine electronic circuits (convergence of nano, bio and information technologies) that opens a broad spectrum of opportunities in materials synthesis, nanoengineering and nanoelectronics.

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University of Texas – Austin, NSF Award 9986563.

Abstr. Pap. Am. Chem. S. 221: 415-INOR Part 1 APR 1 2001.

Abstr. Pap. Am. Chem. S. 222: 53-POLY Part 2 AUG 2001.

Funding Agencies: NSF

B.2. Building DNA Nanomechanical Devices

Researchers at New York University demonstrated the first DNA nanomechanical device, based on the B-Z transition of DNA, in 1999. This device relied on fluorescence resonance energy transfer to demonstrate the molecular motion, and the key stumbling block to its development was finding a component rigid enough so that a well-defined structural transition could be characterized. The green and pink filled circles in the Figure B.3 represent the DNA string pair used to demonstrate motion. In addition to making DNA devices, the same researchers have produced periodic DNA arrays from a variety of motifs. These are 2D arrays, although they are working hard to extend these results to 3D. The key goal is to combine these efforts and incorporate nanomechanical devices into arrays. If this goal is achieved, it would be possible to construct a variety of structural states. Except for a certain amount of chemical nuance in B-Z propensity, the B-Z device will lead to two different structural states, regardless of how many unique molecules are incorporated into the array. Given N different 2-state devices, one should be able to produce 2^N different states. Being able to do this is a first step towards a practical nanorobotics. To this end, the device shown in Figure B.4 was designed. Panel (a) illustrates the two end states available to this system. On the left is a paranemic crossover (PX) DNA molecule, in which two double helices are aligned with twofold symmetry about a central dyad axis, and every possible crossover occurs between helices. In the molecule shown, the system becomes a blue double helix, a red double helix, and a “red” double helix that are inter-wrapped for 1.5 turns. To the right of the PX molecule is a JX_2 molecule, in which two of the crossovers are missing. The consequence of this change in topology is that the molecules wrap only once over the same distance. Thus, although the tops of the two molecules, A and B, are in the same places, the bottoms are rotated 180° from each other; C and D in the PX molecule occupy the same spatial positions as D and C, respectively, in the JX_2 molecule. This is the structural basis of the new device.

The machine cycle and the adjustments to the system to turn it into a device are shown in panel (b) of Figure B.4. For convenience, the red and blue strands each have been combined into a single strand, by the addition of hairpin loops at their ends. More importantly, the red and blue strands have been interrupted for 3 half-turns by a pair of green strands. Removal of these strands is the first step in the operation of the device. The green strands each have a short extension. When the complete complement (including the extensions) to each of the green

strands is added to the PX molecule, as shown in Process I, they are removed from the PX molecule, and the unstructured intermediate shown at the top of the panel is obtained. Adding the purple strands (Process II) leads to the JX_2 state, shown on the right. The machine cycle can be completed by removing the purple strands (Process III) and adding the green strands, again (Process IV). It is very important to realize that the sequences of the blue and red strands that pair with the green and purple strands can be varied, so many different devices can be produced that can be addressed by their particular sets of green and purple strands. Each of the four steps of the machine cycle corresponds to changing the state of the environment. The system responds by achieving the lowest free energy state, given the new circumstances. The proposed nanorobotics approach will lead to methods of making new molecules (chemical fabrication).

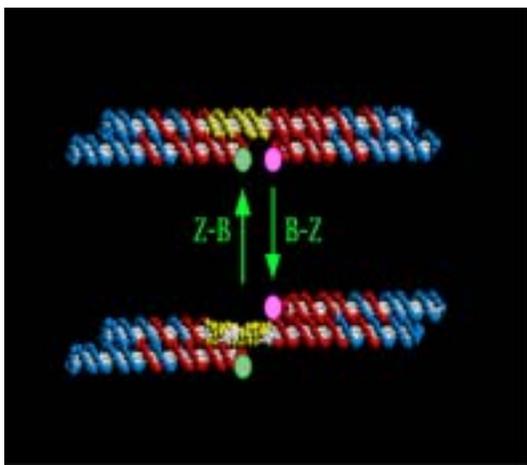


Figure B.3. DNA string pair used to demonstrate motion.

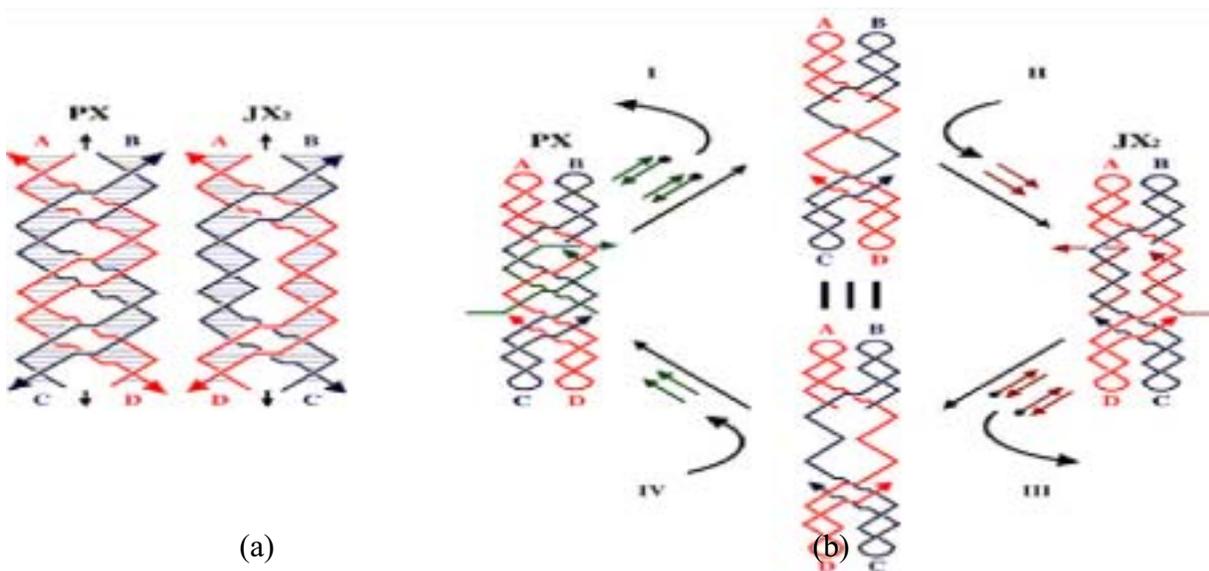


Figure B.4. Nanomechanical DNA device: (a) two states of the system; (b) machine cycle, I – II – III – IV, of the device.

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Funding Agencies: NSF

B.3. Simulation of Biological Ion Channels in Human Body

Biological Ion Channels (BICs) are the nano-transistors of nature. They switch electrical currents and fulfill a multitude of functions in human body. They can regulate the electricity of the heart, they can act as antibiotics and they even fight cancer. BICs have nanometer dimensions in all directions. The NSF Distributed Center for Advanced Electronics Simulation (Descartes) from the University of Illinois at Urbana-Champaign and Stanford University with collaborators from Rush Medical Center (Chicago) have explained the magnitude of the electric currents in several BICs and the connection of these currents to macroscopic cell membrane potentials (see figures B.5 and B.6).

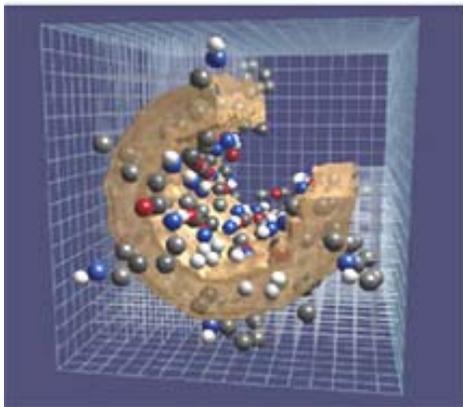


Figure B.5. The atom structure (spheres) of an ion channel is represented together with a computational grid. The shaded area indicates the electrostatic potential corresponding to the channel pore. Inner area is open to ion transport.

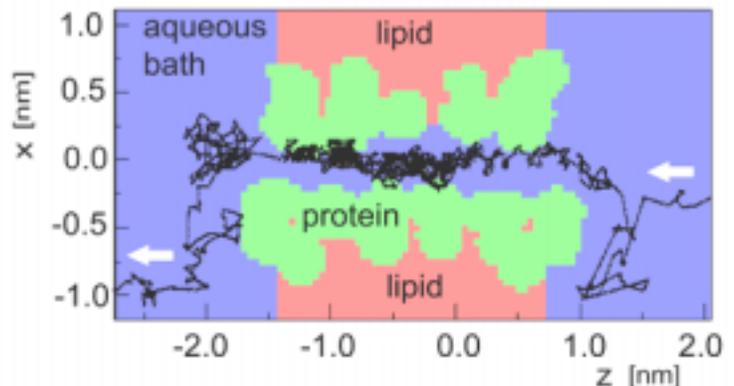


Figure B.6. The actual simulation of a successful ion traversal trajectory in the same channel, obtained by a Monte Carlo simulator utilizing leading expertise acquired in the simulation of semiconductor devices. These simulations resolve the history of individual ions and can explain rare-event phenomena and important properties of BICs like ion selectivity.

The hierarchy of simulation tools that was developed for the design of semiconductor devices permits the simultaneous description of single ion transport in channels of nanometer dimensions as well as the prediction of the macroscopic currents and cell membrane potentials. This opens new horizons for the understanding of ion channel activity in the human body. For example, it should be possible in the future to simulate the known positive influence of increased magnesium-ion concentrations in the blood to reduce atrial arrhythmias of the heart, simply by connecting the nano- and macro-scale by using hierarchical and interdisciplinary simulation tools.

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Funding Agencies: NSF

B.4. Molecular Circuitry Heralded as “Breakthrough of the Year”

Science Magazine awarded its “Breakthrough of the Year for 2001” to the successes in assembling molecules into basic electronic circuits. Before 2001 only molecular devices had been demonstrated; in 2001 a number of laboratories connected molecular devices into more complex circuits.

At an ACS meeting Jim Heath and his colleagues at UCLA reported making semiconducting crossbars with molecules called rotaxanes. By controlling the input voltages to each arm of the crossbar, they showed that they could make working 16-bit memory circuits. Phaedon Avouris of IBM reported making a circuit out of a single semiconducting nanotube. By draping the nanotube over a pair of electrodes and independently controlling their behavior, the team coaxed the device to work like a simple circuit called an inverter, a basic building block for more complex circuitry. Circuits with stronger gain came from Cees Dekker’s team at Delft University of Technology in the Netherlands; they were able to create CNT transistors with an output signal 10 times stronger than the input. Charles Lieber’s group at Harvard constructed circuits with their semiconducting nanowires, made from silicon and gallium nitride.

Backed by this string of accomplishments, molecular electronics is rapidly moving from blue-sky research to the beginnings of a technology. Researchers now face the truly formidable task of taking the technology from demonstrations of rudimentary circuits to highly complex integrated circuitry that can improve upon silicon’s speed, reliability, and low cost. Reaching that level of complexity will undoubtedly require a revolution in chip fabrication. But as chip designers race ever closer to the limits of silicon, pressure to extend this year’s breakthroughs in molecular electronics will only intensify.

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Funding Agencies: DOD, NIST, NSF

B.5. Micro Lens for Nano Research

A silicon lens that is 1/10 the diameter of a human hair, or only a few wavelengths in diameter, has been fabricated and used to image microscopic structures by a team at Stanford University (G. Kino and K. Goodson). Known as solid immersion microscopy, the micro fabricated lens is scanned close to a surface to collect images (see Figure B.7). The lens can focus light to 1/5 of a wavelength with an improvement in definition (over that of standard lens) by a factor of 3.5, and a ratio of intensity of the output to input power at least 1000 times better than existing near-field probes. The lens's combination of high optical efficiency and improved spatial resolution over a

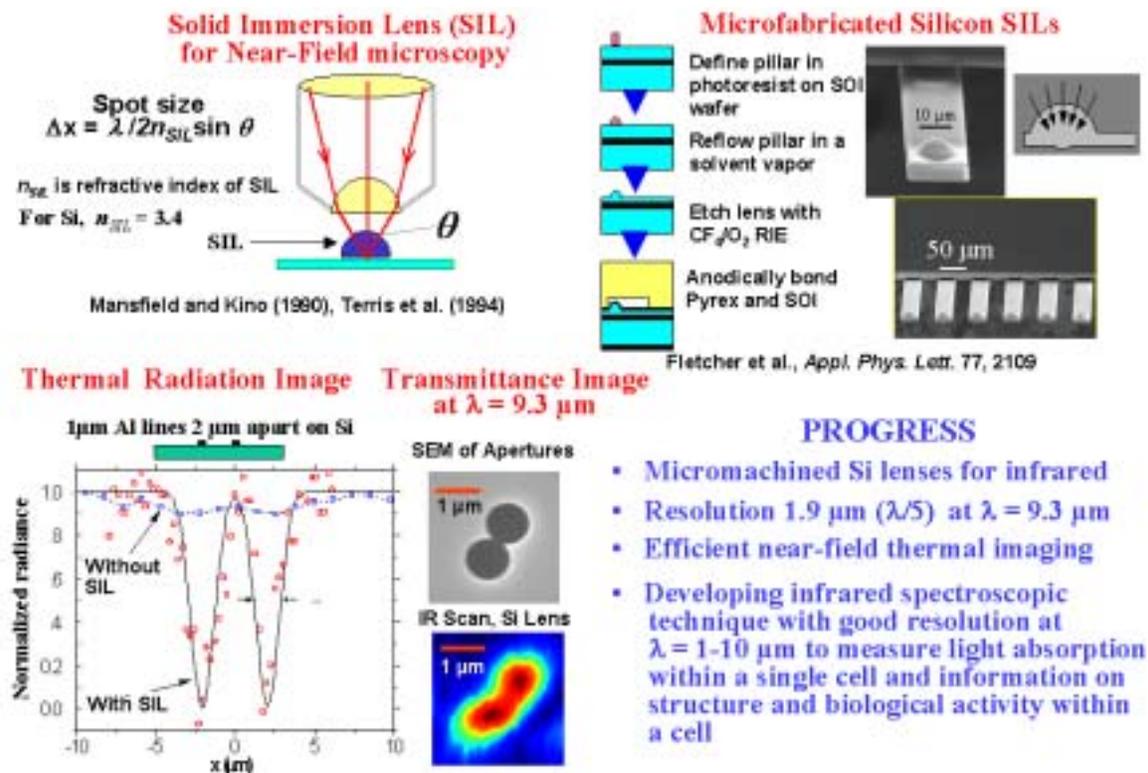


Figure B.7. A near-field infrared microscope using micro lenses.

broad range of wavelengths (1-10 μm) has enabled measurement of infrared light absorption in single cells. This spectroscopic technique can provide important information on chemical composition, structure, and biological activity within a cell. Currently, a modified system is also being designed to give definition of the order of 1/20 of a wavelength.

Reference

J. Microelectromech. Sys 10, 450-459 (2001)

Funding Agency: DOE

B.6. Development of the Biological Force Microscope in Geochemistry

Professor Michael F. Hochella and coworkers (NanoGeoscience and Technology Laboratory, Department of Geological Sciences, VPI&SU, Blacksburg, VA) have developed the first biological force microscope which is capable of quantitatively measuring interfacial and adhesion forces between living bacteria and mineral surfaces, in situ. The image and data in the Figure B.8 and B.9 below were collected using a fluid cell atomic force microscope (AFM) developed at VPI.

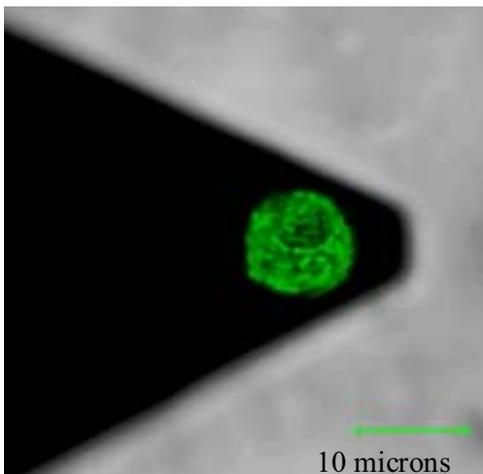


Figure B.8. Image of *E. coli* cells attached to an AFM cantilever.

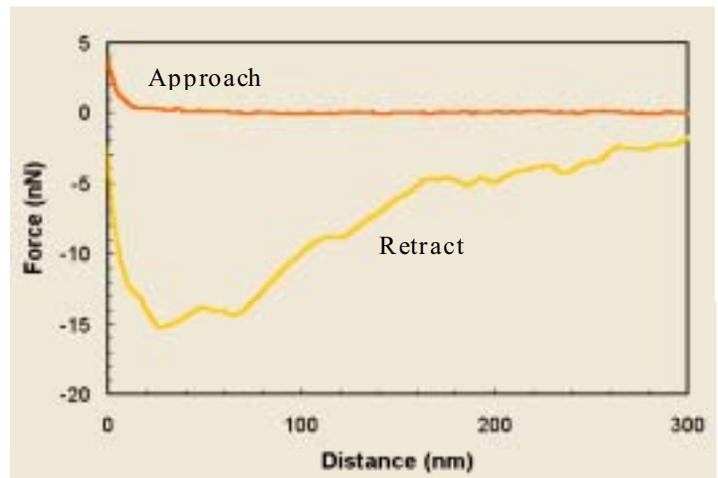


Figure B.9. Repulsive (+) and attractive (-) forces between *E. coli* cells and mineral muscovite in an aqueous solution.

A study by this group was recently published in *Science* (18 May 2001, v. 292, p. 1312-1313 and 1360-1363). Cells of *E. coli* were attached via a polycationic linker molecule to a minute glass bead, then the bead attached to an AFM cantilever to create a biologically-active force-probe (Figure B.8, where individual *E. coli* cells can be seen attached via the bead to the dark triangular AFM cantilever). Figure B.9 illustrates the interaction between this *E. coli* and the mineral muscovite in aqueous solution to simulate how environmentally important, living bacteria interact with mineral surfaces in a soil-like solution. As muscovite and *E. coli* approach one

another, nanometer by nanometer, repulsive forces (positive values in nanoNewtons) begin at a distance of 20 nanometers and reach a magnitude of 5 nN up to surface contact. This is consistent with electrostatic repulsion as both muscovite and *E. coli* have negative surface charges under the pH of this experiment. However, upon contact and subsequent retraction, attractive forces (negative values) of up to 15 nN extend outwards for over 300 nanometers. These data suggest that once contact is established, *E. coli* is able to overcome any repulsive interactions by forming attractive hydrogen bonds with surface hydroxyls on the muscovite surface.

Results such as these suggest that biological force microscopy has the potential to allow researchers, for the first time, to gain fundamental insights into the nanoscale and nanoforce world that exists at the interfaces between microorganisms and minerals in nature. Moreover, because the cells, substrate and fluid properties can be easily varied, this technique will be of interest to biologists, materials scientists, and medical researchers. Applications will be as wide ranging as understanding the mobility of pathogenic bacteria in a groundwater aquifer to determining the affinity of certain kinds of human lung cells to various mineral fibers.

Reference

Geomicrobiol J 18(1), 63-76 (2001)

Funding Agency: NSF

B.7. Electron Picometer Ruler to Measure Atomic Displacements in Crystals

A team at Brookhaven National Laboratory (Y. Zhu, L. Wu, J. Tafto, M. Suenaga, and D. O. Welch) has developed a new interferometric electron beam technique that has measured atomic displacements across interfaces in a bismuth-based superconductor to a record accuracy of 1 picometer, i.e., one one-hundredth of the diameter of an atom. Imperfections in atomic packing such as interfaces and crystal boundaries often determine the properties and behavior of materials, particularly in nano-structured devices and can lead to new insights about chemical bonding and electronic structure at structural imperfections and consequent changes in materials performance. A critical example is the effect of lattice expansion at interfaces between crystallites on the current flow in superconductors. This capability has been made possible by the new interferometric technique, coupling electron diffraction with imaging using a highly coherent electron beam in an electron microscope (Figure B.10). The key to the accuracy of the measurement is its independence of the wavelength of the electrons. This was achieved by a quantitative analysis of interference patterns produced by electron waves, which are scattered by structural imperfections. The result is a greatly enhanced capability to map imperfections and their resulting strain fields in materials ranging from superconductors to multilayer semiconductor devices.

Reference

PRL 85, 5126-5129 (2000)

Funding Agency: DOE

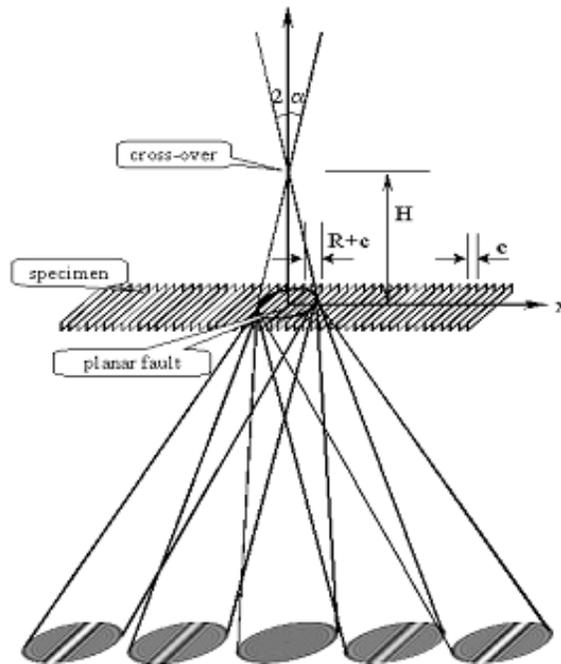


Figure B.10. Atomic displacements have been measured with an accuracy of a picometer (0.001 nm) using a coherent source in the experimental setup shown in this figure.

B.8. Carbon Nanotube Field-Effect Inverters

The first demonstration of a carbon nanotube (CNT) based inverter logic circuit has been completed at NASA Ames Research Center. This breakthrough applies to p-type metal-oxide-semiconductor (PMOS) and complementary metal-oxide semiconductor (CMOS) inverters and it is based on single-walled carbon nanotube field-effect transistors. A carbon nanotube is grown via a chemical vapor deposition (CVD) method and contacted by two metallic source/drain electrodes (Figure B.11). The circuit that uses both CMOS and PMOS platforms has been shown to work at room temperature, and this has significant implications for electronics applications.

Carbon nanotubes may be semiconducting or metallic, and allow readily for making metal-semiconductor, semiconductor-semiconductor junctions. The single wall nanotube is just about 1 nm in diameter and can lead to electronic devices at the nanometer scale. Previous work had used various fabrication approaches to address individual single walled carbon nanotubes. These techniques allowed the production of isolated devices such as single-electron transistors and field effect transistors. However, fabrication of integrated systems requires control on the position and orientation of the nanotubes. The new CVD technique allows such control. The core of this fabrication approach involves depositing catalytic nanoscale iron particles onto a patterned Si/SiO₂ substrate.

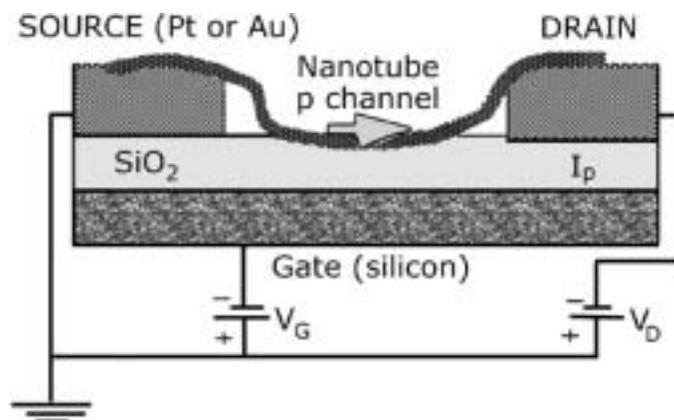


Figure B.11. A carbon nanotube connecting the source and the drain was used to build an inverter logic circuit.

The PMOS inverter is constructed from a carbon nanotube transistor using an external load resistor. The CMOS inverter is constructed by connecting a p-type nanotube transistor with an n-type nanotube transistor. Both types of inverters functioned at room temperature and possess gains equivalent to or greater than 1. This innovation is paving the way for the development of carbon nanotube transistor based integrated circuits and for future computing systems.

Reference

Liu, X.-L., C.-L. Lee, C.-W. Zhou, and J. Han. 2001. *Applied Physics Letters*, 79, 3329.

Funding Agency: NASA

B.9. Peptide Nanotubes as Antibacterial Drugs

Many of our commonly used antibiotics work by defeating the perimeter defenses of the invading bacterial cell. That is, they damage the bacterial cell membrane. But many do so by targeting single types of molecules in the membrane, so if the bacteria can change that molecule slightly, which they usually can, then the bacteria become resistant to the antibiotic.

A research group at the Scripps Research Institute in San Diego, California, with support from the National Institute of General Medical Sciences (NIGMS), NIH, showed last year that nanotubes originally developed for a variety of purposes, including to serve as tiny test tubes (with an opening smaller than 1 nm across!) to study chemistry in molecularly-confined spaces, can also be used to punch holes in bacteria. With holes in their membranes, the bacteria become leaky and die quickly (Figure B.12).

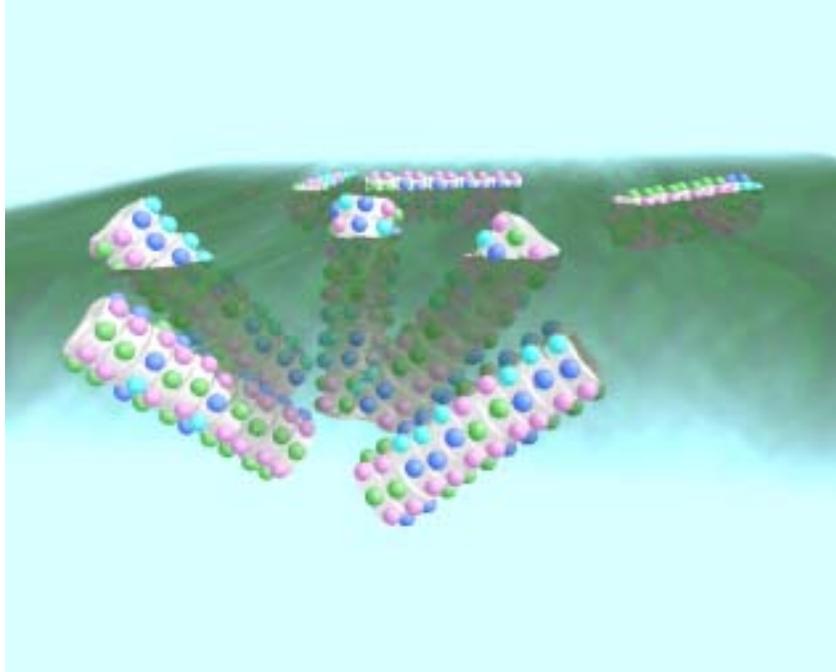


Figure B.12. Polypeptide nanotubes are thought to assemble within the membrane of bacterial cells, forming a channel from inside to outside the cells. The bacteria become leaky and die within minutes (courtesy Art Olson, The Scripps Research Institute).

The nanotubes are built of amino acid subunits very similar to those found in the proteins in our bodies, but with one important difference: alternating subunits have a structure that is the mirror image of the structure of our own amino acids (that is, naturally occurring L-amino acids alternate with D-amino acids). The strings of subunits (called peptides) therefore form small disks, which under the right conditions (such as are found in cell membranes) can stack to form tubes. By controlling the chains that stick out of the nanotubes walls, overall characteristics of the tubes can be fine-tuned. This makes it possible for the nanotubes to perforate bacterial membranes without harming the cells of the animal (in this study, a mouse) that has been infected by the bacteria. Studies continue to determine if these little tubes can be made specific for a wide variety of harmful bacteria, while sparing the cells of the host.

It is thought that it will be harder for bacteria to become resistant to these agents than to many other types of antibiotics, because the bacteria would have to substantially change their membranes, not just alter a particular molecule. The bacteria can probably do this given enough time, but then the structure of the nanotubes can be changed to foil the escape. These tubes have another important property – they are resistant to proteases (protein-digesting enzymes) found in our bodies. If successfully developed, drugs based on this concept might be used to treat millions of cases of otherwise antibiotic-resistant bacterial infections in humans and animals every year, worldwide.

Many steps are needed before this scientific discovery can be harnessed to produce antibacterial drugs. Nevertheless, it is an example of how new ideas emerge in unexpected ways from basic nanotechnology research.

Reference

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Funding Agencies: NIH

B.10. Fluorescent Imaging with Quantum Dots

Recent studies using fluorescent quantum dots (QDs) demonstrate their practical utility for important biomedical applications. These QDs are semiconductor nanocrystals, about 2 to 7 nm in diameter, consisting of just 200-10,000 atoms, that have remarkable properties and promise.

Fluorescent labeling is a powerful method in biomedical research. Most biological molecules are invisible, but by attaching dyes or particles that emit intense fluorescence to them, it becomes possible to track to location of those molecules inside cells, revealing their locations and interactions with other molecules. Fluorescent labeling is also an essential starting point for many analytical techniques, such as DNA sequencing and microarray (sometimes known as “gene chip”) experiments for gene expression and human sequence variation (SNP) analysis. These basic experimental tools have many applications, including disease diagnosis, drug discovery, the study of basic disease mechanisms, and detection of infectious (including bioterror) agents.

In the late 1990s, scientists showed that semiconductor nanocrystals produce intense fluorescence in different colors, depending on particle size, and could be used for labeling biological molecules (Figure B.13). The particles offer several advantages over the fluorescent organic dyes commonly used to label biological molecules. The fluorescent nanoparticles have a core surrounded by a thin shell. In this configuration, the size of the core determines the color of the fluorescence and the shell increases its brightness. Different core diameters result in different colors. Both the intensity and the sharpness of the color spectrum are greater for QDs than for organic dyes. In addition, organic dyes are harder to use, because different ones must be illuminated with different colors of light to make them fluorescence. In contrast, a single color can be used to excite QDs of several different colors. In spite of these promising optical qualities, using QDs in biological experiments has been difficult.



Figure B.13. Members of a family of quantum dots of different sizes, illuminated by a single light source, emit intense fluorescence of different colors (courtesy Felice Frankel, MIT).

In 2001, significant progress was made in showing how to use QDs to obtain useful biological information. One study, supported in part by the National Institute of General Medical Sciences (NIGMS), NIH, demonstrated how to change the QD surface so that it could bind to short DNA strands for use in experiments to detect mutations inside cells (Figure B.14). This method should be generally useful for many different types of biology experiments using DNA and proteins, but much more specific and sensitive than previous methods. A second study, also supported in part by NIGMS, showed how to incorporate very specific ratios of different QDs, or variable but tightly controlled amounts of the same QDs, into tiny (1 micron) plastic beads, and to attach biological molecules to the surface of those beads (Figure B.15). This offers a new way to do gene-chip experiments without the chip – in liquid samples that may be much faster and more flexible, while still allowing study of more than 10,000 different molecules in a single test.

Several laboratories at universities and companies are working with these bright little particles to develop useful tools and products for research, industry, and diagnostics.

References

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Funding Agencies: NIH

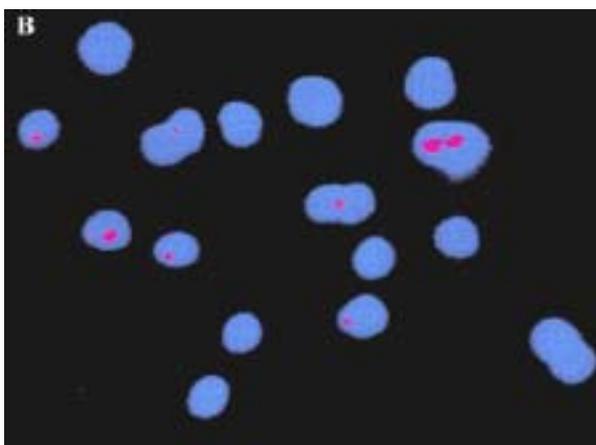


Figure B.14. Fluorescence micrograph of in situ hybridization of red quantum dot probe(s) for the Y chromosome in human sperm cells (Pathak et al. 2001).

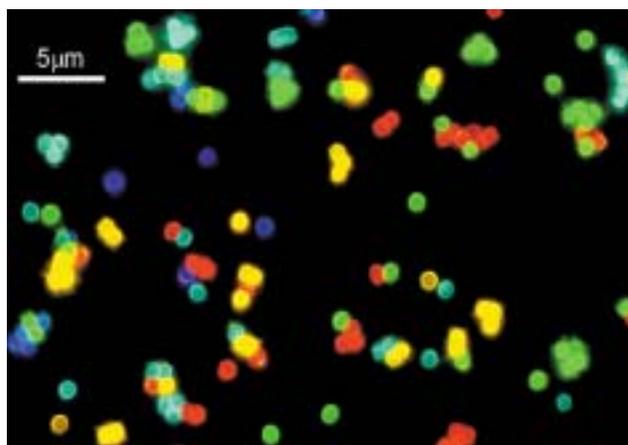


Figure B.15. Fluorescence micrograph of a mixture of CdSe/ZnS QD-tagged beads emitting single-color signals at 484, 508, 547, 575, and 611 nm (Han et al. 2001).

B.11. Nanopores Distinguish Subtle Differences in DNA Sequence

Several groups around the world and in the U.S. collaborated and competed to sequence the human genome, and reported their findings on the first large-scale view of that sequence early in 2001. Those reports emphasized that the sequencing experiments were done in large “factories” full of robots and expensive detection equipment. There are many reasons to sequence much more DNA: to learn about the subtle differences between individual humans that underlie disease, to learn about other organisms that inform our knowledge of human health and disease, and to understand the plants and animals on which our agricultural systems are based and the bacteria that dramatically affect our health and the chemistry of the biosphere. What if we could sequence DNA in devices the size of the DNA molecules themselves, using DNA directly from the cells being studied, rather than by using rooms full of equipment to grow up and purify the samples, run biochemistry reactions on them, and read off the base-pairs?

Two independent research groups made similar, small, but important steps toward developing such a nanopore-based DNA sequencing device in 2001. David Deamer’s laboratory at the University of California, Santa Cruz, with support from the National Human Genome Research Institute (NHGRI), NIH, studied small DNA molecules bent into hairpin structures (Figure B.16). When these molecules interacted with a protein pore that had been inserted into a membrane, and electrical measurements were made across the membrane, it was possible to distinguish between molecules that differed from each other by as little as one DNA base-pair in the length of the hairpin structure, or by one DNA base in the loop at the top of the hairpin. More strikingly, it was possible to distinguish between molecules in which the “stem” of the hairpin structure was perfectly base-paired (A with T and G with C), versus molecules in which the bases were mis-matched (e.g., A with A). That is, by sensing differences in DNA structure, the investigators could distinguish differences in DNA sequence. Meanwhile, Hagan Bayley’s lab at The Texas A&M University tethered a single-stranded DNA molecule within the pore itself (Figure B.17). When a second single-stranded DNA molecule was introduced into the solution surrounding the pore, differences were detected in the electrical signals across the membrane, depending on whether the challenger DNA could base-pair exactly with the tethered DNA or if it contained a mismatch. Further, different mismatches (e.g., T with G versus T with C versus T with A) yielded different signals. Thus, both groups demonstrated the ability to sense DNA sequence-dependent signals using nanopore devices.

These experiments are all based on a series of studies that began with the landmark observations, published in 1996, proposing that a nanopore (the smallest internal diameter of which is approximately 2 nm, about the same as the diameter of a single-stranded DNA molecule) might form the basis of a DNA sequencing device. That early paper demonstrated that reproducible electrical signals from the “device” were correlated with the length and overall DNA-base composition of the DNA molecules being measured. Subsequent research in several laboratories has refined the measurements, so that more information can be obtained with better physical control.

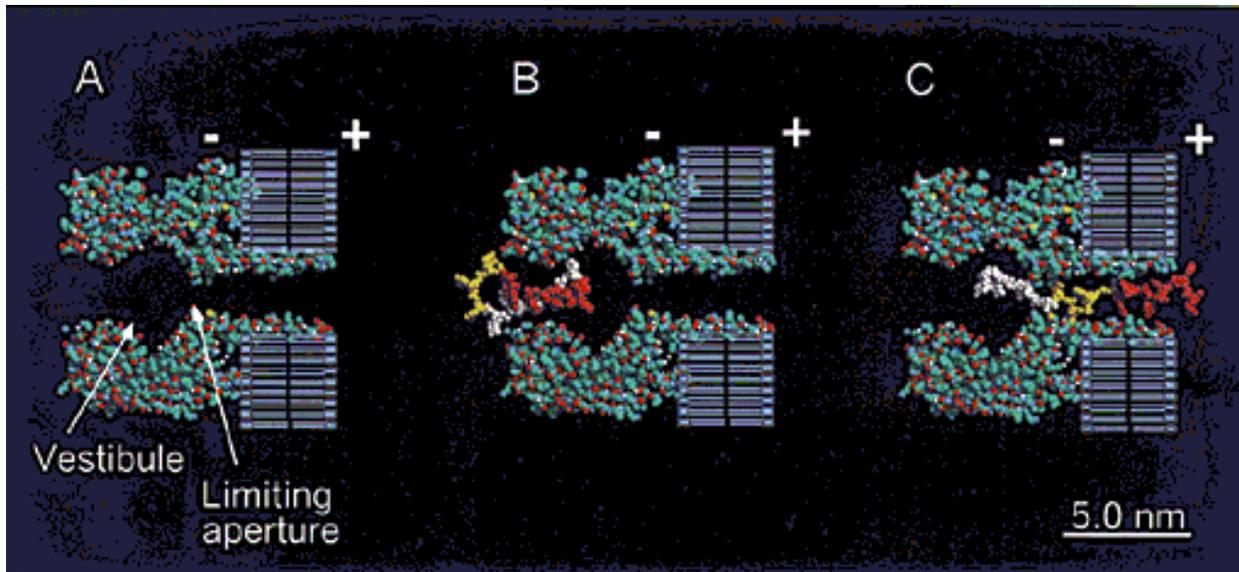


Figure B.16. Protein pore in lipid bilayer membrane (a) shown with a DNA hairpin structure in “vestibule” (b) or with hairpin unwound and passing through narrowest constriction of pore (c). Different electrical signals emanate from structures A, B and C (Vercoutere et al. 2001).

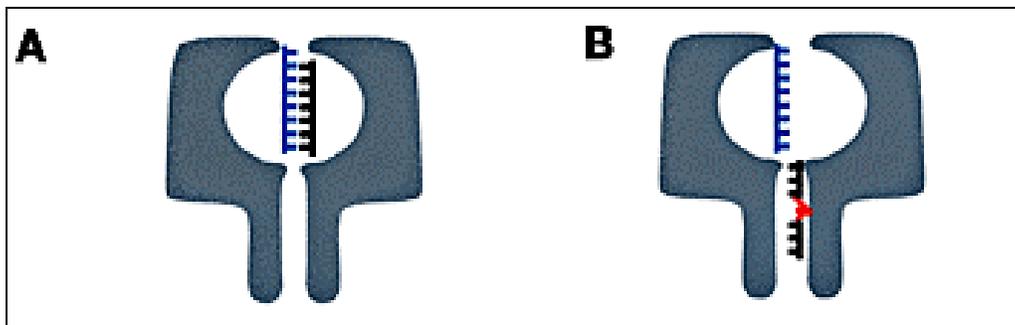


Figure B.17. The electrical signal obtained when (a) DNA strand (black) binds to tethered DNA strand (blue), is different from the signal obtained when (b) black DNA strand fails to bind tightly to tethered strand because of mismatched base (red) (Howorka, Cheley and Bayley 2001).

This research will provide outstanding opportunities for collaborations between biochemists and biophysicists; nanotechnologists who will fabricate robust, synthetic pores to replace the currently-used, relatively fragile biological pores in lipid bilayer membranes, build the sensors directly into the pore structures to make them integrated devices, and create arrays of these integrated devices so they can be implemented at high-throughput; analytical chemists and micro-technologists who will integrate those sensor arrays into micro-scale devices that will liberate DNA from the cellular samples and prepare it for measurement; and computer scientists who will develop the sophisticated signal processing tools and algorithms needed to extract the maximum amount of information from the sensor arrays.

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Funding Agencies: NIH

B.12. Ultrahigh-Density, Radiation-Hard Nonvolatile Memory Based on Silicon Nanocrystals

NASA requirements for computing and memory for microspacecraft emphasize high density, low power, small size, and radiation hardness. Non-volatile memories are ideal because they require power only during read/write operations. Furthermore, by using Si nanocrystal ensembles for the floating gate of a flash memory, the distributed nature of a storage element leads to intrinsic radiation-hardness. Researchers have demonstrated and measured the charge injection into single Si nanocrystals (NC). A quantitative model of the charging process and of the amount of charge injected into a single nanocrystal has been developed. An aerosol fabrication process for Si nanocrystals has been proposed that is compatible with the strict contamination standards of CMOS. Jet Propulsion Lab, California Institute of Technology in collaboration with Lucent Technologies has completed the first generation of non-volatile memory devices incorporating aerosol-synthesized Si nanocrystals (Figure B.18). These represent the first demonstration of nanocrystal memories utilizing size-classified aerosol nanocrystals. This superior synthesis technique resulted in complete functional memory units, which are state-of-the-art for nanocrystal memory devices. The devices were characterized by electrical measurements, indicating excellent lifetime endurance and non-volatility characteristics.

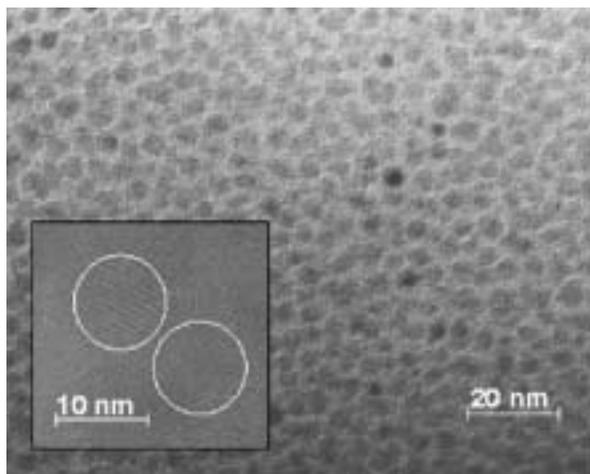


Figure B.18. Transmission electron micrograph of a monolayer of Si NCs deposited on a partially completed memory structure.

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Funding Agency: NASA

B.13. Explosive Detection by Nano-Thermo-Mechanical Signatures

Detecting explosive molecules using a nanomechanical signature is a paradigm shift in explosive detection. The development of atomic force microscopy has led to the detection of minute amounts of chemicals with microfabricated cantilevers (T. Thundat, Oak Ridge National Laboratory – see references). The cantilevers are smaller than the width of a human hair – 100 μm long, 20 μm wide, and 1 μm thickness with a mass of a few tens of nanograms (Figure B.19). The cantilevers are micromachined from single crystal silicon and can include an implanted boron channel for heating the cantilever. Since the thermal mass of the cantilever is small, the cantilevers can be heated to high temperatures in milliseconds using milliwatts of power. If the cantilever is heated to a temperature characteristic of an explosive (a few hundreds $^{\circ}\text{C}$) and the temperature is maintained for an appropriate length of time, the adsorbed explosive analyte undergoes nanodeflagration (nanoexplosion). The transient mechanical motion due to nanoexplosions can be detected at Angstrom resolution by a diode laser beam focused on its apex (Figure B.20).

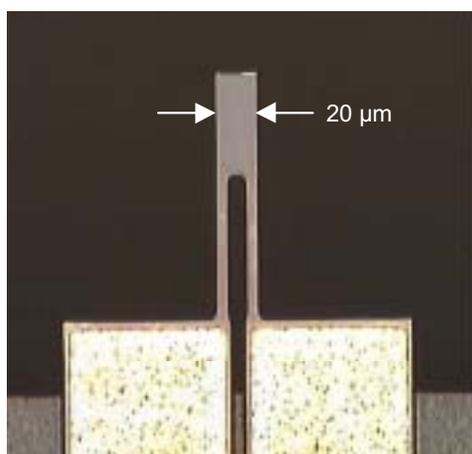


Figure B.19. Micrograph of cantilever.

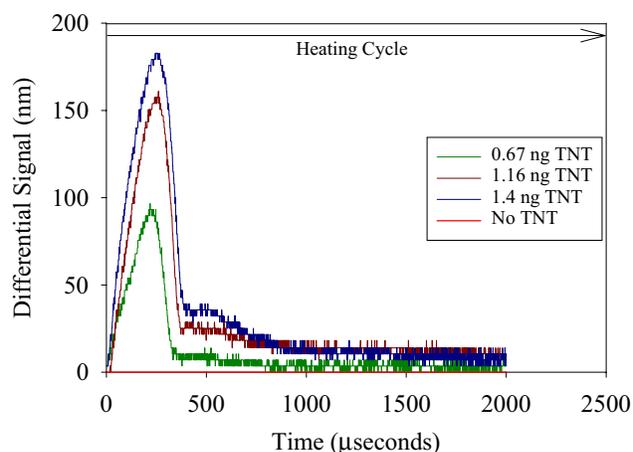


Figure B.20. Cantilever deflection in nanometers as a function of heating cycle with different amounts of TNT adsorbed on its surface.

In addition, explosive vapors have been detected by using microcantilevers coated with chemically selective polymers. Coated cantilevers undergo bending due to differential surface stress due to molecular adsorption. Selectivity is derived from chemically selective coatings.

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Funding Agency: DOT (Transportation Security Administration)

B.14. Nanoparticles for Sensitive, Selective Detection of Chemical, Biological, Radiological, and Explosives (CBRE) Agents

The analytical tools being developed for nanoscience must locate and measure the properties of single atoms – this precision can be adapted to sensing with exquisite sensitivity. Several sensor concepts are under commercial development for chemical and biological agent detection. As an example of chemical sensing, organothiols stabilized nanosized Au clusters have been self-assembled between two microfabricated electrodes. The current flowing between the electrodes depends on electron tunneling through the organic films. Small amounts of chemical agent in the air surrounding the sensor can partition into the organic and cause changes in its dimension or dielectric constant (Wohltjen and Snow 1998; Snow, Wohltjen and Jarvis 2001). Both effects cause exponential changes in electrical current; parts-per-billion of chemical agent has been detected by this approach. Utilizing pattern recognition techniques, an array of sensors – each with a different organic constituent – provides the selectivity. This technology is under commercial development by MicroSensor Systems Incorporated (Figure B.21). As an example of biological sensing, it has been shown that nanosized Au clusters in solution have different colors, depending on their separation. If appropriately chosen strands of DNA are attached to the clusters, the presence of its complement can cause the clusters to be “glued” together and change color (Figure B.22). A lower detection limit for this system of 500 pM for a 24 base single-stranded target and 2.5 nM for a duplex target nucleotide has been demonstrated (Reynolds, Mirkin and Letsinger 2000). It has been shown that anthrax DNA can be sensitively detected by this technique; commercial development is underway by Nanosphere Inc.

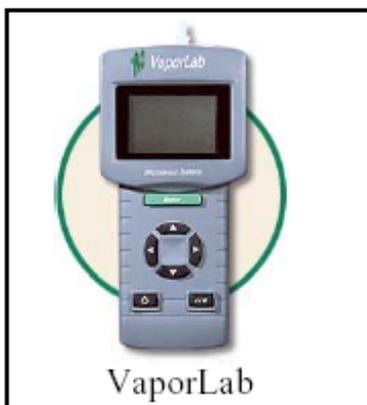


Figure B.21. MicroSensor Systems Inc. handheld chemical sensor based on nanoparticle Au (Snow, Wohltjen, and Jarvis 2001).

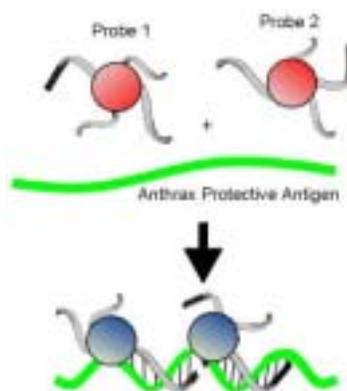


Figure B.22. Color change in Au nanoparticles localized by DNA sequence recognition (Reynolds, Mirkin, and Letsinger 2000).

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Funding Agencies: ARO, ONR, AFOSR, NSF, NIGMS

B.15. Nanoparticles for Chemical and Biological Agent Decontamination

Decontamination and destruction of chemical and biological warfare agents in the field is of great importance to the warfighter and to civilian disaster response teams. During the Tokyo subway attack in the mid-90s, there was a high percentage of casualties from the first responders who did not have proper protective gear. New reactive adsorbents for the effective removal of toxic materials and chemical warfare agents are a priority need (Figure B.23). The most effective adsorbents generally have large surface areas for ready access between agent and adsorbent. Nanoparticles are very small particles with increased surface areas and reactivity; one-quarter ounce can have the same surface area as a football field. Various forms of nanoparticles show extremely promising prospects to provide innovative, highly effective approaches to decontamination. CaO, Al₂O₃, and MgO nanopowders (Wagner et al. 1999; Wagner et al. 2000; Wagner et al. 2001) have been shown to react aggressively with chemical warfare agents, rendering them ineffective (Koper, Lucas and Klubunde 1999; Koper and

Klabunde 2000). The nanoparticle effectiveness is illustrated Figure B.24, which compares destructive absorption of a war gas simulant for MgO and for various activated carbons. These nanoparticles are currently being evaluated by the U.S. Army Edgewood Chemical Biological Centers, the U.S. Army Medical Research Institute for Chemical Defense, and the Natick Soldier Center. Nanoemulsions of water/oil with droplets in the 200-400 nanometer range have been shown effective at disrupting biological threat agents, including anthrax (Hamouda and Baker 2000; Hamouda et al. 2001). The emulsions can be formulated in a variety of carriers allowing for gels, creams, and liquid products. The nanoemulsions can destroy microbes effectively without toxicity or harmful residual effects. The classes of microbes eradicated are virus, bacterial, spores, and fungi. Yet a third type of nanoparticle, highly branched (dendritic) polymer, has been very effective as reactive inclusions in topical skin protective (TSP) creams (Yin et al. 2001). In addition to significantly extending the nerve agent protection time, the inclusion of the dendritic particles made the TSP also effective against mustard agent (HD).



Figure B.23. Powdered adsorbent being used to decontaminate a soldier (Yin et al. 2001).

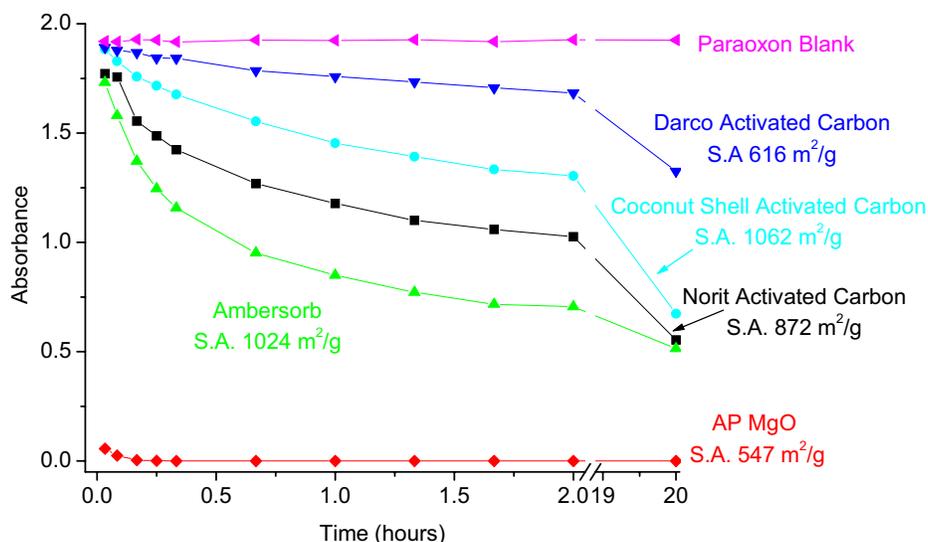


Figure B.24. Destructive adsorption of paraoxon (VX and GD simulant) on Nanoscale Materials' AP-MgO and different types of commercially available activated carbon. Lower absorbance means more complete destructive adsorption (Koper, Lucas and Klabunde 1999).

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Funding Agencies: ARL, ARO

Agencies' Contributions to FY 2001-2003 NNI Implementation Plan

The National Nanotechnology Initiative (NNI) began in FY 2001 (<http://www.nano.gov>). It emphasizes long-term, fundamental research aimed at discovering novel phenomena, processes, and tools; addressing NNI grand challenges; supporting new interdisciplinary centers and networks of excellence including shared user facilities; supporting research infrastructure; and addressing research and educational activities on the societal implications of advances in nanoscience and nanotechnology. Funding is provided on competitive basis with other programs and within NNI.

The FY 2002 nanoscale R&D budget approved by Congress is approximately \$604 million (\$578.9 million reported on February 4, 2001, plus \$25.5 million in associated programs at NASA and USDA). This is a 43% increase over \$422 million enacted by Congress for FY 2001. Agency funding is as follows: National Science Foundation (NSF – \$199 million), Department of Defense (DOD – \$180 million), Department of Energy (DOE – \$91.1 million of which BES \$85 and NNSA 6.1 million), National Aeronautics and Space Administration (NASA – \$46 million), National Institutes of Health (NIH – \$40.8 million), National Institute of Standards and Technology (NIST – \$37.6 million), Environmental Protection Agency (EPA – \$5 million), Department of Transportation (DOT – \$2 million), Department of Agriculture (USDA – \$1.5 million), and Department of Justice (DOJ – \$1.4 million). Budgets for other participating agencies are not available.

NSET has estimated that an increased investment of 30-50% is needed for FY 2002 and 2003 nanotechnology research and development in order to create the infrastructure required in this initial phase in the development of nanotechnology, to maintain U.S. R&D in a competitive international position, and to fully take advantage of the new technology. Three new grand challenges are planned: manufacturing processes at the nanoscale, use of nanotechnology for chemical-biological-radioactive-explosive detection and protection, and development of instrumentation and metrology at the nanoscale. The FY 2003 President's budget request of about \$710 million (\$679 million reported on February 4, 2002, plus \$31.5 million in associated programs at NASA and USDA) for Federal investment in nanoscale science, engineering and technology, a 17% increase over FY 2002, is shown in Table C.1.

Table C.1
 FY 2001 (Budgeted and Actual), 2002 (Current Plan) and 2003 (Congressional Request) for NNI
 (\$ millions)

Reported on	FY 2001		FY 2002		FY 2003	
	2/7/01	2/4/02	2/4/02	2/5/02	2/4/02	2/5/02
NSF	150	150	199		221	
DOD	110	123	180		201	
DOE	93	88	91.1		139.3	
NASA	20	22	22	22 + 24	22	22 + 29
NIH/HHS	39	40	40.8		43.2	
NIST/DOC	10	33.4	37.6		43.8	
EPA		5	5		5	
DOT/TSA		0	2		2	
USDA		1.5	0	+ 1.5	0	+ 2.5
DOJ		1.4	1.4		1.4	
Total	422	464.3	578.9	604.4	678.7	710.2

Note: the “total” includes funding reported on 2/4/02 plus funding in associated nanotechnology programs.

Department of Defense

FY2001 Investment

The past (FY01), present (FY02 current plan) and recommended (FY03) DOD support for nanoscience and nanotechnology is delineated in Table C.2. The principal DOD participants in the NNI are DDR&E, DARPA, Air Force, Army and Navy; the “Other” category in Table C.2 corresponds to BMDO and intelligence agencies.

While the NNI is an initiative focused on fundamental science (i.e., DOD 6.1 funding category), one of the principal NNI goals is to transition science discovery into new technology. The DOD structures its S&T investment into basic research (6.1), applied research (6.2) and exploratory development (6.3); the latter two focus on transitioning science discovery into innovative technology. MANTECH, SBIR and STTR programs are also available for transition efforts. There are nanoscience discoveries for which technology potentials are clear and transition funding is appropriate. Beginning in FY02, the DOD will track and encourage the transitions into these applied programs, under the label “6.2/6.3” in Table C.2.

Table C.2
 DOD Investment in Nanoscience

	2001 (Actual)		2002 (Current Plan)		2003 (Rec.)	
	6.1	6.2/6.3	6.1	6.2/6.3	6.1	6.2/6.3
DDR&E	36		26		28	-
DARPA	28	12	9	88	11	90
Army	6		18	2	18	5
Air Force	6	4	8	7	13	5
Navy	31		21	1	26	5
Other	-		-		-	-
Total	107	16	82	98	96	105

In FY01 the DOD invested \$77 million from its core basic research (6.1) funds, \$30 million from the NNI augmentation, and \$16 million from applied research (6.2) funds in topics germane to the NNI. The DOD NNI funding augmentation was allocated to support university basic research through the University Research Initiatives (URI) program (\$20 million) and DOD laboratory efforts through the Navy basic research program (\$10 million).

The URI program in FY01 added 16 MURI nanoscience projects as part of a Defense University Research Initiative on NanoTechnology (DURINT) competition and another 5 nanoscience projects under the traditional MURI competition. In addition, under the DURINT competition \$6 million was invested in 45 fellowships and \$7 million in university equipment. The Navy invested its \$10 million augmentation as ~\$5 million for equipment competition for the DOD laboratories and ~\$5 million in a collaborative program between university and DOD laboratories addressing miniaturized, intelligent sensing (MIS).

FY 2002 Investment

The DOD URI program will continue the new DURINT programs begun in FY 01 and will support an additional MURI program in nanoscience. The commitment of transition funding (6.2/6.3) ensures the DOD will exceed the previously recommended FY02 goal of \$133 million for the NNI.

DARPA plans a significant enhancement in nanoscience/nanotechnology for its investment portfolio. New programs begin for nanostructures in biology and quantum information devices. The molecular electronics effort transitions from 6.1 into 6.2. The Large Area Printing Program, in which approximately one half of the projects addressed nanoscale issues, comes to a close.

The Air Force is looking to increase its investment in nanoscience; an NAS panel is assisting in the identification of the best investment strategy for FY02. While the panel recommendations are not yet available, it is anticipated that Air Force basic research activities will expand to address topics in the following areas:

- *Nanocomposites.* Hybrid polymer-inorganic nanocomposites for dramatic improvement over the properties of traditional polymers without sacrificing density, processibility or toughness as in conventional composite/blend approaches; dispersed carbon nanotubes in polymer fiber to provide improvement in tensile and compressive properties of high performance polymer fibers.
- *Self-assembly and nanoprocessing.* Advances in organic and organic/inorganic nanoparticles and nanoscale materials and nanoscale materials processing techniques to create the opportunity for development of new paradigms for the realization of 3-D optical and electronic circuitry.
- *Highly efficient space solar cells.* If U.S. satellites could be developed that more efficiently convert light to electrical power, then lower launch costs and heavier payloads could be realized. Nanotechnology may enable space solar cells that can operate at an efficiency of 60%.
- *Nanoenergetics.* Understanding the factors that control reactivity and energy release in nanostructured systems, and developing the structures and architectures to optimize them.

- *Nanostructures for highly selective sensors and catalysts.* Nanostructures for the remote sensing and identification of chemical and physical species, and catalysts to selectively react with compounds to release energy (monopropellants) or destroy them (undesirable chemicals).
- *Nanoelectronics, nanomagnetics and nanophotonics.* Ultra-dense magnetic memory, ultra-fast digital signal processing, nanosensing, spatial and temporal dispersion characteristics of photonic crystals, and a computer architecture based on one-dimensional cellular automata, which offers an important solution to molecular scale limitations.
- *Nanostructured coatings, ceramics and metals.* Tailor the structure of coatings at the nano-scale to provide unique and revolutionary properties, specifically nanostructured adaptive tribological (low friction) coatings for MEMS devices; economical, multifunctional ceramic materials that operate in extreme environments; new material concepts and design tools to impact mechanics issues important to airframes.

The Army will augment its FY01 program by \$10 million in basic research funds for a University Affiliated Research Center (UARC) – Institute for Soldier Nanotechnologies. The purpose of this center of excellence is to develop unclassified nanometer-scale science and technology solutions for the soldier. MIT will host this center, which will emphasize revolutionary materials research toward advanced soldier protection and survivability capabilities. The center will work in close collaboration with industry, the Army’s Natick Soldier Center (NSC), the Army Research Laboratory (ARL) and the other Army Research Development and Engineering Centers (RDECs) in pursuit of the Army’s goals. The research will integrate a wide range of functionalities, including multithreat protection against ballistics, sensory attack, chemical and biological agents; climate control (cooling, heating, and insulating), possible chameleon-like garments; biomedical monitoring; and load management. A large centralized research facility is envisioned that will house world-class scientists and an exceptional research infrastructure.

Among the three services, the Navy has the largest investment in nanotechnology, with an emphasis in the area of nanoelectronics. Reprogramming \$10 million of its core funds, the Naval Research Laboratory has initiated an Institute for Nanoscience to enhance multidisciplinary thinking and critical infrastructure. The mission of the institute is to conduct highly innovative, interdisciplinary research at the intersection of the fields of materials, electronics and biology in the nanometer domain. A new Nanoscience Building is being built to provide modern, state-of-the art facilities dedicated to nanoscience research and nanotechnology development.

FY 2003 Request

As indicated in Table C.2, the DOD investment in nanoscience is planned to increase to \$201 million for FY 03. In its preliminary report, the National Academy of Engineering committee evaluating the NNI has pointed out the importance of multidisciplinary programs. The MURI/DURINT contributions from the DOD are an important contribution to the overall balance of the NNI and funding for those efforts will continue through their potential 5-year lifetimes. It is anticipated that the largest increase in nanoscience programs will be in the more

applied programs that will lead to transition of the basic research findings to new technologies for national security applications.

Nanoscience shows great promise for arrays of inexpensive, integrated, miniaturized sensors for chemical / biological / radiological / explosive (CBRE) agents, for nanostructures enabling protection against agents, and for nanostructures that neutralize agents. The recent terrorist events motivate accelerated insertion of innovative technologies to improve the national security posture relative to CBRE. The NNI has redefined a grand challenge to address this important topic; DOD expects to play a major role in this multiagency effort.

The DOD Advisory Group on Electronic Devices (AGED) has agreed to perform a special technical area review (STAR) on nanoelectronics. A key goal for that review will be guidance for the “Nano-Electronics, -Optoelectronics and –Magnetics” Grand Challenge basic science investment, and for the 6.2/6.3 funding necessary to accelerate the development of information technology devices (with special attention to DOD’s unique needs.)

The NNI investment in nanoscience is highly motivated by the technological consequences. There have already been some successes in transition, e.g., nanocomposite materials with Triton from an AF SBIR, nanoparticle plasma spray coatings with Inframat from ONR support, and improved biological agent detection using nanoscale gold particles and single strands of DNA with Nanosphere from Army URI support. The Inframat product was awarded 2001 R&D100 recognition as one of the top 100 new products in the year 2000. In FY03, the DOD will have additional investment of 6.2/6.3 funds in order to exploit additional opportunities uncovered by the research program. The DOD will also develop topics for further SBIR and STTR transitions.

Department of Energy

FY2001 Investment

The enacted FY 2001 DOE budget of \$93 million (actual \$87.95 million) includes the BES nanoscience program solicitation of about \$36 million. The program solicitation was published on the Web (http://www.er.doe.gov/production/grants/Fr01_03.html; or <http://nano.gov/>). The data on pre-applications and applications are shown below.

- Universities: Total budget \$18 million. Preapplications were received by January 12, 2001, and formal applications by March 14, 2001. 745 preapplications received; 313 encouragement letters and 432 discouragement letters mailed; 417 applications received March 14, 2001.
- DOE Laboratories: competing for \$18 million in research awards. Submissions were restricted to 4 proposals per laboratory. Full proposals were due January 24, 2001. 46 proposals were received.
- DOE has also reviewed proposals for Nanoscale Science Research Centers (NSRCs) in late April. The NSRCs are substantial laboratories associated with DOE user facilities with construction costs in the \$50 to \$100 million range and with annual budgets of about \$15 to \$20 million per year in steady operation. DOE was scheduled to complete its review of the NSRC proposals by the end of April 2001. DOE anticipates initiating about 3 in FY 2002.

A description of each of the DOE centers presented to the Basic Energy Sciences Advisory Committee is on DOE's Web site (<http://www.sc.doe.gov/production/bes/besac/PPT02-26-01.htm>) (items 9 and 10 relate to the NSRCs).

Briefly, the BES Nanoscale Science Research Centers will:

- Advance fundamental understanding and control of materials at the nanoscale
- Support investigators and groups working together on problems of a scope, complexity, and disciplinary breadth not possible working separately, with the whole being greater than the sum of the parts
- Provide state-of-the-art nanofabrication and characterization facilities to in-house and visiting researchers at no cost
- Provide a mechanism for short- and long-term collaborations and partnerships among DOE laboratory, academic, and industrial researchers
- Provide training for students in interdisciplinary nanoscale research in cooperation with regional or national academic institutions
- Advance the strategic vision and build on the core competencies of the host laboratory, particularly the BES user facilities and research programs already in place
- Optimize the use of the BES national user facilities for materials characterization
- Provide the foundation for the development of nanotechnology important to DOE
- Partner with state government and local institutions
- Complement one another and other agency centers (e.g., existing components of the NSF National Nanofabrication Users Network)

NNI Management

The supplement of \$36 million in FY 2001 is managed by Basic Energy Sciences (BES), with advise from the Basic Energy Sciences Advisory Committee.

Collaborations with Other Agencies/Private Sector

- Nanostructured materials - with NSF, DOD
- Quantum computing - with NIST, NASA, NSF and DOD

Special Accomplishments

- *Terabit arrays (one trillion bits per square inch).* A 300-fold increase in magnetic storage density has been achieved using a patented technique of self-assembly of block copolymers under the influence of a small voltage. The new technique is simple, robust, and extremely versatile. The key to this discovery lay in directing the orientation of nanoscopic, cylindrical domains in thin films of block copolymers. By coupling this with routine lithographic processes, large area arrays of nanopores can be easily produced. Electrochemical deposition of metals, such as cobalt and iron, produces nanowires that exhibit excellent magnetic properties, key to ultrahigh density magnetic storage. The nanowires also are being used as field emission devices for displays.
- *Observations of atomic imperfections.* A new electron beam technique has been developed that has measured atomic displacements to a record accuracy of one-hundredth of the

diameter of an atom. Such small imperfections in atomic packing often determine the properties and behavior of materials, particularly in nanostructured devices. This capability has been made possible by a new technique that couples electron diffraction with imaging technology. The result is a greatly enhanced capability to map imperfections and their resulting strain fields in materials ranging from superconductors to multi-layer semiconductor devices.

- *Semiconductor nanocrystals as “artificial leaves.”* Recent experiments demonstrated that carbon dioxide could be removed from the atmosphere with semiconductor nanocrystals. These “artificial leaves” could potentially convert carbon dioxide into useful organic molecules with major environmental benefits. However, to be practical, the efficiency must be substantially improved. New theoretical studies have unraveled the detailed mechanisms involved and identified the key factors limiting efficiency. Based on this new understanding, alternative means for improving efficiency were suggested that could lead to effective implementation of artificial leaves to alleviate global warming and the depletion of fossil fuels.
- *“Magic” values for nanofilm thickness.* A key issue for nanotechnology is the structural stability of thin films and the devices made from nanostructures. It was recently demonstrated that nanofilms are significantly more stable at a few specific values of film thickness. The origin of this effect arises from the confinement of electrons within the film leading to electronic states with discrete energy values, much as atomic electrons are bound to the nucleus at discrete energy levels. Calculations demonstrated that increased stability occurred when the number of electrons present in the film completely filled the set of available states, just as filled electronic shells make the noble gases very stable.
- *Micro lens for nano research.* A silicon lens that is 1/10 the diameter of a human hair has been fabricated and used to image microscopic structures with an efficiency 1,000 times better than existing probes. The combination of high optical efficiency and improved spatial resolution over a broad range of wavelengths has enabled measurement of infrared light absorption in single biological cells. This spectroscopic technique can provide important information on cell chemical composition, structure, and biological activity.
- *Nanofluids.* Nanofluids (tiny, solid nanoparticles suspended in fluid) have been created that conduct heat ten times faster than previously thought possible, surpassing the fundamental limits of current heat conduction models for solid/liquid suspensions. These nanofluids are a new, innovative class of heat transfer fluids and represent a rapidly emerging field where nanoscale science and thermal engineering meet. This research could lead to a major breakthrough in making new composite (solid and liquid) materials with improved thermal properties for numerous engineering and medical applications, to achieve greater energy efficiency, smaller size and lighter weight, lower operating costs, and a cleaner environment.
- *The world’s smallest laser.* A team of materials scientists and chemists has built the world’s smallest laser - a nanowire nanolaser 1,000 times thinner than a human hair. The device, one of the first to arise from the field of nanotechnology, can be tuned from blue to deep ultraviolet wavelengths. Zinc oxide wires only 20 to 150 nanometers in diameter and 10,000 nanometers long were grown, each wire a single nanolaser. Discovering how to excite the nanowires with an external energy source was critical to the success of the project. Ultimately, the goal is to integrate these nanolasers into electronic circuits for use in “lab-on-a-chip” devices that could contain small laser-analysis kits or as a solid-state, ultraviolet laser to allow an increase in the amount of data that can be stored on high-density optical disks.

- Erosion-resistant materials
- Advanced instrumentation facilities

FY 2002 Investment

The current plan is for \$91.1 million. DOE announced a request for applications for FY 2002. Over 500 preapplications were received. About 200 were encouraged to submit grant proposals. The deadline for receipt of formal applications is February 12, 2002. A letter was also sent to the DOE laboratories encouraging submission of proposals. Funding decisions will be made competitively using peer review.

Controlling and manipulating matter at the atomic and molecular scale is the essence of nanoscale science, engineering, and technology (NSET). The Basic Energy Sciences (BES) program has worked with the National Science and Technology Council's NSET Subcommittee, with the Basic Energy Sciences Advisory Committee (BESAC), and with the broad scientific community from academia, industry, and the National Laboratories to define and articulate the goals of this research. The BES program in NSET has the following overarching goals: (1) attain a fundamental scientific understanding of nanoscale phenomena; (2) achieve the ability to design and synthesize materials at the atomic level to produce materials with desired properties and functions, including nanoscale assemblies that combine hard and soft (biological) materials to achieve novel functions; (3) attain a fundamental understanding of the structural, dynamic, and electronic aspects of nanoassemblies, including biomolecular assemblies, associated with unique materials properties, chemical transformations, energy conversion, and signal transduction; (4) develop experimental characterization tools and theory/modeling/simulation tools necessary to understand, predict, and control nanoscale phenomena; and (5) to obtain an integrated structural and dynamic view of nanoassemblies in biological systems, through the development of enhanced imaging tools and nanoscale probes. Nanoscale research funding is also provided by the Office of Scientific Computing Research for both the use of high-performance computers and to support technology transfer of results from nanoscale research and by the National Nuclear Security Agency.

Funding for Nanoscale Science Research Centers (NSRCs) continues in FY 2002 with \$3 million appropriated for engineering design. The NSRCs are designed to be both research facilities and user facilities. They will provide advanced instrumentation and access to facilities for investigators and groups working together on problems of a scope, complexity, and disciplinary breadth not possible working separately. They will collocate researchers and specialized equipment in physics, chemistry, materials sciences, and biology with the goal of fabrication of novel systems at the nanoscale. As with all BES facilities, the NSRCs will operate with no fees for users who intend to make the results of their research widely available.

Based on peer review, three NSRCs were authorized to proceed with conceptual design in June 2001. These centers are the Molecular Foundry ("Foundry") at Lawrence Berkeley National Laboratory, the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory, and the Center for Integrated Nanotechnology (CINT) at Sandia National Laboratories and Los Alamos National Laboratory. Proposals from Argonne National Laboratory and Brookhaven National Laboratory were deemed not ready to proceed with conceptual design.

Based on the review of its conceptual design in December of 2001, the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory was considered ready to initiate construction in FY 2003. The CNMS will be an 80,000 sq. ft. building, including class 100, 1,000, and 10,000 clean rooms; synthesis, processing, and characterization equipment; and physical, chemical, and biological laboratories. The CNMS held a workshop in October 2001 to help define the scientific program; in attendance were 278 scientists from 67 institutions, including 46 universities, 11 government laboratories, and 10 industries. The CNMS will be collocated with the Spallation Neutron Source on Chestnut Ridge at ORNL. Its construction schedule will be integrated with that of the SNS to optimize use of local construction trades and purchase of materials. One of the areas of emphasis of the CNMS will be neutron science. The other two NSRCs will continue engineering design in FY 2003

FY 2003 Request

Total request is \$139.3 million, including funding of \$6.3 million for defense programs.

In FY 2003, fundamental research to understand the properties of materials at the nanoscale will be increased in three areas: synthesis and processing of materials at the nanoscale, condensed matter physics, and catalysis. In the area of synthesis and processing (Materials Sciences and Engineering subprogram), new activities will develop a fundamental understanding of nanoscale processes involved in deformation and fracture, synthesis of ordered arrays of nanoparticles using patterning techniques, and synthesis of nanoparticles of uniform size and shape. In the area of condensed matter physics (Materials Sciences and Engineering subprogram), new activities will focus on understanding how properties change or can be improved at the nanoscale and how macromolecules reach their equilibrium configuration and self assemble into larger structures. In the area of catalysis (Chemical Sciences, Geosciences, and Energy Biosciences subprogram), new work will focus on fundamental research to understand the role nanoscale properties of materials play in altering and controlling catalytic transformations. In FY 2003, requests for applications in these research areas will be issued to DOE laboratories by letter and to universities through a notice inviting grant applications. The combination in a single coordinated research program of individual investigators at universities and interdisciplinary groups at DOE's laboratories is a proven excellent mechanism for incorporating advanced basic research, cutting-edge instrumentation, access to facilities, and the needs of energy technologies. Included also is nanoscale research in the National Nuclear Security Agency.

In addition to the increases for research in FY 2003, the FY 2003 request includes \$35 million for centers. Construction will begin on one Nanoscale Science Research Center (NSRC), and engineering and design will continue on two others. NSRCs are user facilities for the synthesis, processing, fabrication, and analysis of materials at the nanoscale. NSRCs were conceived in FY 1999 within the context of the NSTC Interagency Working Group on Nanoscale Science, Engineering, and Technology as part of the DOE contribution to the National Nanotechnology Initiative. They involve conventional construction of a simple laboratory building, usually sited adjacent to or near an existing BES synchrotron or neutron scattering facility. Contained within NSRCs will be clean rooms; chemistry, physics, and biology laboratories for nanofabrication; and one-of-a-kind signature instruments and other instruments, e.g., nanowriters and various research-grade probe microscopies, not generally available outside of major user facilities. NSRCs will serve the nation's researchers broadly and, as with the existing BES facilities, access

to NSRCs will be through submission of proposals that will be reviewed by mechanisms established by the facilities themselves. Planning for the NSRCs includes substantial participation by the research community through a series of open, widely advertised workshops. Workshops held to date have been heavily attended, each attracting up to 300 researchers. Funds are requested for the start of construction of the NSRC located at Oak Ridge National Laboratory and for the continuation of engineering and design for NSRCs located at Lawrence Berkeley National Laboratory and at Sandia National Laboratories (Albuquerque) and Los Alamos National Laboratory. These NSRCs were chosen from among those proposed by a peer review process.

Nanoscale research efforts nationwide will benefit significantly from these NSRCs. For example, the NSRC at Oak Ridge National Laboratory will provide direct access to sample preparation for neutron scattering, which is ideal for magnetic structures, for soft materials and for residual stress in materials; Oak Ridge also has a combination of electron beam microcharacterization instruments that are needed to characterize nanoscale particles and dislocations. The NSRC at Lawrence Berkeley National Laboratory will provide synthesis capabilities to explore the phenomena of macromolecular conformation and assembly and will provide ready access to the Advanced Light Source, the National Center for Electron Microscopy, and other characterization instruments. The NSRC at Sandia/Los Alamos National Laboratories will provide sample preparation capabilities for thin films, electron transport, patterning, and magnetic layered structures. This NSRC will also have an array of characterization instruments for nanoelectronics, thin films, and magnetic structures; in the case of magnetic materials, the NSRC will provide ready access to the National High Magnetic Field Laboratory at Los Alamos. The research activity will also benefit from new work proposed in FY 2003 by the Office of Advanced Scientific Computing (ASCR) in the area of computational nanoscale science engineering and technology. ASCR will develop the specialized computational tools for nanoscale science.

The estimate of FY 2003 DOE funding includes \$6.3 million in the Office of Defense Programs (NNSA), 0.2 million over FY 2002, and \$1.35 million over FY01. The amount is an estimate of the fraction of the work supported at Sandia, Los Alamos, and Livermore that is in this area.

Department of Justice

The Department of Justice's National Institute of Justice (NIJ) has two separate project areas that incorporate or will incorporate nanotechnology – DNA Research and Development and Chemical and Biological Defense.

FY2001 Investment

The FY 2001 amount of funding for nanotechnology related projects in DOJ/NIJ was \$1 million (NIJ Base Budget).

Activities

DNA Research and Development. NIJ continues the research and development of chip based or micro device technologies that will be used to analyze DNA in forensic applications. Nanotechnology has or will be a significant part of the device under development that will eventually be integrated into the current crime laboratory processes and protocols to analyze forensic DNA samples. FY01 budget: \$1 million for nanotechnology related projects in forensic DNA analysis development.

Nanotechnology Initiative Management

Chemical and Biological Defense. The Chemical and Biological Defense program is being managed by the National Institute of Justice's Office of Science and Technology. This program is funded through the Local Law Enforcement Block Grant Technology Set-aside.

DNA Research and Development. The DNA research and development for forensic applications is being managed by the National Institute of Justice's Office of Science and Technology. This program is funded through NIJ's base budget.

All NIJ projects. Proposals received in response to solicitations are reviewed by peer panels consisting of both practitioners and technologists. Proposals approved by the NIJ Director are awarded as cooperative agreements to university and industry based organizations for development and demonstration of nanotechnology related projects.

Collaborations with Other Agencies/Private Sector

DNA Research and Development. The NIJ DNA Research and Development program has been coordinated with the FBI Laboratory, the National Institute for Standards and Technology (NIST), as well as state and local forensic laboratories.

Chemical and Biological Defense. NIJ, in collaboration with the Technical Support Working Group, is sponsoring development of chemical and biological defense technologies.

Success Stories in R&D

Hundred-fold faster DNA analysis (Principal Investigators: Dr. Daniel Erlich, Whitehead Institute, and Dr. Ronald Sosnowski, Nanogen). NIJ has been developing two chip-based technologies that use nanotechnologies for forensic applications of DNA analysis. The first chip, created at the Whitehead Institute, uses a capillary based system similar to that employed in existing forensic DNA laboratories, but on a chip format that will ultimately lead to greater efficiencies in speed of processing and in use of forensic DNA labs. This project has a working prototype chip that allows for simultaneous analysis of 16 DNA samples for all of the 13 short tandem repeat (STR) genetic markers required to search the National DNA Index System (NDIS) containing convicted offender and unsolved casework DNA. The Whitehead DNA chip is entering its evaluation phase by the forensic DNA community. The second chip, under development by Nanogen Corp, is a hybridization chip that has the potential for higher resolution

power than a capillary system. With three of the 13 STR genetic markers already embedded in this format, the developers are looking at the addition of new markers, called single nucleotide polymorphisms (SNPs), for future use as investigative aids at the crime scene. These DNA analysis chips will provide portability, smaller instrument footprints, and higher DNA analysis throughput to effectively and efficiently address the expected increased use of DNA analysis in the criminal justice system.

FY 2002 Investment

The FY 2002 DOJ budget for nanotechnology is \$1.4 million (NIJ Base Budget and the Local Law Enforcement - Block Grant Technology Set-aside).

DNA Research and Development. NIJ will continue the research and development as well as the demonstration of chip based or micro device technologies to analyze DNA in forensic applications. Nanotechnology is or will be a significant part of the device under development that will eventually be integrated into the current crime laboratory processes and protocols to analyze forensic DNA samples. FY02 budget planned: \$1 million.

Chemical and Biological Defense Program. NIJ is developing a wearable, low-cost device to provide warning of exposure to unanticipated chemical and biological hazards in sufficient time for its wearer to take effective protective measures. The current approach relies on an enzymatic reaction. It is based on vapor exposure of an immobilized enzyme surface. Evolving nanotechnology may be used to address limitations of the enzymatic approach. FY02 budget planned: \$400,000.

FY 2003 Request

- Forensic (DNA analysis on a chip R&D): FY03 \$1,000,000
- Counterterrorism (chem/bio threat detectors – Study and Research): \$400,000

Total request in FY 2003 for nanotechnology-related projects: \$1,400,000.

Department of Transportation

The Department of Transportation's nanoscale R&D program supports one of the agency's most critical missions today: ensuring the security of our nation's air transportation system.

FY 2002 Investment

Nanoscale R&D is critically needed in aviation security to improve the detection of explosives and chemical/biological weapons. The Department's Transportation Security Administration (TSA) is pursuing research, development, test, and evaluation programs to detect explosives and hazardous chemicals at the nanometer level and to characterize the interactions of explosives on material surfaces at this scale. Further research will yield sensor technologies that are cheaper and lighter – and yet far more sensitive, selective, and reliable – than current systems.

In FY 2002 DOT's budget for nanoscale R&D is approximately \$2 million. Activities include the following:

- An initiative with NASA's Ames Research Center involves R&D on carbon nanotubes as the active nanowire-detector for single molecule detection of trace levels of explosives. The nanowire is part of a transistor bridge, whereby the difference in conductance of the wire junction is monitored for presence of the molecule/cluster of explosive. This is an early attempt at utilizing nanostructures for explosives and chemical detection.
- In collaboration with the National Safe Skies Association, DOT is funding an evaluation at Oak Ridge National Laboratory (ORNL) of an explosive vapor detection system that uses nanoexplosions on microcantilever surfaces. In addition, the TSA and Bureau of Alcohol, Tobacco, and Firearms (ATF) are collaborating on a jointly funded project to develop an efficient vapor and particle collection/preconcentrator system for the ORNL microcantilever system.
- Another microcantilever study involves an interagency collaboration among DOT, ORNL, ATF, and Naval Research Laboratory (NRL). This project uses a different type of microcantilever to collect and measure the presence of explosives and hazardous chemicals (i.e., the incorporation of thin polymer coatings that selectively absorb explosive vapor, hence providing a sensor for monitoring explosives and other hazards). The interaction of the surfaces with the explosive molecules is at the nanoscale, and critical studies of this interaction will assist in further developments and understanding of the phenomena that occur.
- Under a DOT grant, Fisk University is studying adsorbed molecules of explosives on surfaces. These nanoscale characterizations are performed using a variety of techniques, including FT-infrared spectroscopy (FT-IR) and atomic force microscopy (AFM). The study of the interaction between the explosive molecules and a wide variety of surfaces assists in characterizing the physical and chemical properties involved in this process.
- Similar work is studying explosive molecular bonding and interactions at surfaces with techniques such as scanning electron microscopy and Raman microprobe microscopy (along with more common techniques such as FT-IR). Knowledge of these surface interactions is important for R&D of calibrants and standards for trace explosives systems.
- DOT is co-funding a miniaturized, handheld detection system being developed by Sandia National Laboratory (SNL). This system is based on the SNL micro "Chem-Lab-on-a-Chip." The new system is being designed to detect explosive particles/vapor, hazardous chemicals, and chemical agents. It is based on nanoscale surface interactions on a variety of detection platforms – surface acoustic waveguides (SAW detection), miniature ion mobility spectrometer (IMS), and gas chromatography separation/detection.
- Another co-funded effort involves collaboration among the Defense Advanced Research Projects Agency (DARPA), the Army Research Laboratory (ARL), and DOT on a MEMS-based "Mass Spectrograph on a Chip." This system, being developed by Northrop Grumman and ARL, will be used to detect both chemical agents and explosives. Each segment of the mass spectrograph research and development involves critical molecular and surface interactions on the nanoscale.
- Nanoscale R&D projects are ongoing with two universities: the University of Puerto Rico and Fisk University. Each uses state-of-the-art characterization systems to study explosive particle/molecule surface interactions. These analytical tools include STM/AFM, Raman microprobe, electron spectroscopy, and other assorted surface techniques.

- Other projects include providing technical guidance to the ATF for several nanoscale R&D programs. One involves an effort with the University of Massachusetts/Lowell to develop a “Micro Thermal” trace explosives detection system. This system will have an array of micro thermal surfaces, whereby nanoclusters of explosive vapor will be detected via differential thermal analysis. This project will also include several MEMS-based platforms, such as the NIST MEMS-based “Micro Hot Plate” detector.

NNI Management

Currently, the TSA manages the department’s nanoscale R&D program. In addition, DOT’s Research and Special Programs Administration works with the TSA to leverage the R&D of other NNI participants in areas central to the department’s missions through outreach and interagency collaboration.

Collaborations with Other Agencies/Private Sector

DOT currently is working with NASA, ORNL, ARL, ATF, NRL, SNL, DARPA, and NIST on its nanoscale-related activities (see above). Programs proposed for FY 2003 would expand this collaboration to other agencies participating in the NNI, as well as to other research institutions and industry.

Success Stories in R&D

Work with ORNL has already demonstrated the approach’s feasibility by measuring explosive vapor at the parts-per-trillion level. This shows promise for a future low-cost, highly selective and sensitive explosive detector.

FY 2003 Request

The NNI activities proposed for FY 2003 (approximately \$2.0 million) will build on current efforts to expedite the fielding of far more accurate and effective security technology at our nation’s airports. In particular, DOT plans to apply novel chemical detectors based on nanoscale and MEMS integrated circuits to sense trace levels of explosives and chemical/biological weapons at checkpoints and in checked bags; investigate nanoscale detection (building on current research in “nanoexplosion”/detection with microcantilever surfaces) with MEMS remote receive/transmit systems embedded on the chip; study monolayer and cluster nanolayers of selective polymers on surfaces to selectively collect, preconcentrate, and detect trace levels of explosives and other hazards; and characterize molecular detection mechanisms to investigate novel miniature inlet/preconcentrator systems (with MEMS) for enhanced sensitivity and selectivity. DOT will also work to transfer the most successful detection technologies to other transportation modes.

Environmental Protection Agency

The mission of the United States Environmental Protection Agency is to protect human health and the environment. EPA conducts and supports research to ensure that there is a sound scientific basis for its actions to carry out this mission. EPA's research is organized around the risk assessment/risk management paradigm. Research on human health and environmental effects, exposure, and risk assessment is combined to inform decisions on risk management. Research on environmental applications and implications of nanotechnology can be addressed within this framework. Nanotechnology may offer the promise of improved characterization of environmental problems, significantly reduced environmental impacts from "cleaner" manufacturing approaches, and reduced material and energy use. However, the potential impacts of nanoparticles from different applications on human health and the environment must also be evaluated.

FY 2001 Investment

In FY 2001 EPA announced its first solicitation for research on nanotechnology. This solicitation was under the Science to Achieve Results (STAR) program announcement on "Exploratory Research to Anticipate Future Environmental Issues." The program solicitation closed on June 18, 2001. Peer reviews for submitted proposals were held from September 24 through September 27, 2001.

Under this solicitation EPA planned to award approximately \$6 million for 16 research projects. Research categories include synthesis and processing, characterization and manipulation, modeling and simulation, and device and systems concepts. In addition, EPA has awarded several contracts under its Small Business Innovative Research (SBIR) program for Phase I projects on nanotechnology that were selected under an FY 2001 solicitation.

FY 2002 Investment

EPA has issued a second STAR solicitation in early 2002 with an estimated budget of \$5 million (<http://es.epa.gov/ncer/rfa/02nanotech.html>). Four research areas have been identified:

1. *Green manufacturing and processing.* Nanotechnology that eliminates or minimizes harmful emissions from industrial processes.
2. *Remediation/treatment.* Techniques to effectively remediate and/or treat environmental pollutants.
3. *Sensors.* Novel sensing technologies or devices for pollutant and microbial detection.

Proposals for smaller grants are requested in the following topic area:

4. *Environmental implications of nanotechnology.* Environmental benefits and potential harmful effects of nanotechnology at a societal level.

NNI Management

EPA's nanotechnology research is managed by the Office of Research and Development. The STAR grant solicitation and Small Business Innovation Research (SBIR) programs are managed

by the National Center for Environmental Research (NCER). In-house research currently includes the National Exposure Research Laboratory and the National Risk Management Research Laboratory, and may expand to other ORD laboratories in the future.

Collaborations with Other Agencies/Private Sector

EPA has plans to explore collaborations in nanotechnology research with other agencies. In particular, USDA and EPA share some common interests in nanotechnology research, for example, in the areas of biotechnology applications, pesticide monitoring, and food safety.

FY2003 Request

Nanotechnology research is not yet a separate item in EPA's budget. The current grant solicitation is part of the STAR Exploratory and Futures research activity. In-house research is a natural extension of ongoing exposure and risk management research. FY 2003 research is expected to be at a level similar level to FY 2002, but is dependent upon overall research funding levels indicated by the Presidential FY 2003 budget request. Accordingly, FY 2003 research is expected to be approximately \$5 million.

National Aeronautics and Space Administration

FY2001 Investment

In FY 2000 NASA's program was only about \$5 million across a variety of small activities encompassing sensors, materials and information technology. These activities were largely focused on exploring the application of emerging basic nanoscale science and technology to NASA's long-term needs.

In FY 2001 the agency received a \$15 million augmentation: \$5 million in OAT focused on nanotechnology for advanced space systems; and \$10 million in OBPR focused on bio-medical applications (including the joint NASA/NCI activity) and research into biological processes related to nanotechnology.

NASA identified three principal programs for its FY01 NNI funding of \$20 million:

1. \$10 million devoted to a joint effort with the NIH NCI (which planned to contribute an additional \$10 million) to develop understanding of the molecular signatures important to medicine and health
2. The second program focused on cost effective, reduced weight materials
3. The third program focused on nanostructures for information processing with 70% funding in universities and 30% in NASA laboratories

In FY2002 and onwards, NASA indicated that its total investment in nanoscience and nanotechnology research needed to be in excess of \$46 million in order to accomplish the goals and objectives set forth in this document.

FY 2002 Investment

Currently NASA's program is split primarily between the Office of Aerospace Technology (OAT) with a focus on *nanotechnology* research and applications and the newly formed Office of Biological and Physical Research (OBPR) with a focus on basic research in *nanoscience* related to biomedical applications. Furthermore, the OAT program integrates nanotechnology development in three areas: (1) Materials and Structures, (2) Nanoelectronics and Computing, and (3) Sensors and Spacecraft Components.

A major focus at NASA is to advance and exploit the *zone of convergence between nanotechnology, biotechnology and information technology*.

A summary of the contents of the above program follows:

Materials and Structures (OAT). A major emphasis for NASA over the next 5 years will be the production scale-up of carbon nanotubes; the development of carbon nanotube reinforced polymer matrix composites for structural applications; and the development of analysis, design and test methods to incorporate these materials into new vehicle concepts and validate their performance and life. However, NASA will also explore the use of other nanotubes such as boron nitride for high temperature applications; and will research the use of crystalline nanotubes to ultimately exploit the full potential of these materials. NASA studies indicate that nanotube composites can reduce the weight of a reusable launch vehicle by a factor of 2 over the best composite systems today and by 80% over current aluminum structures. Early studies also indicate that the dry weight of a large commercial transport could similarly be reduced by about half, resulting in a fuel saving of about 25%. In the long term, the ability to create materials and structures that are biologically inspired provides a unique opportunity to produce new classes of self-assembling material systems without the need to machine or process materials. Some unique characteristics anticipated from biomimetics ("mimicking" biology) include multifunctional material systems, hierarchical organization, adaptability, self healing/self-repair, and durability. This will allow tailoring the mechanical properties to meet the design requirements and revolutionize aerospace and spacecraft systems. Exploiting the characteristics of biological systems, new materials will enable the development of adaptable, self healing/self-repair, and durable structures.

Nanoelectronics and Computing (OAT). NASA has requirements for computers that offer extraordinary computational speed and memory capacity, as well as powerful new electronic science tools. These computers must be manufactured from nanoelectronic devices that feature *both* low power consumption and resistance to harsh radiation environments, revolutionizing the way NASA accomplishes its missions. For example, future aerospace transportation vehicles could have all of their electronic systems on a single tiny chip, where the computing and memory necessary for guidance, navigation, communications and integrated vehicle health management (IVHM) reside. Clearly, such a capability will enable inexpensive, powerful microspacecraft. Much of technology to accomplish this is envisioned to come from knowledge of biological systems. They can be up to a million times more power and space efficient than conventional electronics, but also self-assemble, self-adapt to changing conditions and self-repair when damaged.

Today, biologically inspired neural nets have been developed in laboratory demonstrations that allow computers to rapidly account for loss of aircraft control elements, understand the resulting aerodynamics and then teach the pilot or autopilot how to avoid the loss of the vehicle and crew by an innovative use of the remaining aerodynamic controls. Such approaches, coupled with the advances in computing power anticipated from nanoelectronics, will revolutionize the way “aerospacecraft” deal with condition-based maintenance, aborts and recovery from serious in-flight anomalies. While aircraft do not require electronic devices that can tolerate the space radiation environment, spacecraft exploration for the Space Science and HEDS Enterprises, e.g., vehicles exploring Mars, the outer planets and their moons, will require such capabilities. NASA mission planners view such capability as enabling to conduct in-situ science (without real-time Earth operators) where huge amounts of data must be processed, converted to useful information, and then sent as knowledge to Earth without the need for large bandwidth communication systems. A longer-term vision incorporates the added complexity of morphing devices, circuits and systems whose characteristics and functionalities may be modified in flight. NASA will support work at the underlying device level, in which new device configurations with new functionalities may be created through intra-device switching. Combined research in the “zone of convergence” of nanotechnology, biotechnology and information technology will lead to the development of new nanoelectronics and computing devices to meet NASA’s unique requirements.

Sensors and spacecraft components (OAT). NASA’s challenge to detect ultra-weak signals from sources at astronomical distances make every photon or particle a precious commodity which must be fully analyzed to retrieve all the available information it carries. Nanostructured sensing elements in which each absorbed quantum generates low-energy excitations that record and amplify the full range of information, provide an approach to achieve this goal. NASA will also develop field and inertial sensors with many orders of magnitude enhancement in sensitivity by harnessing quantum effects of photons, electrons and atoms. A gravity gradiometer based on interference of atom beams is currently under development by NASA, with the potential for space-based mapping of the interior of the Earth or other astronomical bodies.

Miniaturization of entire spacecraft will entail reduction in the size and power required for all system functionalities, not just for sensors. Low-power, integrable nano devices are needed for inertial sensing, power generation and management, telemetry and communication, navigation and control, propulsion and in-situ mobility, etc. Integrated nano-electro-mechanical systems (or NEMS) will be the basis for future avionics control systems incorporating transducers, electromagnetic sources, active and passive electronic devices, electromagnetic radiators, electron emitters, and actuators.

Basic Nanoscience (OPBR). Foremost among the technological challenges of long-duration space flight are the dangers to human health and physiology presented by the space environment. Acute clinical care is essential to the survival of astronauts who must face potentially life threatening injuries and illnesses in the isolation of space. Currently we can provide clinical care and life support for a limited time, but our only existing option in the treatment of serious illness or injury is expeditious stabilization and evacuation to Earth. Effective tertiary clinical care in space will require advanced, accurate diagnostics coupled with autonomous intervention and, when necessary, invasive surgery. This must be accomplished within a complex man-machine

interface, in a weightless environment of highly limited available space and resources, and in the context of physiology altered by microgravity and chronic radiation exposure. Biomolecular approaches promise to enable lightweight, convenient, highly focused therapies, guided with the assistance of artificial intelligence enhanced by biomolecular computing. Nanoscopic, minimally invasive technology for the early diagnosis and monitoring of disease and targeted intervention will save lives in space and on Earth. Prompt implementation of specifically targeted treatment will insure optimum use and conservation of therapeutic resources, making the necessity for invasive interventions less likely and minimizing possible therapeutic complications.

Specifically the NASA Basic Nanoscience program comprises of two research areas. The first is in Bio-Molecular Systems Research, which is a joint NASA/NCI Initiative, and the second is in Biotechnology and Structural Biology. The NASA/NCI Initiative emphasizes research in the following areas:

- Identification of bio-molecular signatures, sensors and markers for early detection of human diseases (genetic mutations)
- Development of in-situ and remote molecular imaging techniques for monitoring human health
- Signal amplification and processing
- Micro/nano systems for in-situ human health exploration
- Data storage, knowledge extraction and visualization

Emphasis in the second area of research focus, i.e., Biotechnology and Structural Biology, is in the following areas:

- Macromolecular crystallization and imaging (atomic force microscopy)
- Membrane protein crystallization
- Self-assembling mechanisms
- Molecular motors

FY 2003 Request

FY2003 investment is approximately \$51 million.

In FY2002, NASA plans to invest a total of \$51 million in basic nanoscience and nanotechnology research, of which \$22 million appear as line items in the agency's budget.

Similarly, in FY2003, in addition to the \$22 million in both basic nanoscience and nanotechnology research (which remains as line items in the budget), the agency plans to invest approximately an additional \$29 million in the area of nanotechnology *science* and *applications*. These investments, however, have not been line itemized specifically in the budget, but instead are embedded within several program areas and within the Office of Biological and Physical Research and the Office of Aerospace Technology.

The planned agency resources for next five years in the various areas of nanoscience, research and technology are as shown in Table C.3 below.

Table C.3
Current and Planned NASA Investments (\$ million)

Topic / Fiscal Year	2002	2003	2004	2005	2006
Nanostructured Materials	10	10	11	11	11
Nano Electronics and Computing	9	9	10	10	10
Sensors and Microspacecraft Components	8	8	9	9	9
University Aerospace Research Centers	9	9	9	9	9
Basic Nanoscience	15	15	15	15	15
Total \$	51	51	54	54	54

Opportunities for Collaboration with Other Agencies

Collaboration is particularly important for NASA, since it recognizes the importance of importing technologies from other Federal agencies. Given the infancy of nanotechnology, there is a huge area of basic research knowledge performed by other Federal agencies (particularly NSF, DOD, NIH, and DOE) that would benefit NASA. Due to NASA’s relatively modest budget, the agency will focus primarily on NASA-unique needs; examples are low power devices and high strength materials that perform with exceptional autonomy in the hostile space environment. (A joint program in non-invasive human health monitoring via identification and detection of molecular signatures is currently being developed with NCI based on a common interest in this area.) The agency plans to aggressively forge such partnerships in the future. Examples of potential areas for collaboration are as follows:

<u>Area of Common Interest</u>	<u>Potential Collaborators</u>
Aerospace structural materials	DOD
Radiation tolerant devices and materials	DOD
High resolution imagery	DOD
Terrain and environmental characterization	DOD
Large space optics and antennas	DOD
Biosensors, lab-on-a-chip, environmental monitoring	DOE, DOD, NIH, NSF
Targeted therapeutic delivery	NIH
Exploratory computational architectures	DOD, NSF
Micro spacecraft systems	DOD
Efficient energy conversion and storage	DOE
Basic research in nanostructures	NSF

Grand Challenges

NASA expects to allocate the majority of its nanotechnology program funds to address priority challenges of future robotic and human aerospace systems, as well as applications needed to advance the field of aeronautics. In addition to specific overlap in applications requirements with various government agencies (specifically NSF, NIH and DOD), NASA expects to leverage the nation’s investments in basic research as starting points for much of its investment in applications-oriented grand challenges, including the following specific topics within the grand challenge areas:

Nanostructured Materials “By Design.” NASA’s focus in this area is on high strength-to-mass, “smart” structural materials in the context of:

- Safer, more reliable, multifunctional and eventually self-repairing aerospace vehicle structures
- Truly smart and agile materials with programmable optical, thermal and/or mechanical properties
- Ultra-large space structures such as antennas, solar sails and gossamer spacecraft
- Materials for special environments, e.g., low/high temperature, low/high pressure, low/high gravity, high radiation and chemically reactive

Nano-Electronics, Optoelectronics and Magnetics. Priority areas for NASA are in nanoscale devices and novel computational architectures for:

- Quantum-limited sensors of electromagnetic radiation and fields, able to capture multiparameter information in detecting single quanta
- Low-power, ultra-high-speed signal processing devices and computers
- High-density, radiation-tolerant memory technologies
- Devices for special environments, e.g., low/high temperature, low/high pressure, low/high gravity, high radiation and chemically reactive

Advanced Healthcare, Therapeutics and Diagnostics. The challenge of ensuring astronaut health and performance drives NASA to a focus on biochemical signatures of incipient problems, on nanoscale *in vivo*, and on minimally invasive biochemical sensors and therapy effectors in the context of:

- Early detection of incipient health and performance problems of astronauts
- Targeting and delivery of preventative and curative therapeutics
- In-situ detection and characterization of life beyond Earth’s biosphere

There is strong overlap with NIH in this area, and a joint program is being planned with NIH/NCI in the general area of detection and imaging at the molecular level. There is also overlap with biosensor development outside of the medical arena in DOD and DOE covered under the bio-nanosensor category, below.

Efficient Energy Conversion and Storage. NASA is interested in high-efficiency, low-mass solar and thermal energy conversion for space power, high-mass-efficiency power storage and distribution, and efficient low-temperature refrigeration for ultra-sensitive space-based sensors. DOE shares the goals of high-efficiency energy conversion and storage.

Microspacecraft Space Exploration and Industrialization. NASA’s focus in this area is on low-mass, low-power, devices, subsystems and systems with the following goals:

- Reduction in size and energy consumption of capable spacecraft by a factor of 10
- Greatly increased on-board capability for signal processing, real-time decision making and autonomy
- Low-power, miniature spacecraft systems including sensors, signal processing, avionics, inertial guidance, propulsion and communications
- Bio-mimetic evolvable space system architectures that can adapt to new environments and mission needs, and eventually to self-replicate using local resources at distant locations

There is overlap with microspacecraft goals of DOD, and cooperative programs will be considered.

Bio-Nanosensor Devices for Communicable Disease and Biological Threat Detection. NASA's focus in this area is on nanoscale sensors and integrated laboratories for the purpose of monitoring and controlling human space habitat environments. Agencies with overlapping interests are DOD (detection of biochem-warfare agents), and DOE (lab-on-a-chip for detecting environmental pollutants and biological threats).

Economical and Safe Air Transportation. NASA's focus in this area is on smart materials and advanced aircraft avionics for economical air (commercial) transportation, Earth-to-orbit and deep-space transportation based on more reliable materials, smart systems for condition-based maintenance, and lower overall mass. Agencies with overlapping interests are DOD (low-cost air and space transportation) and DOT (low-cost, clean and secure air transportation).

Program Planning and Implementation Approach

NASA will typically use open solicitations and peer-reviewed competition for allocating basic research funds. Coherent, applications-oriented development programs with strong NASA center participation will be established to address specific grand challenges. The selection of challenges to address will be aligned with science priorities of the agency enterprises. NASA will also seek external scientific, engineering and biomedical expertise in determining the technical content of the program, and in reviewing the progress of the work to ensure quality. Opportunities will be sought with university research centers to arrange for student and postdoc participation in NASA's grand challenge research, including opportunities to work at NASA centers.

NASA has ongoing programs with several universities with a focus on applications of nanotechnology to aerospace vehicle structures, batteries and energy storage and nanodevices for microspacecraft. Collaboration opportunities of potential mutual benefit include the following:

<u>Area of Common Interest</u>	<u>Potential Collaborators</u>
Bionanotechnology, nanostructured materials, nanodevices, exploratory computational architectures	Universities
Microspacecraft technologies	Small and large aerospace industry
Biochips	Biotechnology industry

In addition, NASA will significantly increase university participation in agency nanotechnology programs by competitively awarding three University Research, Engineering and Technology Institutes (RETIs) in FY 2003. NASA plans to select one RETI in each of three areas: (1) aerospace materials, (2) electronics and computing, and (3) bio-nanotechnology fusion. Each award will for about \$3 million/yr. for 5 years with the option to extend award for up to an additional 5 years.

NASA's interaction with international activities is typically in international space missions, which are negotiated among the space agencies of the collaborating nations, and are implemented with no exchange of funds. It is NASA's intent to extend such space mission collaborations into the arena of nano and bio-technology.

National Institutes of Health

FY2001 Investment

For FY 2001, NIH continued to receive nanoscience and nanotechnology grant applications under several existing and some new programs. These programs were managed individually by the institutes and centers, with peer review for most of them conducted by the Center for Scientific Review. Overall program coordination occurred through the NIH Bioengineering Consortium (BECON). The NIH nanoscience program announcements were summarized at <http://www.nano.gov/nihnano.doc> and http://grants.nih.gov/grants/becon/becon_funding.htm.

NIH's nanotechnology-specific program entitled "Bioengineering Nanotechnology Initiative" (PA00-018) was an SBIR program under which several awards were made.

The majority of nanotechnology research at NIH was supported under a wide variety of programs, in which nanoscience and nanotechnology were among the numerous relevant enabling approaches. For example, several awards for nanotechnology research were made under the "Bioengineering Research Partnerships" (PA01-024, applications due February 16, 2001, and August 14, 2001) and "Bioengineering Research Grants" (PA99-009, applications due February 1, June 1, and October 1, annually) solicitations.

Additional programs were announced that year to encourage submission of grant applications for nanotechnology research, including a pair of program announcements on single molecule detection and manipulation (PA-01-049 for R01 grants, PA-01-050 for SBIR and STTR grants). These programs are described in more detail below (see FY 2002 description).

Another new program that was expected to include support for nanotechnology research was on "Fundamental Technologies for Development of Biomolecular Sensors." The purpose of this collaborative interagency program between the National Cancer Institute and NASA was to advance the development of technologies and informatics tools to enable minimally-invasive detection, diagnosis, and management of disease and injury, using technology platforms for biomolecular sensors that can function in the living body to measure, analyze, and manipulate molecular processes. The program was announced as NCI/NASA BAA No. N01-CO-17016-32 (<http://rcb.nci.nih.gov/appl/rfp/17016/Table%20of%20Contents.htm>). Awards were announced in 2002 (see below).

FY 2002 Investment

For FY 2002, NIH will receive nanoscience and nanotechnology grant applications under existing and renewed programs. These programs are managed individually by the institutes and centers, with peer review conducted for the most part by the NIH Center for Scientific Review.

Overall nanotechnology program coordination occurs through the NIH Bioengineering Consortium (BECON). The NIH nanoscience program announcements are available from <http://www.nano.gov/nihnano.doc> and http://grants.nih.gov/grants/becon/becon_funding.htm.

The NIH nanotechnology-specific SBIR program entitled “Bioengineering Nanotechnology Initiative,” originally issued in 1999, will be revised and reissued in 2002. Application deadlines are on April 1, August 1 and December 1, annually.

Additional nanotechnology research at NIH is supported under a wide variety of programs, in which nanoscience and nanotechnology are among the relevant enabling approaches. Two trans-NIH program announcements were developed with coordination by BECON, and specifically solicit nanoscience and nanotechnology research grants; both of these announcements were re-issued early in FY2002. The “Bioengineering Research Partnerships” program, PAR-02-010 issued October 11, 2001, with receipt dates on January 24, 2002, and August 12, 2002, solicits basic and applied multidisciplinary research addressing important biological or medical research problems, applying an integrative systems approach to developing knowledge and or methods to prevent, detect, diagnose, or treat disease, or to understand health and behavior. The parallel “Bioengineering Research Grants” program, PA-02-011 issued October 11, 2001, and with application receipt on February 1, June 1, and October 1, supports multidisciplinary research in single laboratories or conducted by small numbers of investigators, with science and technology goals similar to those of the Bioengineering Research Partnerships program.

Several institutes and centers of the NIH published grant solicitations in 2002 in topic areas appropriate for nanoscience and nanotechnology research, such as tissue engineering, sensors, genomics, imaging, and general instrument development. An example is the paired program announcements on single molecule detection and manipulation (PA-01-049 for R01 grants, PA-01-050 for SBIR and STTR grants), originally issued in 2001, and continuing through February 1, 2004. These programs solicit investigator-initiated proposals for basic research on detection and manipulation of single molecules to provide fundamentally new information about biological processes for understanding cellular function, including real-time measurements of single molecules in living cells and the development of the collateral chemistry and instrumentation. Led by the National Institute of General Medical Sciences, the National Institute on Deafness and Other Communication Disorders and the National Human Genome Research Institute are also participating. Applications for R01 grants are due February 1, June 1, and October 1, annually, and for SBIR/STTR grants on April 1, August 1, and December 1. Some of the nanotechnology areas emphasized in this announcement are focused on the development of highly luminescent semiconductor nanocrystals, or “quantum dots,” carbon nanotubes for use as AFM tips for increasing the resolution of this method, optical tweezers, multiphoton spectroscopy optimization for optical sectioning in the 50 nm range, and the improvement of instruments needed to optimize high resolution measurements in the 1-100 nm scale.

Based upon a shared vision of the future of human health care, NASA and the NCI have formed a partnership, and created the “Fundamental Technologies for Development of Biomolecular Sensors” Program. Through this partnership, NCI and NASA will jointly support the development of minimally invasive technologies to scan the body for the earliest signatures of emerging disease and support immediate, specific intervention. These technologies should

support a seamless interface between detection, diagnosis and intervention. NCI and NASA have awarded approximately \$21 million over three years to develop new biomedical technologies to detect, diagnose and treat disease inside the human body.

The selected proposals will develop and study nanoscale biomedical sensors that can detect changes at the cellular and molecular level and communicate irregularities to a device outside the body. The contracts awarded to date under this program place a strong emphasis on multifunctional nanoparticles and molecular beacons. These nanoparticles would have the ability to identify and target cancer cells, provide contrast enhancement for imaging, deliver a therapeutic, and monitor status post treatment. Nanoparticles of various size and composition are proposed. Plans include particle synthesis and preliminary testing in animals.

Training of scientists and engineers to conduct multifaceted nanotechnology research is essential. NIH, through BECON, is re-issuing a program solicitation, “Mentored Quantitative Research Career Development Award,” to support career development of investigators with quantitative scientific and engineering backgrounds who have made a commitment to focus their research on biomedical (basic or clinical) or behavioral research. The awards support supervised study and research to assist investigators in making this career transition.

Additional effort to work across disciplines to enhance nanoscience and nanotechnology research opportunities is exemplified by the topic of the 2002 BECON Symposium, Sensors for Biological Research and Medicine (June 24-25, 2002). The symposium is designed to present medical and biological perspectives on the technology needs, and the technological state-of-the-art, to focus discussion on near- and longer-term opportunities to develop integrated sensors to detect, monitor, and treat disease. Nanotechnology is one of the most fruitful areas in modern biosensors research. Therefore, this symposium will provide additional insights into specific opportunities for nanotechnology research supported by the NIH, and provides unique opportunities for interaction and development of scientific collaborations across the disciplines.

NNI Management

Each of the institutes and centers of the NIH funds and manages a research portfolio designed to fulfill its mission, and nanotechnology research is incorporated in the majority of these portfolios. Trans-NIH coordination of nanoscience and nanotechnology programs is the responsibility of BECON, the NIH Bioengineering Consortium, in particularly close collaboration with the newly formed National Institute of Biomedical Imaging and Bioengineering (NIBIB).

Collaboration with Other Agencies/Private Sector

- Three agencies, NSF, DOE, and NIST participate in monthly BECON meetings at which NIH plans for developing bioengineering, bioimaging, and technology development programs generally, and nanoscience and nanotechnology programs specifically. These agencies provide their perspectives on our programs and information on theirs. BECON members and other NIH staff meet with representatives of various companies and agencies to explore and explain program goals and research opportunities at monthly BECON meetings.

- The National Cancer Institute (NCI) and NASA signed a Memorandum of Understanding to jointly develop new biomedical technologies that can detect, diagnose and treat disease here on Earth and in space, based on nanotechnology-based “microscopic explorers” that would travel through the human body looking for disease. This agreement was bolstered by a joint NCI/NASA workshop on Sensors for Biomolecular Signals. One manifestation of this collaboration is a joint broad agency announcement, described above, on fundamental research to develop biomolecular sensors. NCI has also funded a contract at NASA’s Ames Research Center to study how nanotechnology can be used in the detection of cancer cells. NCI and NASA also host a Web-based Biotechnology Forum that brings together NCI and NASA scientists, technologists, and engineers.
- NIH representatives speak at industry (e.g., small business and state-run economic development/university partnership-promoting), professional society, and other agencies’ conferences to describe the agency’s vision for nanotechnology in biomedicine, and research, funding, and partnership opportunities to achieve that vision.

Success Stories in R&D

- Antibacterial agents from controlled self-assembly of novel amino acid analogues (Scripps Research Institute)
- Quantum dot bar codes (Indiana University)
- Single DNA nucleotide discrimination by nanopores (University of California Santa Cruz; Texas A&M University)

Activities and Budget Plans for FY 2003

Through trans-NIH announcements such as those developed through BECON, and through individual institute programs (cited above), NIH is developing focus in several promising areas. These include the following:

- *Nanomaterials.* Nanomaterials science to interface with living tissues, deliver pharmaceuticals, enable tissue engineering, and for contrast and biologically active agents
- *Nano-imaging.* Real-time intracellular imaging of structure, function and metabolism
- *Cell biology.* Nanoscale research on cellular processes, including biophysics of molecular assemblies, membranes, organelles, and macromolecules
- *Molecular and cellular sensing/signaling.* Technologies to detect biological signals and single molecules within and outside cells
- *Nanomotors.* Understanding structure/function, self-assembly, and power supplies
- *Prosthetics.* Mechanical, chemical, and cellular implant nano-technologies to achieve functional replacement tissue architectures
- *Nano-bio processors.* Implantable nanoscale processors that can integrate with biological pathways and modify biological processes
- *Nanosystem design and application.* Fundamental principles and tools to measure and image the biological processes of health and disease; and methods to assemble functional nanosystems

NIH anticipates that increasing interest in and capabilities of nanoscience and nanotechnology research will result in larger numbers of applications in response to our several program

announcements, and therefore an increase in the number of quality projects that will be funded. The current estimate is for an increase from \$40 million in FY2002 to \$43 million in FY 2003. This specific nanoscience and nanotechnology investment is in addition to much larger NIH investment in understanding biology at the molecular (nanoscale) level, which is part of NIH's ongoing research that is not categorized within the nanotechnology program, but reveals the nanoengineering principles developed by nature over the millennia that may be used as the basis for biomimetics in nanotechnology projects across the agencies and disciplines.

National Institute of Standards and Technology

FY 2001 Investment

In FY 2001, in addition to its initial estimated core funding of \$8 million in nanotechnology, NIST received a \$2 million NNI augmentation. The NIST Laboratories were asked in December 2001 to submit their nanotechnology budgets for FY 2001, FY 2002 and FY 2003. The numbers were significantly higher than those reported previously, due in part to more accurate interpretation of the definition of nanotechnology. As a result, the total NIST investment in FY 2001 was revised at \$33.4 million. The \$2 million of NNI funds was distributed using a competitive process across the NIST Laboratories. \$1 million of NNI funds were used to supplement in-house efforts while the other \$1 million was used to leverage external support of internal work (\$1 million) in the following areas:

- Molecular electronics
- Quantum computing
- Nanomagnetodynamics
- Nanotribology
- Autonomous atom assembly

The nanotechnology projects supported only by NIST core funds cover a broad range of measurement and standards activities in these and other areas, and involve a large range of industry interactions.

NIST's mission for measurements and standards for industry and other scientific interests was established by the U.S. Congress in 1901. As such, NIST needs to ensure the accuracy and precision of nanoscale characterization through scientific development, standards, and calibration sources. By working with industry, academia, and other government agencies, NIST is addressing these metrology issues. For example, through the National Nanotechnology Initiative, NIST is developing a broad range of metrologies in areas ranging from molecular electronics to nanomagnetodynamics. As an agency of the U.S. Department of Commerce, NIST works to help facilitate international trade by working with international standards organizations and national metrology institutes. Key issues in the future for international trade, with respect to nanotechnology, will be traceability of measurements and "harmonization" of international standards.

FY 2002 Investment

The total FY 2002 NIST nanotechnology investment was revised in December 2001 at \$37.6 million, of which \$2 million appear as the NNI line item in the agency's budget. The remaining \$35.6 million represents longer-term NIST investments in nanoscale metrology embedded within several programs across the institute. Approximately half of the \$2 million of NNI funds has been used to increase current efforts in several research areas and half will be used to leverage existing efforts with external partners. The following projects received NNI funding:

- Molecular electronics
- Quantum computing
- Nanomagnetodynamics
- Nanotribology
- Autonomous atom assembly

In addition to these projects, NIST has measurement and standards activities related to all of the grand challenges of nanotechnology, as defined by the NSET:

- Nanostructured materials "by design"
- Nanoelectronics, optoelectronics and magnetics
- Advanced healthcare, therapeutics and diagnostics
- Nanoscale processes for environmental improvement
- Efficient energy conversion and storage
- Microspacecraft exploration and industrialization
- Bio-nanosensors for communicable disease and biological threat detection
- Economical and safe transportation
- Chemical, biological, radiological and explosive detection and protection
- Nanoscale instrumentation and metrology
- Manufacturing at the nanoscale

NNI Management

As NIST received slightly under \$2 million for nanotechnology in fiscal year 2002, it was deemed that there was no reason to set up an office to centrally manage the funds. The funds are therefore distributed, using a competitive process, across the NIST Laboratories. Work encompasses the following areas:

- NIST will develop the critical enabling infrastructural measurement, standards, and data for nanomagnetics, nanocharacterization, and new information technologies, including quantum computing, which will replace semiconductor electronics in the future.
- Nanomagnetics research will provide measurement and standards for current and near-term applications of nanotechnology in the semiconductor, communications, and health care industries.
- Nanocharacterization research will produce standards and tools for visualization and characterization at the nanoscale, which are in high demand by a broad base of U.S. industries.
- Research will be conducted to provide fundamental measurements needed for future generations of information technology hardware that will be needed to replace semiconductor electronics technology in a decade or so.

- In order to leverage internal efforts, NIST will develop stronger strategic alliances and collaborations with universities, businesses, and other government agencies that possess leading expertise in nanotechnology. NIST plans to direct half of the new nanotechnology funding to these external organizations to conduct much of the specific work required to meet the goals of this initiative and avoid developing costly, complex in-house capabilities that may only be used once.

Collaborations with Other Agencies/Private Sector

NIST has a large range of collaborations with industry. Expected benefits to industry are:

- This initiative is designed to broadly benefit most sectors of the U.S. economy through new innovations in nanotechnology, which is a critical enabler for information technology, manufacturing, health care, defense applications, automotive, communications, plastics, and many other economic sectors.
- The nanotechnology measurements, standards, and data developed at NIST will help U.S. industry maintain and improve leadership of the \$200 billion computer and peripheral market and \$400 billion telecommunications industry, and improve the U.S. market share in the \$35 billion magnetic data storage market.

R&D Success Stories

- Developed a Nanoscale Recording System applicable to the retrieval of information from damaged or altered audio tapes.
- Developed prototype critical dimension reference materials for calibrating linewidth metrology instruments used in manufacturing semiconductor devices.
- Developed SPM oxidation method for lithographic patterning with capability for producing 10 nm to 40 nm linewidths on silicon for application to nanometrology standards, nanoelectronic device structures and templates.
- Demonstrated the importance of measuring and controlling oxygen partial pressure during the deposition of multilayer GMR read/write heads; the process is used by all major hard-disk drive manufacturers.

FY2003 Request

In FY2003, NIST plans to invest a total of \$43.8 million in nanotechnology, of which \$6 million appears as a line item in the agency's budget. The additional \$37.8 million represents longer-term NIST investments in nanoscale metrology embedded within several programs in the institute.

National Science Foundation *Nanoscale Science and Engineering*

FY2001 Investment

The FY 2001 (actual), FY 2002 (current plan) and FY 2003 (WH request) per directorates are shown in Table C.4.

In FY 2001, NSF invested \$149.68 million in a wide range of research and education activities in nanoscale science and technology, including approximately 10 large nanotechnology research centers, which focus on electronics, biology, and optoelectronics.

Table C.4
NSF Nanoscale Science and Engineering Investments (\$ million)

	FY 2001 Enacted	FY 2002 Current Plan	FY 2003 Request
Biological Sciences	2.33	2.33	2.98
Computer and Information Science and Engineering	2.20	10.20	11.14
Engineering	55.27	86.30	94.35
Geosciences	6.80	6.80	7.53
Mathematical and Physical Sciences	83.08	93.08	103.92
Social and Behavioral Sciences	0.00	0.00	1.11
Education and Human Resources	0.00	0.00	0.22
Total, Nanoscale Science and Engineering	\$149.68	\$198.71	\$221.25

NSF distributed its \$150 million roughly 1/3 to multidisciplinary groups and centers and 2/3 to individual PIs. The funds were allocated as follows:

- \$97 million in the core research and education programs
- \$53 million for a NSF-wide program solicitation (new activity in FY 2001)
- In addition, about \$4 million awards were made through the SBIR/STTR program solicitation with nanotechnology as an area of focus.

The program announcement can be found at <http://www.nsf.gov/nano> (then click on NSF 00-119):

- Nanoscale Interdisciplinary Research Teams (NIRT, 250-500K/yr. for up to four years) received 379 proposals; 43 awards.
- Nanoscale Science and Engineering Centers (NSEC, \$1-4 million/yr. for up to five years) received 69 preproposals; 6 awards.
- Nanoscale Exploratory Research (NER, \$100K/yr. for 1 year) received 260 proposals; 50 awards.

The success rate is expected to be in the range 10-15 %. Younger faculty and interdisciplinary teams are the most active groups.

NNI Management

NSF's Nanoscale Science and Engineering (NSE) Group coordinates the NNI activities. Each directorate has two representatives in the NSE Group. The Chair of the Group is the NSF representative to NSEC.

Examples of Collaborations with Other Agencies/Private Sector

- Quantum Computing, with DARPA
- MRSEC materials centers with DOD
- SRC and ERCs

- GOALI awards (collaboration with private sector)
- Two NSEC centers co-funded with DOD

Success Stories in R&D

- *Scientific breakthroughs*
 - New form of DNA (S.A. Benner)
 - Bio-inspired methods to assemble materials (A. Belcher)
 - Electric signal on surfaces
 - Assembling DNA into devices
 - Environmental nanostructures
- *Accomplishments with relevance*
 - Catalysts
 - Nanoparticle synthesis at high rate production
 - Nanostructured conducting polymers (U. Penn)
 - Hybrid bio-inorganic devices (Cornell U.)
 - NNUN for users and education
 - Network of six nanoscale science and engineering centers

FY 2002 Investment

NSF has been a pioneer among Federal agencies in fostering the development of nanoscale science, engineering and technology. In FY 2002, NSF is investing \$198.7 million in a wide range of research and education activities in nanoscale science and technology, including approximately 16 nanotechnology research centers, which focus on electronics, biology, and optoelectronics. NSF is distributing its allocation roughly 1/3 to multidisciplinary groups and centers and 2/3 to individual PIs.

The program announcement can be found at <http://www.nsf.gov/nano> (NSF 01-157):

- Nanoscale Interdisciplinary Research Teams (NIRT, 250-500K/yr. for up to four years) received 387 proposals.
- Nanoscale Exploratory Research (NER, \$100K/yr. for 1 year) received 407 proposals.

This investment will be expanded to develop and strengthen critical fields and to establish the science and engineering infrastructure and workforce needed to exploit the opportunities presented by these new capabilities. Support will be focused on interdisciplinary research and education teams, national science and engineering centers, exploratory research and education projects, and education and training.

FY 2002 topics of emphasis are in five programmatic focus areas as follows:

- **Fundamental Research and Education.** The FY 2002 request includes \$107.72 million for fundamental research and education, with special emphasis on:
 - *Biosystems at the Nanoscale* – \$19.0 million
 - *Nanoscale Structures, Novel Phenomena and Quantum Control* – \$36.72 million
 - *Device and System Architecture* – \$25.50 million

- *Nanoscale Processes in the Environment* – \$9.50 million
- *Multi-scale, Multi-phenomena Theory, Modeling and Simulation at the Nanoscale* – \$17.0 million
- **Grand Challenges.** Approximately \$7.90 million will fund interdisciplinary activities to focus on major long-term challenges: nanostructured materials “by design,” nanoscale electronics, optoelectronics and magnetics, nanoscale-based manufacturing, catalysts, chemical manufacturing, environment and healthcare.
- **Centers and Networks of Excellence.** \$29.39 million will provide support for research and education centers, a multidisciplinary, multi-sectoral network for modeling and simulation at the nanoscale.
- **Research Infrastructure.** \$19.90 million.
- **Societal and Educational Implications of Nanoscience and Nanotechnology.** Approximately \$8.80 million.

FY 2003 Request

This investment will be expanded in FY 2003 to develop and strengthen critical fields and to establish the science and engineering infrastructure and workforce needed to exploit the opportunities presented by these new capabilities. In addition to single investigator research, support will be focused on interdisciplinary research and education teams, national science and engineering centers, exploratory research and education projects, and education and training.

Long-term objectives include building a foundation of fundamental research for understanding and applying novel principles and phenomena for nanoscale manufacturing and other NNI grand challenges; ensuring that U.S. institutions will have access to a full range of nano-facilities; enabling access to nanotechnology education for students in U.S. colleges and universities; and catalyzing the creation of new commercial markets that depend on three-dimensional nanostructures. These goals will enable development of revolutionary technologies that contribute to improvements in health, advance agriculture, conserve materials and energy, and sustain the environment.

FY 2003 Areas of Emphasis

NSF’s planned investment for Nanoscale Science and Engineering in FY 2003 is \$221.25 million. NSF’s five programmatic focus areas are as follows:

- **Fundamental Research and Education.** The FY 2003 request includes \$140.93 million for fundamental research and education, with special emphasis on:
 - *Biosystems at the Nanoscale* – Approximately \$20.7 million to support study of biologically-based or inspired systems that exhibit novel properties and potential applications. Potential applications include improved drug delivery, biocompatible nanostructured materials for implantation, exploiting of functions of cellular organelles, devices for research in genomics, proteomics and cell biology, and nanoscale sensory systems, such as miniature sensors for early detection of cancer.
 - *Nanoscale Structures, Novel Phenomena and Quantum Control* – Approximately \$53.5 million to discover and understand phenomena specific at the nanoscale, create new materials and functional nanoscale structures and to exploit their novel properties.

Potential applications include quantum computing and new devices and processes for advanced communications and information technologies.

- *Device and System Architecture* – Approximately \$27.8 million to develop new concepts to understand interactions among nanoscale devices in complex systems, including the physical, chemical, and biological interactions between nanostructures and device components. Interdisciplinary teams will investigate methods for design of systems composed of nanodevices.
- *Nanoscale Processes in the Environment* – Approximately \$9.6 million to support studies on nanoscale physical and chemical processes related to the trapping and release of nutrients and contaminants in the natural environment. Potential benefits include artificial photosynthesis for clean energy and pollution control, and nanoscale environmental sensors and other instrumentation.
- *Multi-scale, Multi-phenomena Theory, Modeling and Simulation at the Nanoscale* – Approximately \$20.84 million to support theory, modeling, large-scale computer simulation and new design tools and infrastructure in order to understand, control and accelerate development in new nanoscale regimes and systems.
- *Manufacturing Processes at the Nanoscale* - Approximately \$8.49 million to support new concepts for high rate synthesis and processing of nanostructures, fabrication methods for devices, and assembling them into nanosystems and then into larger-scale structures of relevance in industry and in the medical field.
- **Grand Challenges.** Approximately \$10.70 million will fund interdisciplinary activities to focus on major long-term challenges: nanostructured materials “by design,” nanoscale electronics, optoelectronics and magnetics, nanoscale-based manufacturing, catalysts, chemical manufacturing, biological-chemical detection and protection, environment and healthcare.
- **Centers and Networks of Excellence.** Approximately \$37.94 million will provide support for four new research and education centers, and a multidisciplinary, multi-sectoral network for modeling and simulation at the nanoscale. These funds will support the nanofabrication user facilities that come on line in FY 2002.
- **Research Infrastructure.** Approximately \$21.70 million will support instrumentation and facilities for improved measurements, processing and manipulation at the nanoscale, and equipment and software for modeling and simulation. University-industry-national laboratory and international collaborations will be encouraged, particularly for expensive instrumentation and facilities.
- **Societal and Educational Implications of Nanoscience and Nanotechnology.** Approximately \$9.98 million will support student assistantships, fellowships and traineeships, curriculum development on nanoscience and engineering and development of new teaching tools. The implications of nanotechnology on society will be analyzed from social, behavioral, legal, ethical, and economic perspectives. Factors that stimulate scientific discovery at the nanoscale, ensure the responsible development of nanotechnology, and converging technologies to improve human performance will be investigated. The development and use of nanoscale technologies is likely to change the design, production and use of many goods and services, ranging from vaccines to computers to automobile tires.

U.S. Department of Agriculture

USDA conducts its research both extramurally through the partnership between Cooperative State Research, Education, and Extension Service (CSREES) and Land Grant Universities (LGUs), and in-house at Agriculture Research Service (ARS) national laboratories. The CSREES also provides leadership and financial support in education and outreach in all the states and territories of the United States through the LGUs. According to the USDA Current Research Information System (CRIS) database, the combined research expenditure related to nanoscale science and technology was about \$9.2 million in FY 2001.

FY2001 Investment

Activities

Development of new materials

- Textile materials based on fibers of agricultural origin and polymers for environmental compatibility and human health and safety. The formation of nano particles in fibers has been achieved using doped fibers and UV light. These processes are reversible and have potential applications in electronics, computerized clothing and in data storage devices.
- Bionites made from *Bacillus subtilis* fibers that use drawn bacterial thread as the substrates for mineralization. Two unique products, silica fibers and magnetic fibers, were made of nano-particles that became assembled using bacterial thread to align and compress them.
- Wheat biopolymer (starch) composites for industrial and food applications. Methods for isolating and characterizing cellulose microfibrils as nanocomposites were developed and exploited for the first time.
- Textile fibers based on soybean protein and poly(vinyl alcohol). To develop a knowledge base to provide direction for using inexpensive renewable resource plant protein for manufacturing hydrophilic textile fibers. The work includes use of majority component soybean protein as well as processing a ternary blend fiber of soybean protein/PVA/nano carbon fibers.
- Integrating nano particles into biodegradable polymers to improve the physical and mechanical properties of the resulting polymers.
- Nanocrystalline reinforcing agents from sugar refining waste products. To establish the influence of modified and unmodified nanoparticles (cellulose nanocrystals) on the modulus and elongation at break of silicon rubbers and acrylate polymers using dynamic mechanical analysis.
- Topochemically modified cellulose nanoparticles for polymer composite. Modified cellulose microfibrils.
- Development of a scaleable thermal process with improved thermal efficiency to produce nanostructured silicon carbide using rice husk as the precursor. The effort has yielded a novel technology to produce value-added nanoscale powders in general, and silicon carbide in particular. The effort developed a technology establishing that rice husk has significant commercial potential as a precursor to advanced ceramics.
- Self-assembled cellulosic films by surface segregation.

Fundamental studies

- DNA-enzyme interactions – single molecule studies. RecBCD enzyme is a processive helicase and nuclease that participates in the repair of chromosomal DNA via homologous recombination. Visualization of translocation and DNA unwinding by single DNA helicase molecules permits study of the stochastic properties of individual molecular motors, or “nano-machines,” that is obscured in the population-average of steady-state, bulk phase measurements. The movement of individual RecBCD enzymes on single molecules of duplex DNA (dsDNA) has been directly visualized.
- Mechanisms of plant virus transmission and assembly. Expanded the understanding of the assembly and disassembly of spherical plant viruses. The results have allowed developing a completely new use of viruses as constrained reaction vessels for nano material synthesis and release. The results have greatly expanded the use of viral protein shells for applications in biotechnology and nano engineering. For example, we are developing this technology to create a combined non-invasive cancer MRI imaging agent and drug delivery system. In addition, we are exploring the synthesis of nano materials of great interest to the electronics industry using viral protein cages as organic templates.
- Biomolecular motor powered nano-mechanical devices: to create, develop and demonstrate the technology for constructing engineered hybrid living/non-living nanoelectromechanical devices.
- Structural and immunochemical characterization of quadruplex DNAs: making self-assembling “nanowire” structures.

Separation of bioproducts

- Develop novel and industrially useful separation techniques for both macro- and micro-scale uses. The scope includes use experimental knowledge and mathematical models to design, build, and validate micro-scale bioseparation systems associated with biochips.

Development of biosensor and sensing systems

- Use biochips to probe foods and other materials for pathogenic organisms. Combine fundamental principles of protein/solid phase interactions with models of nanoscale mass transfer phenomena to develop biochips capable of handling fluids derived from plant and animal tissues or products.
- Integrated gas sensor on porous silicon; photoluminescence for monitoring food products. The capability of light emission from silicon nanoparticles fabricated from porous silicon raises several technologically important possibilities, especially the fabrication of a truly integrated chemical sensor. The aim of the program is to develop a sensitive and durable optical sensor based on porous silicon that can detect gas phase chemicals and odorants. Several different surfaces combined in an array and the attendant optics will be interfaced to an electronic nose instrument using pattern recognition signal processing. The final form of the device will be compatible with the size and power requirements of a portable system and versatile enough to screen a wide range of chemicals.
- Microfluidic devices for biosensor development for food safety and environmental protection. A microfluidic device will be developed using standard nano- and microfabrication processes. First prototypes will be made on silicon wafers being the best understood nanofabrication substrate.

- Nanobiotechnological devices. To create nano and microscale devices that interface with biological systems, explore microfluidic systems to transport biological samples, and develop novel materials that are suitable for fabrication. Devices are fabricated at the Nanofabrication Facility using silicon and nonsilicon-based materials and tested for performance properties consistent with their application.
- Liposome-amplified bioanalysis of toxic chemicals and pathogens using nanofabrication approaches.
- Signal transduction via ionic changes and the cytoskeleton in plant cells. Using novel nanobiosensors placed next to or in plant cells to measure different parameters to study cell motility and the cytoskeleton and their relations to signal transduction in plant cells, and to develop better photonic imaging methods.
- Colloidal metal particles for high resolution biological labeling. This project seeks to develop effective labeling strategies that will allow simultaneous visualization of multiple molecular species so the way in which they fit together in the cell can be determined.

Education

- Educating young researchers for sustainable agriculturally-based bioindustries. The general goal of the program is to create a cadre of young engineers and scientists who can participate in the rational design of bio-based industries through the integration of science and engineering concepts across the scale from nanobiotechnology to industrial ecology.
- The Alliance for Nanomedical Technologies brings together academia and the private sector of New York State to develop basic components as well as integrated systems that will be the next generation of medical devices. Beyond its research program the Alliance will create user facilities and help to formulate educational programs to train workers whose skills will be needed to establish New York as the premier location for this new industry.

Infrastructure building

- Several nanotechnology centers. General research, bioselective surfaces, sparse cell isolation, microanalysis of biomolecules, selective molecular filtration.

Applications

- Use of iodinated resins for potable water and clean air production. Investigation of iodinated resin disinfectants in conjunction with nanoparticle technology to disinfect microorganisms on dry surfaces.
- Use of nanoparticles consisting of organic biocides dispersed in a polymer phase as carriers in wood preservative pressure treatments.
- Use of nanosensors to study signal transduction via ionic changes and the cytoskeleton in plant cells and nuclear structure of plant cells.
- Food safety in processing. Adhesive-specific nanoparticles for removal of *Campylobacter jejuni* from poultry.

Bioremediation of metals and pesticides

- Preparation and utilization of cysteine-glutathione or phytochelatin-capped nanocrystals in photodegradation experiments. The primary aims of the project were to understand the fundamental processes involved in detoxification of metals, ultimately to develop processes suitable for the phytoremediation of soils contaminated with heavy metals. In the study, the

possibility of using biomolecularly-capped nanocrystalline materials in photodegradation of organic contaminants was explored. A unique procedure for the synthesis of uniformly sized nanocrystalline materials that has proven very effective in photodegradation of pesticides and other contaminants was devised.

Mathematical modeling and computation in nanoporous media

- Understanding the stability of soil minerals provides a basis for predicting their formation, decomposition, and bioavailability to plants, animals, and bacteria. The manganese oxides studied in this work are important catalysts for chemical processes in soils.
- Studying the underlying mechanisms that govern sorption of nonionic organic compounds to soil natural organic matter (NOM) and to mineral surfaces using soils and model sorbents, including development of models to predict co-condensation of organic vapors and water in nanoporous solids. The existence of specific sites in SOM has potentially far-reaching consequences for modeling the behavior of chemicals in the environment and managing polluted sites. The results are likely to have an impact on vadose zone transport models, prediction of long-term persistence in soil, bioavailability, and assessment of risk to humans and the environment associated with contaminated soil.
- Correlating the nanopore structure of oxide minerals with the adsorption of organic compounds. The initial objectives are to attain a range of pore modifications on iron minerals as a function of freeze-thaw treatment. The relative humidity of the pore sizes will be varied before the freeze-thaw cycles. The long-range objectives are to elucidate the effects of nanopore size distributions and structure of iron hydroxide minerals on the entrapment of a model organic compound. The model compound is 2,4-dichlorophenol (DCP), and the primary minerals studied will be goethite and akaganeite. Entrapment will be evaluated based on adsorption/desorption isotherms and on changes in the pH-dependent edges.
- The physics of fluids in hierarchical porous media: modeling swelling porous media such as foods, soils, and drug delivery substrates; use of computational statistical mechanics in the mixed grand isostress-isostrain ensemble to simulate liquid-gas phase equilibria in finite split-pores and between nanowires; and understanding how unsaturated systems work on the nanoscale.
- Pesticide fate and weed management: develop predictive capability for herbicide movement.
- Adsorption and abiotic degradation of organic chemicals on soil mineral surface. Self-assembly of layered aluminum silsesquioxanes: clay-like organic-inorganic nanocomposites.

Engineering properties of nano-materials

- Energetics of oxide nanoparticles in soils. Measure heat capacities and dehydration energetics by differential scanning calorimetry as appropriate; calculate thermochemical parameters. Identify systematic trends and link to structural features; use thermochemical data in models of reactivity (e.g., high temperature reaction calorimetry applied to metastable and nanophase materials).

NNI Management

USDA currently does not have a formal structure in coordinating and leading nanotechnology related research and education initiatives. Dr. H. Chen of CSREES was invited to represent

USDA on the NSET Subcommittee at the AIChE annual meeting in November 2001. He has participated in NSET's monthly meetings since then.

Collaborations with Other Agencies/Private Sector

Numerous collaborative opportunities are easily perceivable. The researchers at our LGUs have already successfully obtained grants and participated in the research projects sponsored by other Federal agencies and by industry. More collaboration will be fostered as soon as a nanotechnology initiative is formed at USDA.

Success Stories in R&D

Economical synthesis of advanced ceramics from agricultural materials (Principal Investigator: X. Fan, Nanomaterial Research Corporation, Colorado. A scaleable thermal process with improved thermal efficiency has been developed to produce nanostructured silicon carbide using rice husk as the precursor. Effects of major variables: temperature, pressure, feed rate, feed size, quench rate, and residence time on the yield, and the quality of the produced nanostructured silicon carbide are investigated. A quantitative analysis of this project will lead to the optimization of various factors influencing the quality of produced nanostructured silicon carbide. This effort was funded under an SBIR award entitled, "Economical Synthesis of Advanced Ceramics from Agricultural Materials." The project sought two primary objectives: (1) to develop an industrial process that is able to convert agricultural residue, namely, the rice husk and/or hull ash, into value-added industry raw materials; and (2) to produce nanosize SiC powders from the process mentioned above. The focus was to produce nanoscale powders. This effort completed the system design and installation that made it possible to produce nanopowders of various compositions on an industrial scale (100 g/hr). The formation condition for SiC nanopowders (from rice husk) has been investigated. The nanopowders made from rice husk and hull ash via a patented thermal quench process have been characterized. The engineering economics analysis of the process has also been conducted. The effort has yielded a novel technology to produce value-added nanoscale powders in general, and silicon carbide in particular. The effort developed a technology establishing that rice husk has significant commercial potential as a precursor to advanced ceramics.

Integrated gas sensor on porous silicon photoluminescence for monitoring food products (Principal Investigator: J.C. Misfud, Alpha M.O.S. American Inc., New Jersey). In 1998, the U.S. food and beverage industry was expected to spend more than \$300 million in diagnostic systems and reagents. Clearly, there are needs for real-time methods for monitoring, quantitating and performing differential analysis of gas mixtures from chemical processes and products. Although various chemical instruments such as fast GCs have emerged recently, particularly for volatile organic measurements, it is obvious that presently available analytical instrumentation cannot meet commercial criteria such as high selectivity and sensitivity, rapid recovery times, long lifetimes if not single use, low cost, no reagent additions required and no sample preparation. This project investigated the capability of light emission from silicon nanoparticles fabricated from porous silicon, raising several technologically important possibilities, especially the fabrication of a truly integrated chemical sensor. The aim of the program was to develop a sensitive and durable optical sensor based on porous silicon that can detect gas phase chemicals

and odorants. Several different surfaces combined in an array and their attendant optics were interfaced to an electronic nose instrument using pattern recognition signal processing. The final form of the device will be compatible with the size and power requirements of a portable system and versatile enough to screen a wide range of chemicals.

FY 2002 Investment

USDA CSREES currently welcomes and encourages nanotechnology research proposals initiated by individual researchers in the existing competitive and formula programs. The researchers' enthusiasm is evident as shown in the CRIS database. Increased activities are expected. Funding levels should be increased significantly to take advantage of the rapid development in nanotechnology to strengthen the USDA mission and goals. The investment, both for FY 2002 and 2003, should be estimated immediately.

It is necessary and extremely beneficial for CSREES to conduct a workshop involving its research scientists, LGUs administrators and USDA national research staff members to develop a strategic vision, working plan and funding recommendation. This workshop will be held in the fall of 2002.

FY 2003 Request

The estimated budget is \$2.5 million.

Agencies' Contributions to FY 2001, 2002 and 2003 Budgets

Tables C.5, C.6, and C.7 summarize contributions that participating agencies have made to the NNI since its inception in FY 2001.

Table C.5
FY 2001 NNI Investments by Agency

Topic / Agency	NNI total	DOD	DOE	DOJ	DOT	EPA	NASA	NIH	DOC/ NIST	NSF	USDA
Fundamental Research	152.5	11	32				5	8		95	1.5
Biosystems	33.5	3					5	8		16	1.5
Phenomena, structures, and tools	66	8	18							40	
Devices and systems	37	0	14							23	
Theory, modeling, and simulation	16									16	
Grand Challenges	150.6	61	27	1		5	12	19	19	7	
Nanostructured Materials by Design	35.5	15	8	0.5			5		5	2	
Nanoelectronics, Optoelectronics, Magnetics	47.5	35	4	0.5			2		5	1	
Advanced Healthcare, Therapeutics	20							19		1	
Environmental Improvement	6					5				1	
Energy Conversion/Storage	16	1	15								
Microcraft & Robotics	5						5				
CBRE Protection/Detection (was Bionanodevices)	10	10									
Instrumentation & Metrology	11								9	2	
Manufacturing Processes											
Centers/Networks	71	27	14					1		29	
Infrastructure*	76.8	21	15	0.4			5	10	12.4	13	
Societal and Education**	13	3						2	2	6	
TOTAL	464.3	123	88	1.4		5	22	40	33.4	150	1.5

Table C.6
FY 2002 NNI Investments by Agency

Topic / Agency	NNI total	DOD	DOE	DOJ	DOT	EPA	NASA	NIH	DOC/ NIST	NSF	USDA
Fundamental Research	213.5	20	35				15	15		127	1.5
Biosystems	48.5	5					5	15		22	1.5
Phenomena, structures, and tools	90	15	20				5			50	
Devices and systems	48		10				5			33	
Theory, modeling, and simulation	27		5							22	
Grand Challenges	234.5	116	31.1	1.4	2	5	26	18.8	25.6	9	
Nanostructured Materials by Design	52.5	30	5.1	0.4			10		5	2	
Nanoelectronics, Optoelectronics, Magnetics	92.5	72	5	0.5			9		5	1	
Advanced Healthcare, Therapeutics	19.8							18.8		1	
Environmental Improvement	11		5			5				1	
Energy Conversion/Storage	11	2	9								
Microcraft & Robotics	7						7				
CBRE Protection/Detection (was Bionanodevices)	15.5	12		0.5	2					1	
Instrumentation & Metrology	13.6		2						10.6	1	
Manufacturing Processes	12		5						5	2	
Centers/Networks	91	37	15				5			34	
Infrastructure*	51	5	10					5	10	21	
Societal and Education**	14	2						2	2	8	
TOTAL	604.4	180	91.1	1.4	2	5	46	40.8	37.6	199	1.5

Table C.7
Proposed FY 2003 NNI Investments by Agency

Topic / Agency	NNI total	DOD	DOE	DOJ	DOT	EPA	NASA	NIH	DOC/ NIST	NSF	USDA
Fundamental Research	227.5	20	35				15	15		140	2.5
Biosystems	50.5	5					5	15		23	2.5
Phenomena, structures, and tools	94	10	20				5			59	
Devices and systems	53	5	10				5			33	
Theory, modeling, and simulation	30		5							25	
Grand Challenges	266.7	136	31.3	1.4	2	5	27	21.2	31.8	11	
Nanostructured Materials by Design	62.5	40	5.3	0.4			10		4.8	2	
Nanoelectronics, Optoelectronics, Magnetics	96.5	79	5	0.5			9		2	1	
Advanced Healthcare, Therapeutics	22.3							21.2		1	
Environmental Improvement	11		5			5				1	
Energy Conversion/Storage	12	2	9							1	
Microcraft & Robotics	8						8				
CBRE Protection/Detection (was Bionanodevices)	19.5	15		0.5	2					2	
Instrumentation & Metrology	23		2						20	1	
Manufacturing Processes	12		5						5	2	
Centers/Networks	108	38	23				9			38	
Infrastructure*	92	5	50					5	10	22	
Societal and Education**	16	2						2	2	10	
TOTAL	710.2	201	139.3	1.4	2	5	51	43.2	43.8	221	2.5

NNCO Budget Proposal for FY 2003

Estimated: \$1 million

Budget (\$K)
(One Year – 1 January to 31 December)

By Function	
Support to NSET (staff, travel, operating)	310*
Implementation plan and five-year plan integration	
Integration, proofing, printing and distribution of reports	
Response to inquiries on NNI	
External Appraisal (NRC)	200
Homepage revision/updates (NCO contractor, AMPTIAC,)	60
Database development (staff, operating)	130
(NSET requests, meeting calendar,	
funding programs, academic centers,	
government laboratory centers, ...)	
Global awareness (Non-US programs, ATIP)	60
Other: industrial outreach, market assessment, ...	140
Office costs (NSF cost reimbursement)	100
Total	1000

*Anticipated Staff	
Part-time (1/2) Technical Director (with travel)	130
Full-time Assistant (for database development, document preparation)	150
Part-time (1/2) secretary/receptionist (FT person shared with NCO, IT)	30
Total	310