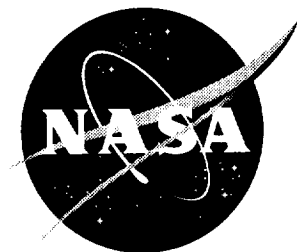


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Nanobiotechnology

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Preface

This document contains the proceedings of the Training Workshop on Nanobiotechnology held at NASA Langley Research Center, Hampton, Virginia, June 14-15, 2000. The workshop was jointly sponsored by the University of Virginia Center for Advanced Computational Technology and NASA. Workshop attendees came from NASA, other government agencies, industry, and universities. The objectives of the workshop were to give overviews of the diverse activities in nanobiotechnology and to identify their potential for future aerospace systems.

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Overview of Nanobiotechnology

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Outline

The ability to manipulate matter at the atomic and molecular levels is likely to change the way almost everything is designed and made, from computers to engineering systems to objects not yet imagined. For nanometer-scale objects, biological systems provide a rich storehouse of interesting ideas and strategies, and this is why there has been synergistic coupling between nanotechnology and biotechnology. The field of nanobiotechnology is garnering much interest around the world. In January 2000, the President announced the establishment of the National Nanotechnology Initiative and has made it a top priority.

An attempt is made in this overview to define some of the buzzwords and set the stage for the succeeding presentations. This presentation is divided into four parts (see Fig. 1). The first part identifies the major characteristics of future aerospace systems that distinguish them from the current systems. The second and third parts describe the revolutionary and key technologies and future research and learning environments required for the realization of future systems. The fourth part lists the objectives of the workshop and the sources of information about nano and biotechnologies.

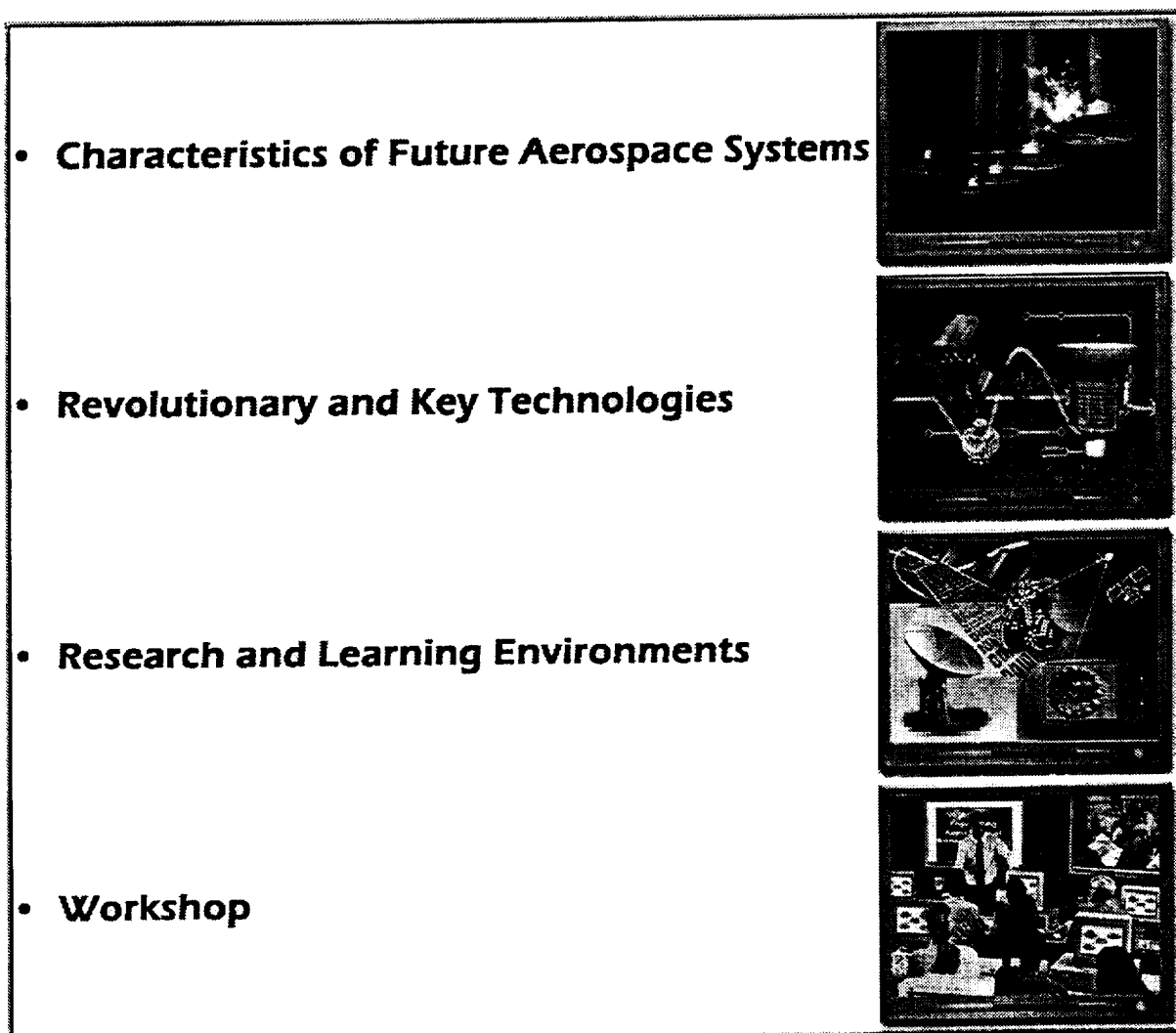


Figure 1

Characteristics of Future Aerospace Systems

The early part of this century will witness a new era of aviation systems, space transportation and space exploration, including sustained in-depth scientific studies performed in increasingly remote environments with very ambitious goals. The realization of these goals with the current national budget constraints will require new kinds of missions and aerospace systems that use novel technologies and manage risks in new ways. Future aerospace systems must be autonomous, evolvable, resilient, and highly distributed (Fig. 2). Space systems must also be able to perform their missions with no (or extremely infrequent) ground support; exploit and use local resources; and routinely close decision loops in real time to handle contingencies and replan mission tasks when necessary.

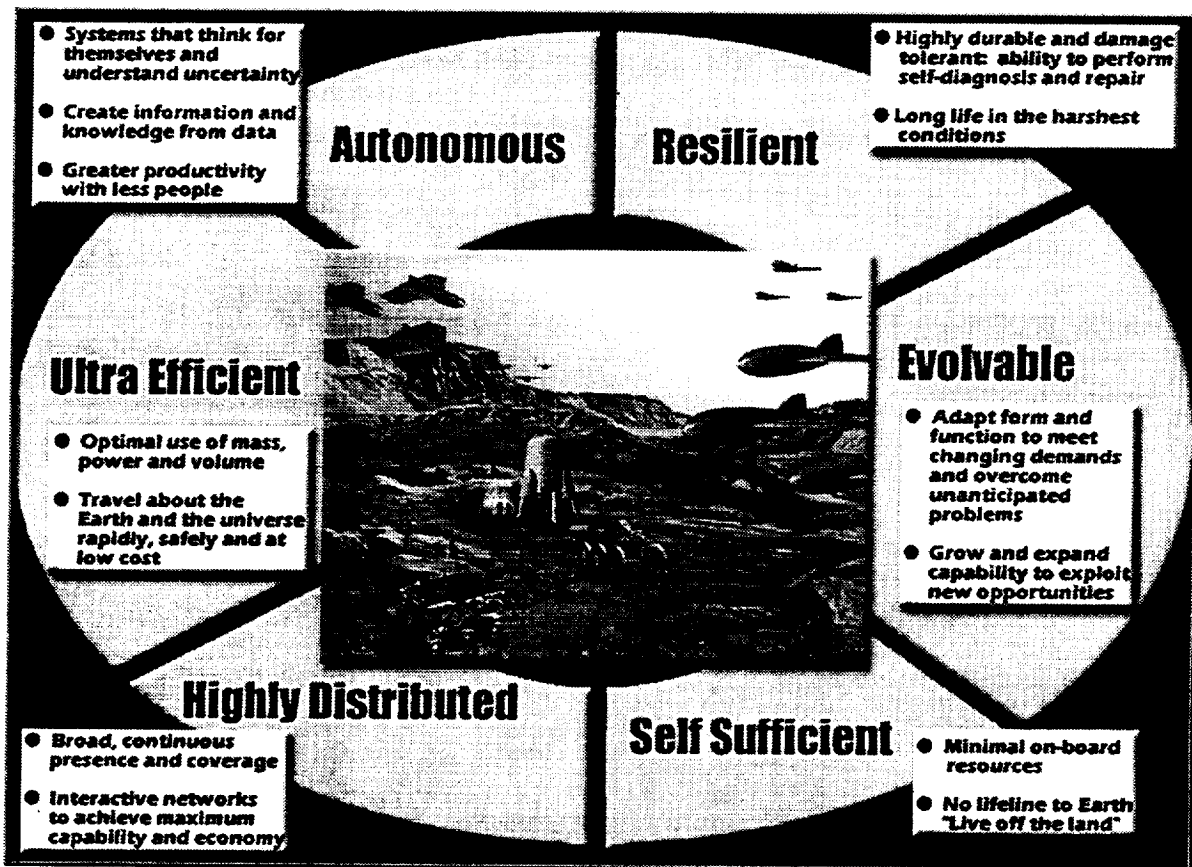


Figure 2

Revolutionary and Key Technologies

The characteristics of future aerospace systems identified in Fig. 2 are highly coupled and require the synergistic coupling of the revolutionary and other leading-edge technologies listed in Fig. 3. The three revolutionary technologies are nanotechnology, biotechnology and information/knowledge technology. The other leading-edge technologies are high-performance computing, high-capacity communication, modeling, simulation and visualization, intelligent software agents, human performance, and human-computer interfaces and communication.

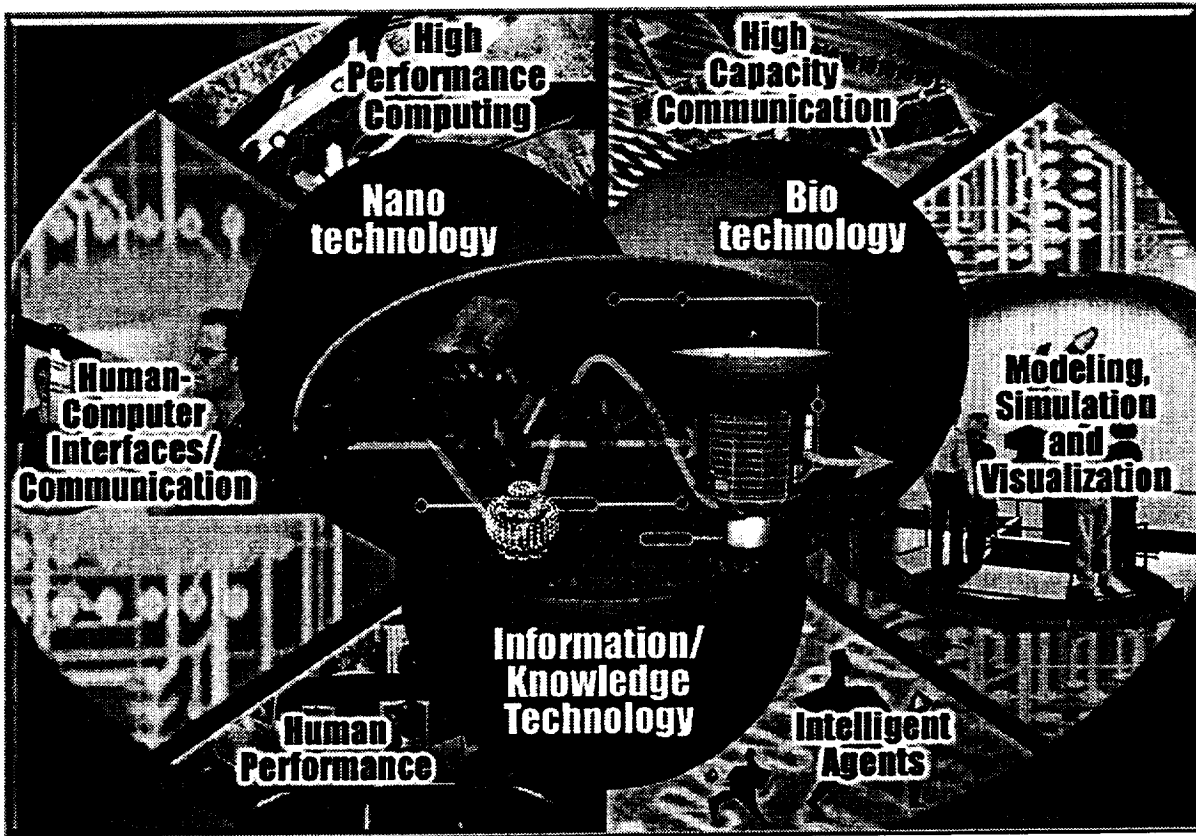


Figure 3

Definition and Evolution of Nanotechnology

The term nanotechnology has often been used to refer to any technique able to work at sub-micron scale. Herein, nanotechnology is defined as an innovative technology aimed at (see Fig. 4):

- Creation of useful materials, devices and systems through the control of matter at the nanometer length (atomic or molecular) scale. This is accomplished by having every atom or molecule in a designed location; and

- Exploitation of novel properties and phenomena developed at that scale.

The utilization of functional structures with at least one characteristic dimension measured in nanometers results in materials and systems that can be rationally designed to exhibit novel and significantly improved physical, chemical, mechanical and electrical properties, phenomena and processes.

The current nanotechnology revolution is a result of the continuing efforts at size reduction and miniaturization, and the development of nanoscience for understanding, visualizing and controlling matter at the atomic and molecular scales (Fig. 4).

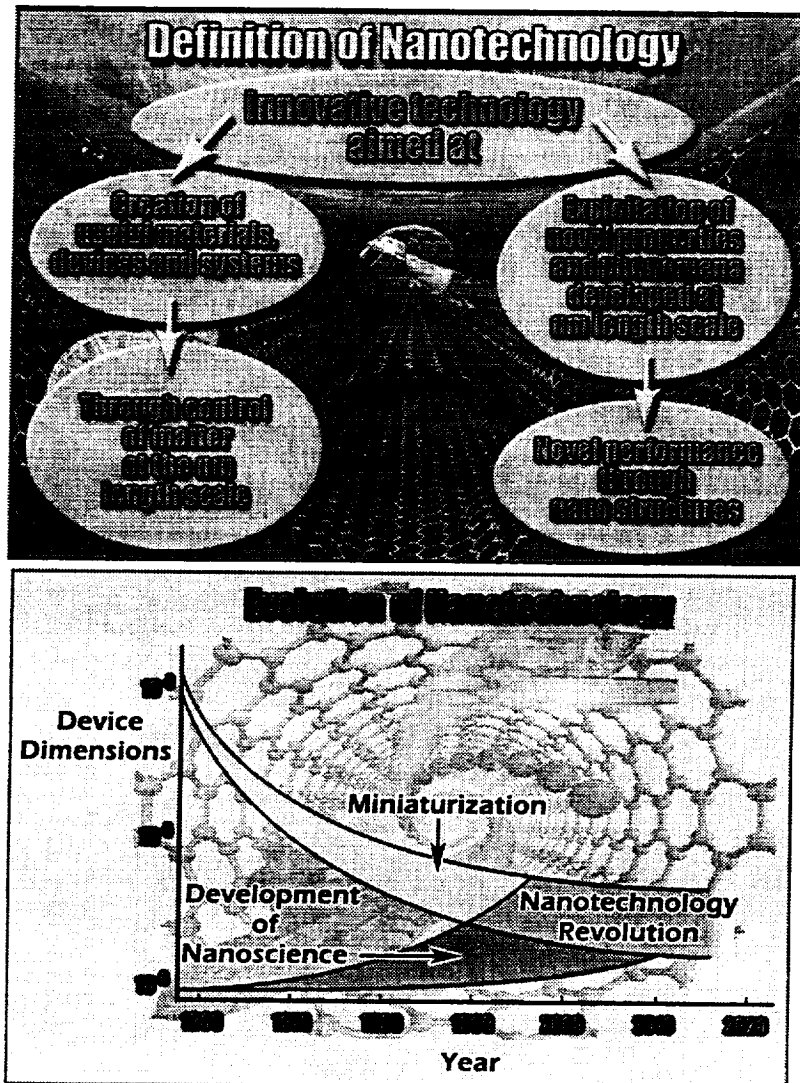


Figure 4

Nanoscale Building Blocks

Figure 5 shows some of the nanoscale building blocks. These are:

- Nanotubes, a new class of molecular-scale fibers with potential mechanical, chemical and electronic applications. The diameter of the nanotube is of nanometer size, and the length can be more than a micrometer. Carbon nanotubes exhibit extraordinary mechanical properties. Young's modulus, over one Tera Pascal, as stiff as diamond, and tensile strength ~ 200 GPa.
- Nanostructured materials are solids composed of structural elements, mostly crystallites, with a characteristic size (in at least one direction) of a few nanometers.
- Ordered nanocavities and nanopore arrays for growth templates.
- Nanoscale particles. These are 1-10 nm in diameter, and are made up of from 10 to 10,000 atoms. Their properties are different from either atoms or the bulk material.
- Molecular building blocks for self-assembling materials.

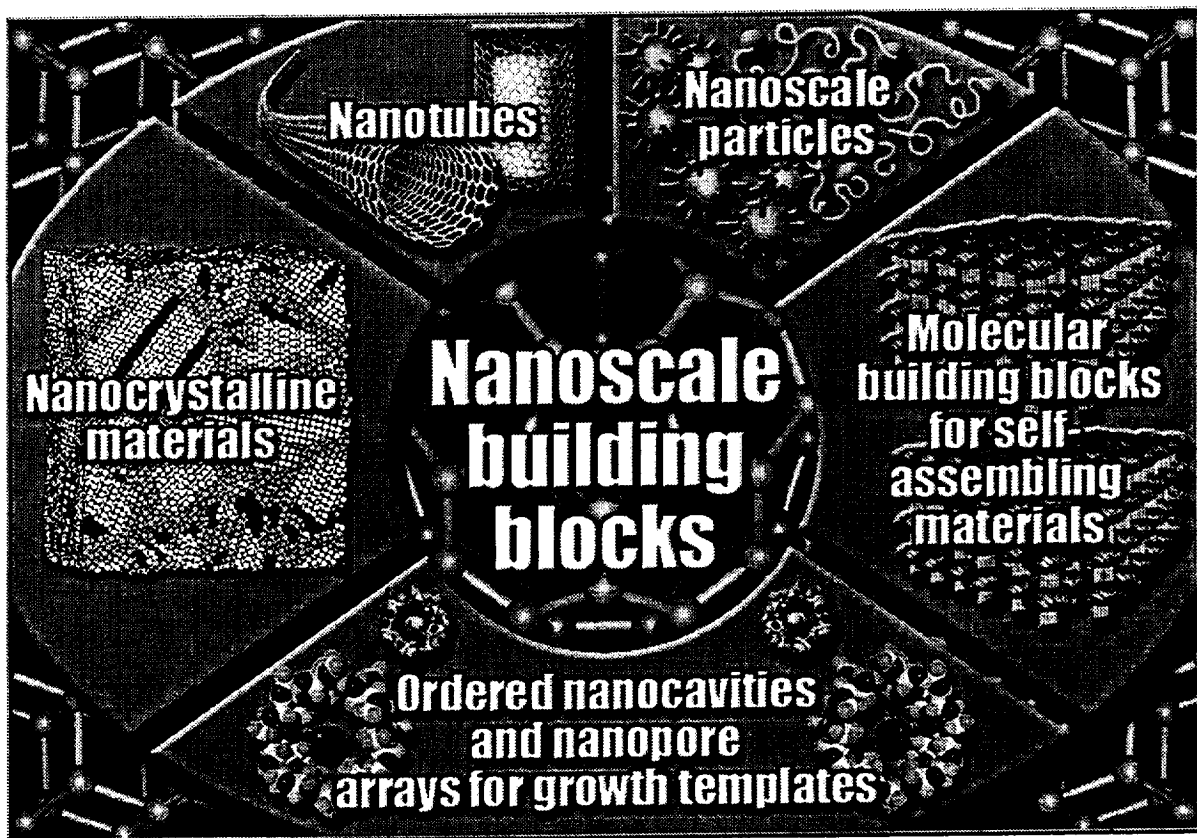


Figure 5

Nanoscale Tools

The nanoscale tools can be grouped into three categories (Fig. 6):

- Detection, imaging (atomic resolution) and characterization.
- Fabrication and manipulation.
- Modeling and simulation, including atomistic-scale modeling and molecular dynamics simulations. Scanned probe microscopy enabled viewing and moving atoms.

The devices that image, characterize nanoscale materials and move them (provide programmable positional control) are:

- Scanning Tunneling Microscope (STM) - used for characterization of nanoscale materials.
- Atomic Force Microscope (AFM) - used for characterization of nanoscale materials.
- Scanning Probe Microscope (SPM) - used for imaging individual atoms and molecules, manipulating and arranging them one at a time.

Because of the interdisciplinary nature of these activities, it is anticipated that future research will involve collaboration between geographically dispersed teams.

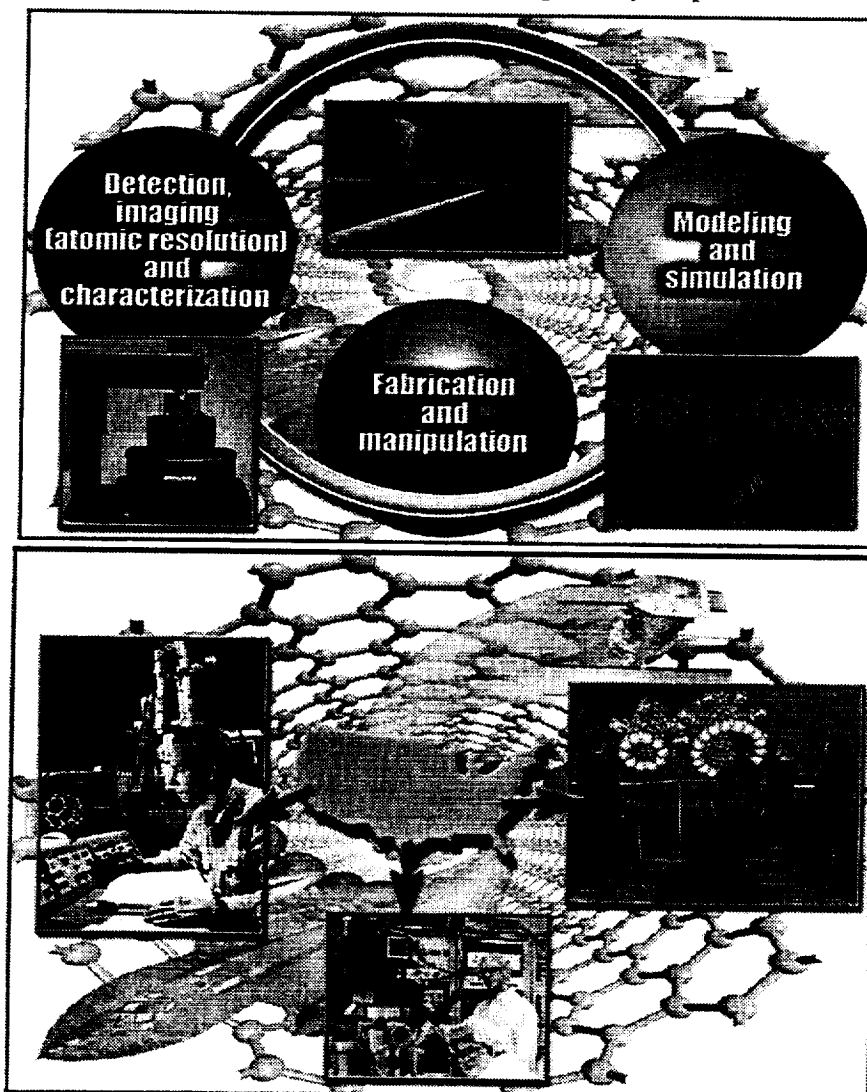


Figure 6

Development of Nanostructure Materials, Devices and Nanosystems

The use of nanoscale tools and nanoscale building blocks will enable the development of nanostructured materials (e.g., nanostructured metals, composites and ceramics, active and self-repairing materials); nanostructure devices (e.g., inexpensive tiny fast computers, sensors and actuators); and eventually low-cost nanosystems (e.g., diamondoid structured vehicles that can carry substantially more payload - Fig. 7).

Among the challenges to be met in realizing these goals are:

- Synthesis of materials by design.
- Determination of the nanoscale initiatives of materials failure.
- Development of cost effective and scalable production techniques.

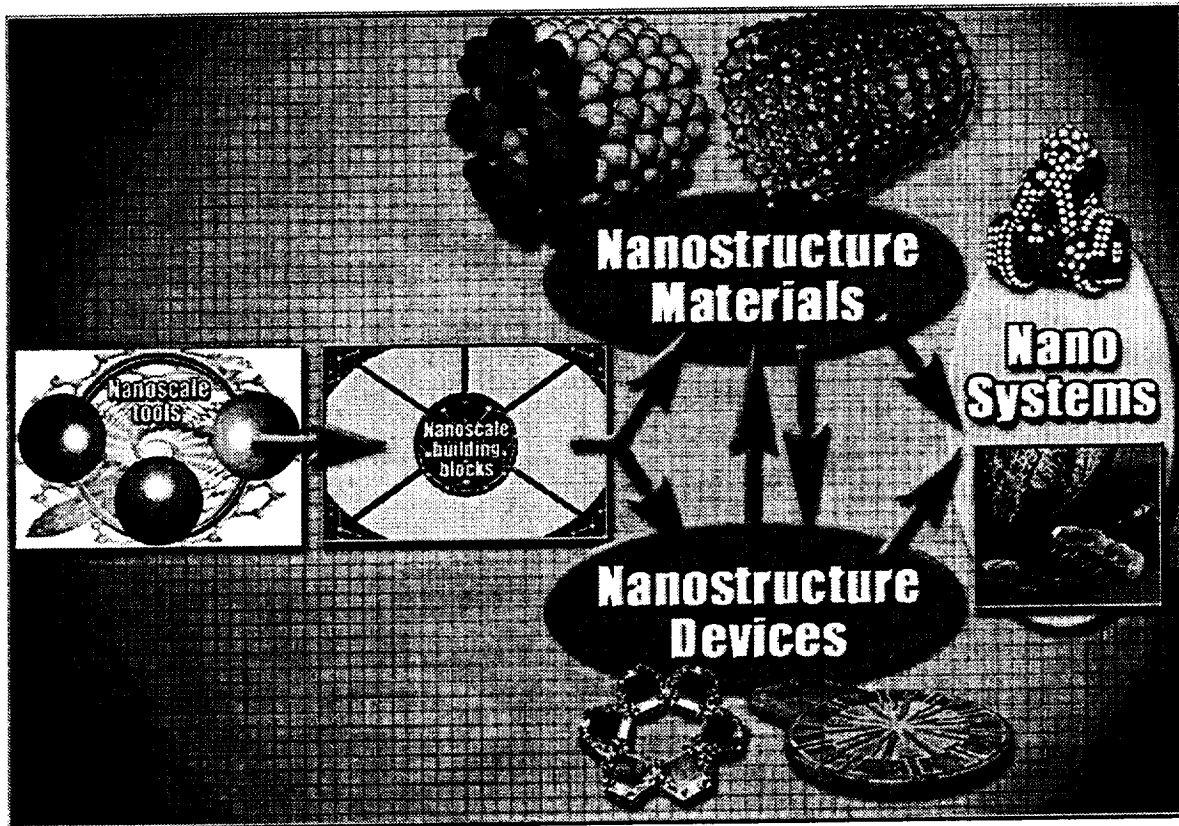


Figure 7

Enabling Technologies/Challenges

Among the enabling technologies/challenges for the development of nanotechnology are (see Fig. 8):

- Characterization and chemical analysis at finer size scales.
- Manipulation of matter at the atomic/molecular scale.
- Multiscale modeling of nanostructuring, from atomic to mesoscopic to macroscopic level, and the resulting material properties at each of these levels.
- Control of nanostructure size and size distribution.
- Roles of surfaces and interfaces in nanostructured materials.
- Thermal, chemical and structural stability of nanostructured materials and devices in the face of temperature and other environmental changes.
- Reproducibility and scalability of nanoparticle synthesis and consolidation processes.

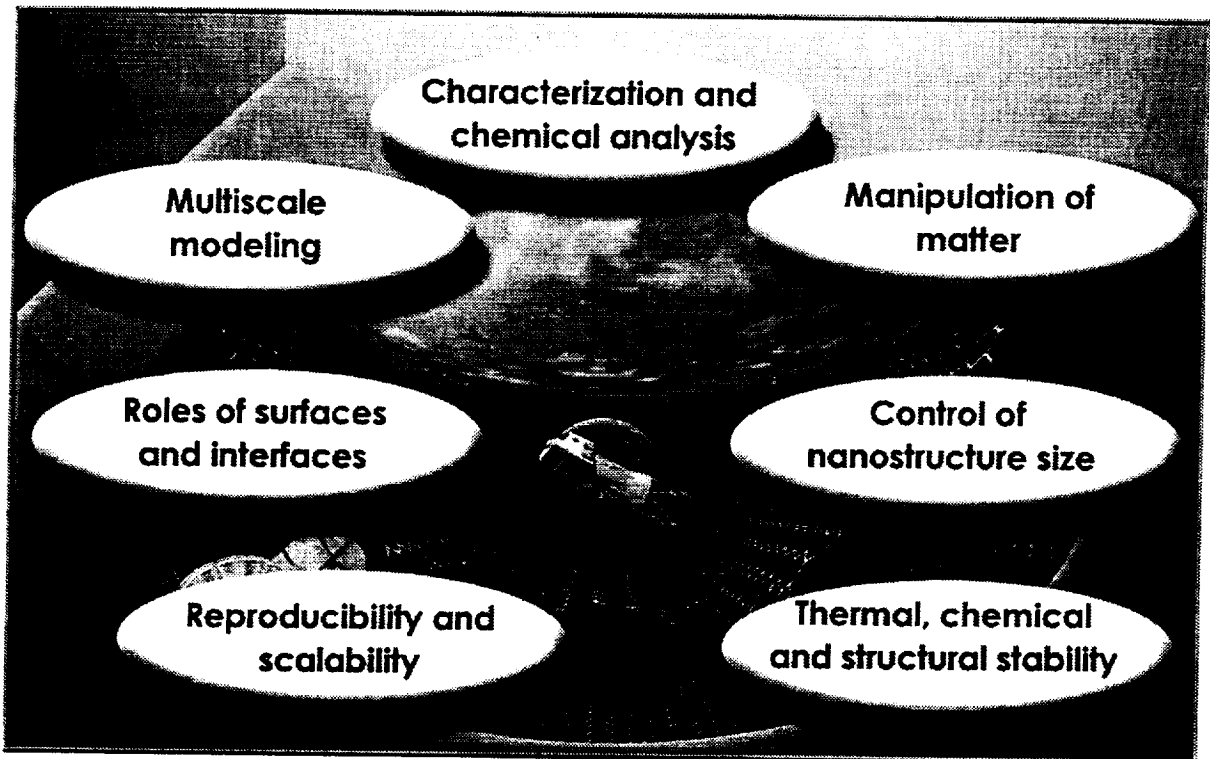



Figure 8

Definition of Biotechnology

Since biology can be viewed as a way of making things work on a very small scale, biotechnology can be defined as the application of biological knowledge and techniques to produce innovative engineering materials, devices and systems (Fig. 9). Biology does not just supply a metaphor, but an actual implementation technology for engineering systems.

Definition of Biotechnology

- Application of biological knowledge and techniques to produce innovative engineering materials, devices and systems.



- Biology is not just used as a metaphor, but as an actual implementation technology for engineering systems.

Figure 9

Hierarchical Biological Structures

The hierarchical biological structures are shown in Fig. 10, starting with the carbon atom as the chemical building block of all matter. Next comes the molecule (e.g., ATP - Adenosine Triphosphate) which is a group of atoms with specific properties. Molecules are collected into organelles (10 ~ 100 nm in size). Organelles are collected and work together in cells, which are the basic units of life. Cells aggregate into tissue. The next level is the organ, which is the structure in an organism performing a specific function. The organism (e.g., fish) is a living entity. A localized group of organisms of the same species form a population. Interacting populations form a community. Future robotic and robotic-human outposts can be thought of as communities in the same sense.

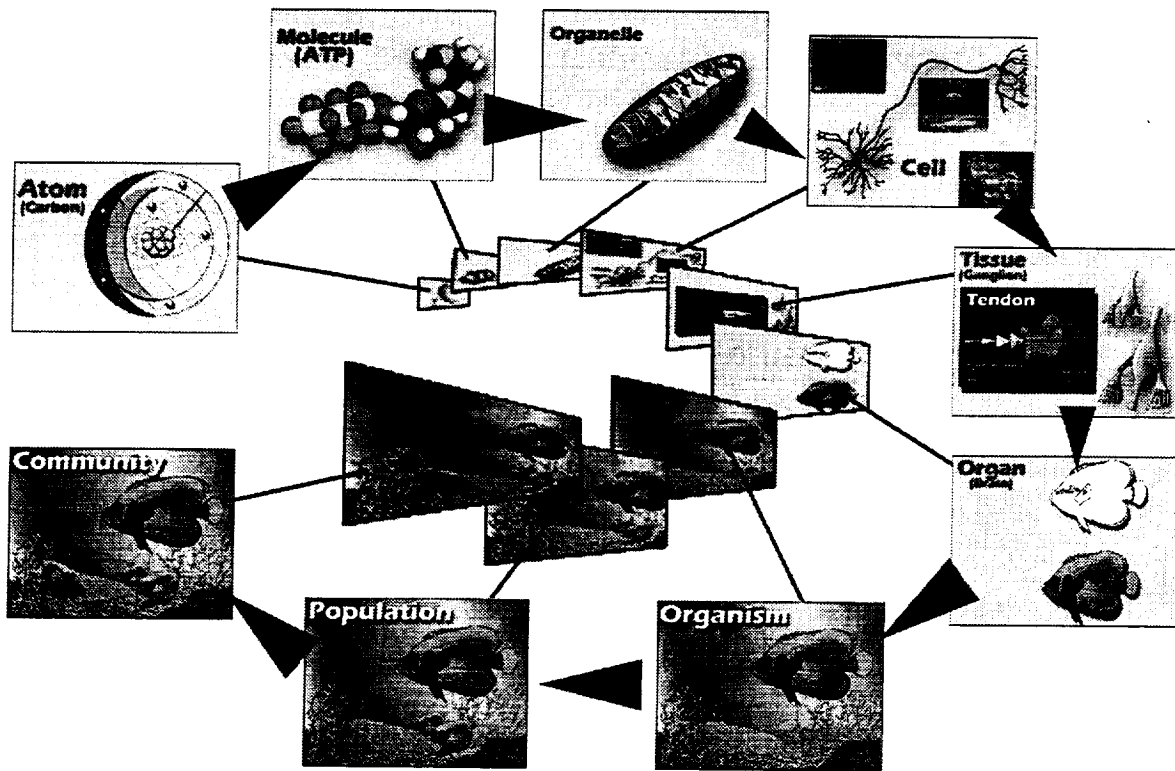


Figure 10

Examples

Three examples of application of biotechnology are shown in Fig. 11:

- Biomolecular materials are designed to have molecular-level properties and characteristics, such as self-assembly of biological materials.
- Biosensors that combine a biological recognition mechanism with a physical transduction technique.
- Chemical and biochemical computers that process information by making and breaking chemical bonds. They store logic states of information in the resulting chemical (i.e., molecular) structures. Examples of biochemical computers are DNA-based and protein-based computers.


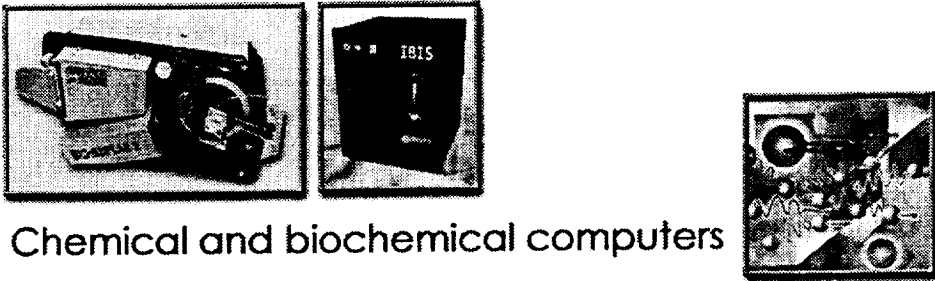
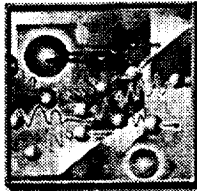
- Biomolecular materials - designed to have molecular-level properties and characteristics (e.g., self-assembly) of biological materials.

- Biosensors - combine a biological recognition mechanism with a physical transduction technique.

- Chemical and biochemical computers


Figure 11

Three Levels of Biotechnology Applications

Three levels of biotechnology applications can be identified (Fig. 12):

- The first is to mimic biological systems (both animal and plant). Applications include: nanoscale, intelligent biologically inspired sensors and instruments (neuromimetic silicon chip - biologically inspired object tracking systems, fully integrated visually aware system - eye-brain module of a thinking spacecraft); and biorobots (robotic systems that are designed as models of particular biological systems).

- The second is to embed biological elements to create hybrid systems. An example of that is a hybrid nanomechanical device (integration of biological motors with NEMS).

- The third is to create fully biological and life like systems. Examples include embryological electronics (with reproduction, adaptation and evolution); protective sensitive material for radiation shielding; and highly intelligent structures that design themselves.


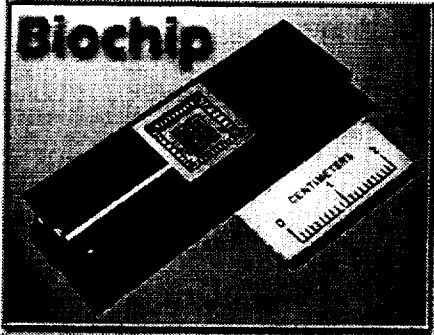
- Mimic biological systems 
- Embed biological elements to create hybrid systems (e.g., hybrid nanomechanical devices - integration of biological motors with NEMS)
- Create fully biological and life-like systems.
Examples:
 - Embryological electronics, with reproduction, adaptation and evolution
 - Highly intelligent structures that design themselves

Figure 12

Biomimetics

Biomimetics refers to mimicking biological synthesis in producing man-made materials. This technology aims at developing novel synthetic materials by understanding and exploring the processes with natural (biological) structural systems employed to build strong and durable structures. This requires knowledge of how biological organisms organize, create, and synthesize systems with smart functions (systems that contain inherent receptors for information).

Some of the unique characteristics of biological systems that are important for future aerospace systems (Fig. 13) are:

- Multi-functionality. Individual components participate in more than one function. This is manifested by the integration of material capabilities, structural and functional requirements.

- Hierarchical organization. A tendon, for example, which serves as a link between muscle and bone, has a very complex structure.

- Adaptability. A bone adapts slowly to a change in loading by changing its own mass and microstructure while maintaining its primary function.

- Self-healing/self-repair.

- Durability.

One of the important characteristics of biologically structured systems is that they do not distinguish between materials and structures. The design and development of natural organisms is an integrated process in which component functions are multiple, and result in a cost effective and durable structure whose performance matches the demands brought upon the living system.

- Mimicking biological synthesis in producing human-made materials
- Some unique characteristics
 - Multifunctionality
 - Hierarchical organization
 - Adaptability
 - Self-healing / Self-repair
 - Durability


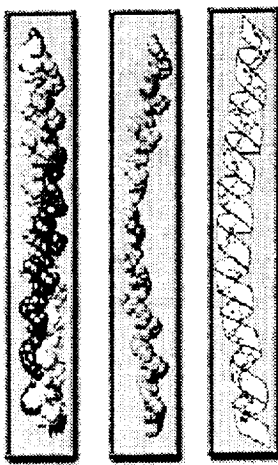


Figure 13

Engineering Applications of Nanobiotechnology

Realizing the potential of nanobiotechnology in engineering systems requires multidisciplinary teams of experts in a number of areas (Fig. 14):

- Condensed matter physics/solid state chemistry - to perform the synthesis of more complex molecules.
- Molecular biology - to manipulate with great precision, a wide range of molecular phenomena occurring in living organisms.
- Materials science - to develop stronger, lighter, more useful materials.
- Molecular manufacturing - to build better small devices at lower cost.
- Engineering disciplines - to create innovative device and system concepts.

The integration of these activities can lead to precise molecular control, and to building large structures to complex atomic specifications (by direct positional selection of reaction sites).

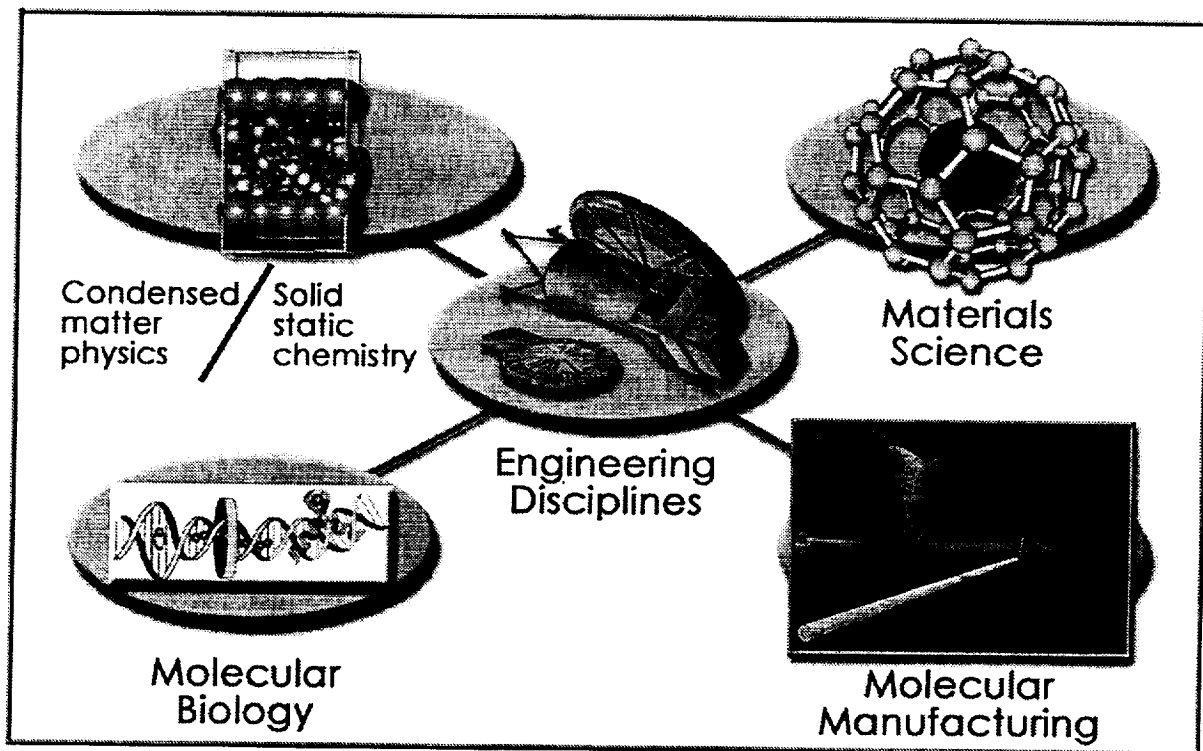


Figure 14

Computing Alternatives Beyond Silicon

The number of transistors per chip has been steadily increasing, in accordance with Gordon Moore's predictions (Moore's Law). It is expected that by 2008, over 16 billion devices will be packaged on a single chip. This means fabricating features that are smaller and smaller. A few years thereafter (2012), the limit of Moore's Law will be reached - one electron per device (Fig. 15). Therefore, in order to continue the trend of miniaturization, alternatives to silicon have to be identified. Among the alternatives being studied are quantum computing (using quantum dots); molecular computing; and biological and DNA computing. All of these alternatives are in the domain of nanobiotechnology.

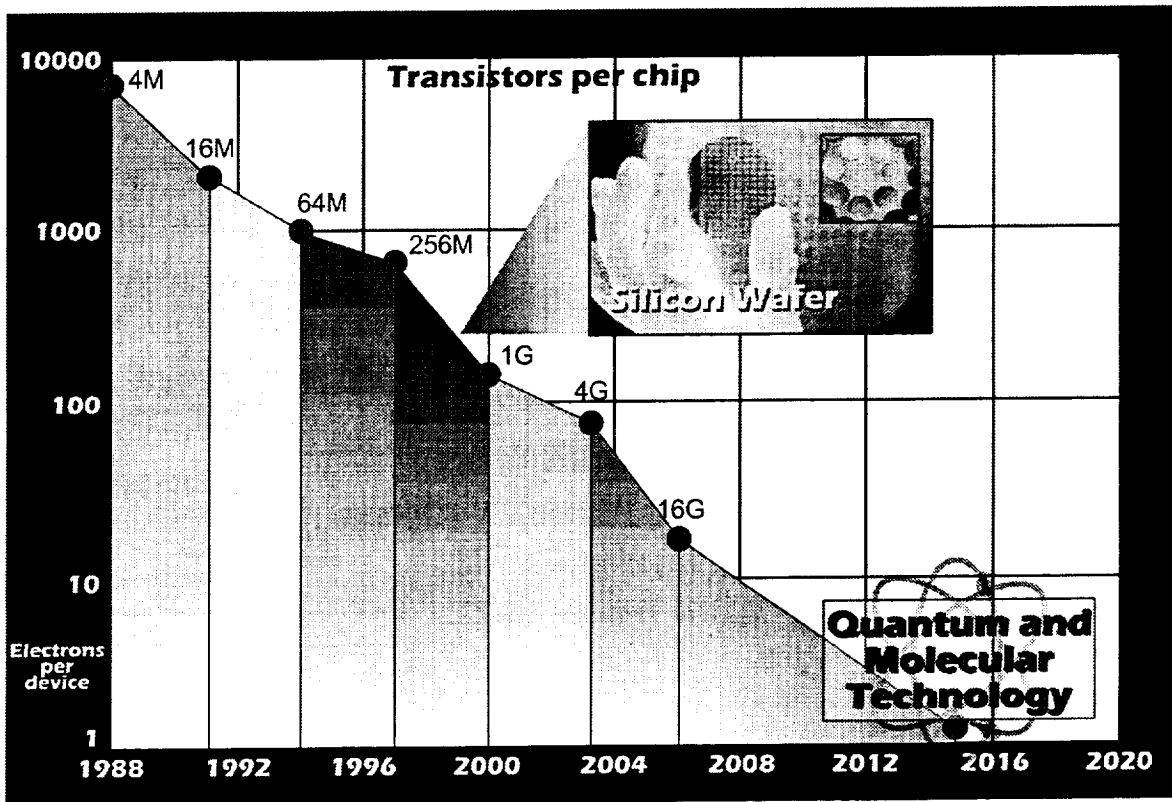


Figure 15

Molecular Electronics (Moletronics)

The field of molecular electronics (moletronics) seeks to use individual molecules to perform functions in electronic circuitry now performed by semiconductor devices. Individual molecules can conduct and switch electric current and store information. Electronic devices constructed from molecules will be hundreds of times smaller than their semiconductor-based counterparts. Figure 16 shows Mark Reed's depiction of a molecular electronic circuit with memory elements and electrical connectors. A general purpose molecular computer has three components: switching device, memory, and interconnects. Examples of the three components are shown in Fig. 16. Moletronics exploits what molecules are good for: self-assembly, thermodynamic equilibrium, and charge storage media.


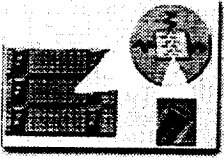
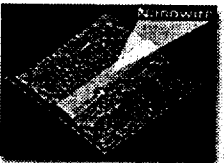

<ul style="list-style-type: none">• Individual molecules can<ul style="list-style-type: none">- Conduct and switch electric current- Store information	
<ul style="list-style-type: none">• General-purpose molecular computer has<ul style="list-style-type: none">- Switching device (like a transistor)- Memory- Interconnects (connecting arbitrarily large numbers of devices and memory elements)	 
<ul style="list-style-type: none">• Moletronics exploits what molecules are good at<ul style="list-style-type: none">- Self assembly- Thermodynamic equilibrium- Charge storage media	

Figure 16

Current State and Potential of Moletronics

In July 1999, researchers from Hewlett Packard and the University of California at Los Angeles built an electronic switch consisting of a layer of several million molecules of an organic substance called rotaxane. The device had only two terminals. Complex logic circuits require more than two terminals.

Although at the present time no methods exist for connecting large numbers of devices, moletronics has the potential for overcoming physical limitations associated with feature size reduction, power consumption, switching speed and cost of foundry (Fig. 17).

- **Current state**
 - Individual molecule switches (with only two terminals) and memory elements. Complex logic circuits require more than two terminals
 - No methods exist for connecting large numbers of devices

- **Has potential for overcoming physical limitations:**
 - Feature size reduction
 - Power consumption
 - Switching speed
 - Cost of foundry

Figure 17

Teramac Configurable Custom Computer

Teramac is a one Tera Hertz massively parallel experimental computer built at Hewlett Packard Laboratories to investigate a wide range of computational architectures (Fig. 18). It is constructed with conventional silicon integrated circuit technology, but many of its problems are similar to challenges faced by nanoscale computing paradigms. It contains 220,000 (3%) hardware defects, any one of which could prove fatal to a more conventional machine. It incorporates a high communication bandwidth that enables it to easily route around defects. It operates 100 times faster than a high end single processor workstation (for some of its configurations). It demonstrates that it is not necessary to chemically synthesize devices with a 100% yield and assemble them into a completely deterministic network in order to obtain a reliable and powerful system.

Teramac Configurable Custom Computer

- **Massively parallel experimental computer built at Hewlett-Packard Labs**
- **Contains 220,000 hardware defects**
- **Incorporates a high-communication bandwidth that enables it to easily route around defects**
- **Operates 100 times faster than a high-end single-processor workstation (for some of its configurations)**

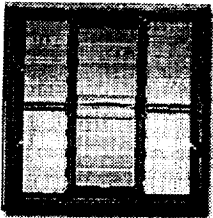

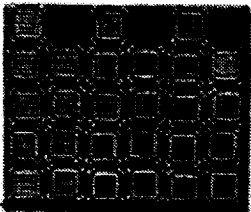
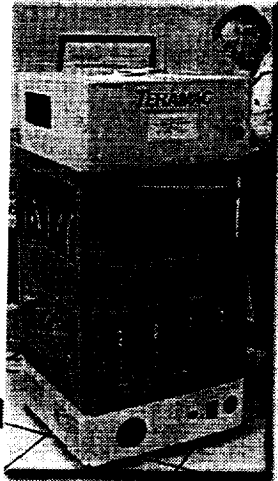


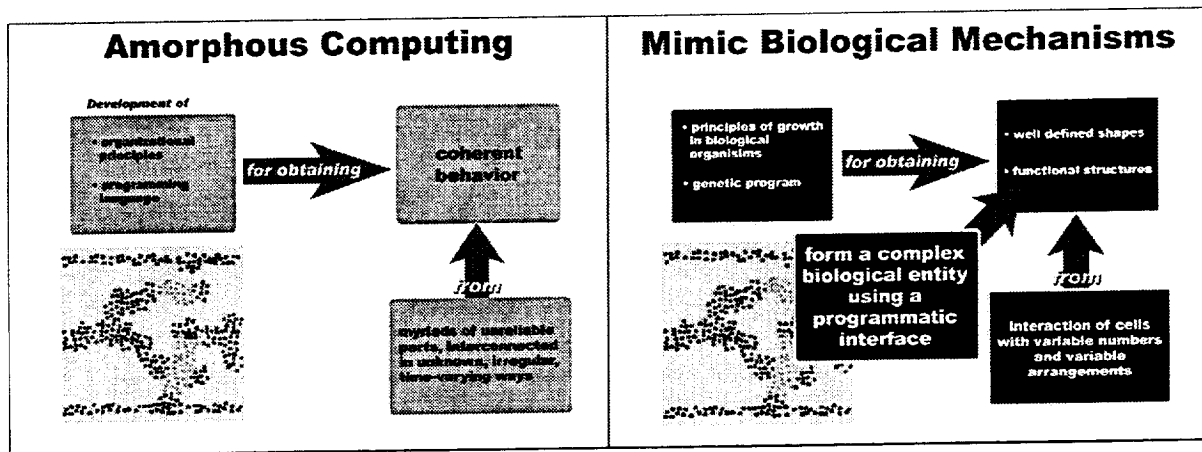
Figure 18

Amorphous Computing Paradigm

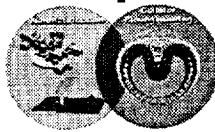
Amorphous computing refers to the development of organizational principles and programming languages for obtaining coherent behavior from a myriad of unreliable parts, interconnected in unknown, irregular time varying ways. This is analogous to the fact that principles of growth in biological organisms and genetic programs are used for generating well defined shapes and functional structures from the interaction of cells with variable numbers and variable arrangements. The basic concept is to mimic the formation of a complex biological entity using a programmatic interface.

Through the integration of nanofabrication and cellular bioengineering, amorphous computing has the potential of:

- Tailor making biological cells to function as chemical factories for the assembly of nanoscale structures.
- Assembling systems incorporating a myriad of information processing units (sensors, actuators and communication devices).
- Mixing these with structural and other materials producing super-intelligent programmable materials (senses and reports on the environment and structural integrity).



Potential of Amorphous Computing



- ➔ **Tailor-making biological cells to function as chemical factories for the assembly of nanoscale structures**
- ➔ **Assembling systems incorporating myriads of information processing units (sensors, actuators, and communication devices)**
- ➔ **Mixing these with structural and other materials produces super-intelligent programmable materials (senses and reports on environment and structural integrity)**

Figure 19

Interagency Working Group on Nanoscience and Engineering (IWGN)

In 1997, the United States conducted 40% of the world's research and development but spent less than 27% on government sponsored nanotechnology research. By contrast, Europe and Japan sponsored 29% and 28% on nanotechnology research. In recognition of the potential impact of nanotechnology on our economy and our society, an interagency working group on nanoscience, engineering and technology (IWGN) has been established. The proposed research and development funding on nanotechnology for FY 01 is \$495 million. IWGN recommended a steady increase of investment, reaching \$2.786 billion in FY 05. NASA's share of the research and development nanotechnology funding in FY 01 is 4%. Among the research areas to be addressed by NASA are nanostructured materials and thin films; nano and bioinspired devices; radiation tolerant electronics; self-healing systems; nanosensors and biomedical nanotechnology.

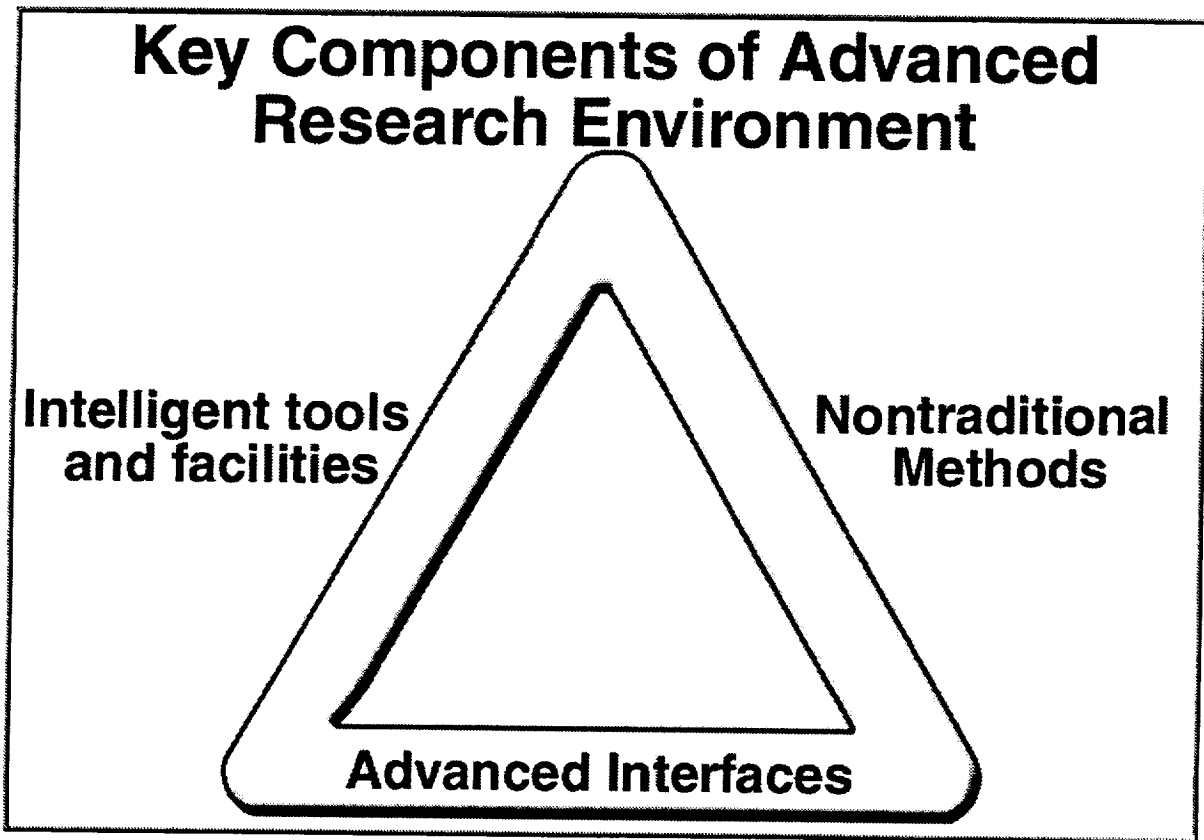


Figure 20

IWGN Grand Challenge Areas

IWGN identified nine grand challenges as essential for the advancement of nanotechnology (as listed in Fig. 21):

- Nanostructured materials include smart multifunctional materials.
- The goal of nanoelectronics is to improve computer speed and efficiency by a factor of millions, increase the memory storage/unit surface area by a factor thousands fold, and increase the communication bandwidth a hundred times.
- Nanostructured and smart materials can potentially build lighter and more efficient transportation vehicles, corrosion free bridges and no-maintenance roads.
- The development of biosensors and new imaging techniques and tiny smart medical devices will contribute to major advances in health care.

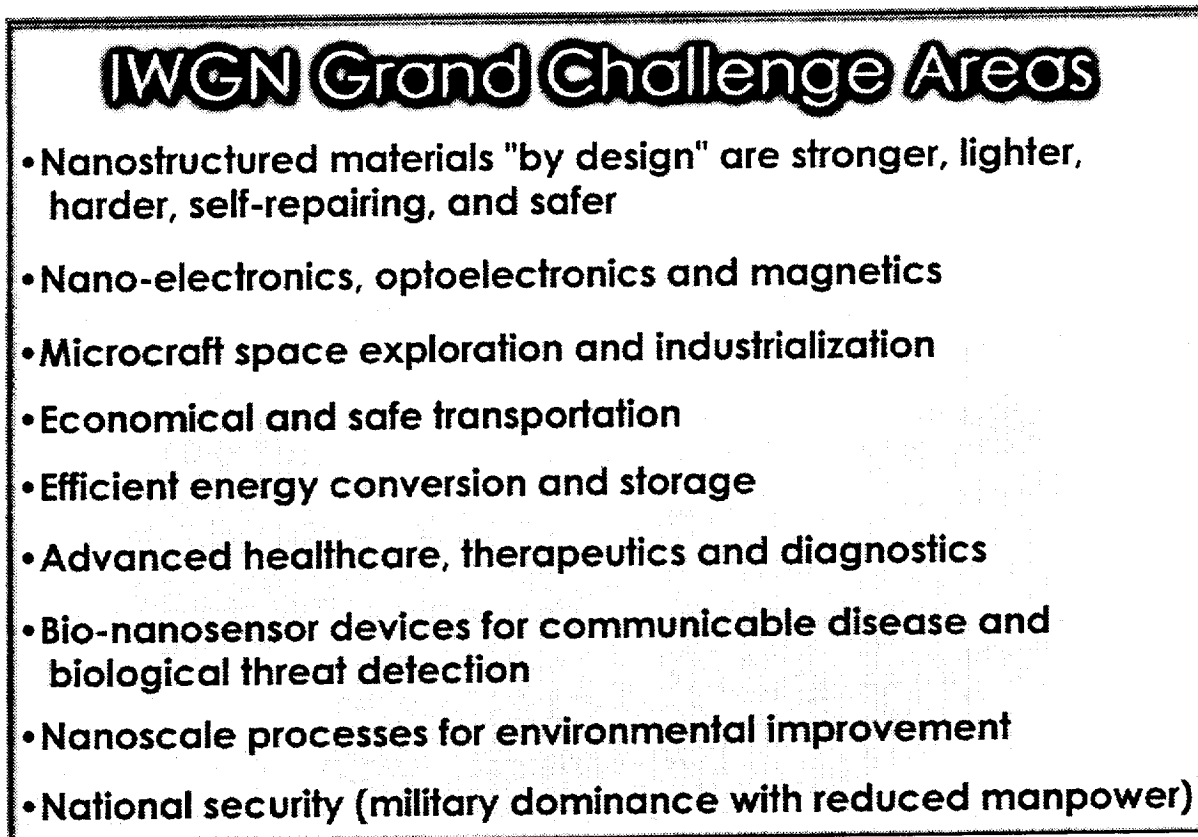


Figure 21

Forces Driving a Change in Research and Learning Environments

After decades of evolutionary change, revolutionary changes are both needed and possible for creating effective research and learning environments. The change is driven by four categories of forces (Fig. 22):

- **Changes in high tech organizations.** Quality was the focus of high tech organizations in the 1980's. In the 1990's, the move from the industrial to the knowledge era shifted the focus to re-engineering and streamlining the processes, and then to managing knowledge and creation of high-performance workplaces. In the future there is likely to be a move to the biological and advanced materials era (referred to as the bioterials era). The focus of high tech organizations will shift to explorations in the cellular and subatomic universe - architecting matter. Facilities will be developed for temporal compression and global diffusion.
- **Economic pressures.** Economic stresses and customer demands for cheaper, better, faster products have driven high tech organizations from mass production to mass customization, and to the adoption of lean production system concepts. They have integrated simulation and design tools with other tools and facilities for lean engineering, manufacturing, and supplier management.
- **Impact of advances in technology.** The synergistic coupling of several leading edge technologies will have a significant impact on future products and engineering systems. To realize the potential of this synergism, high tech organizations will have to provide effective diverse team collaboration facilities and interdisciplinary research networks, as well as a conducive life long learning environment in the workplace.
- **Paradigm change in human/machine/network interaction.** Wireless connectivity among diverse teams and embedded devices, including thousands of embedded nanodevices per person, will become the norm. Consequently, there is a move from human-centered (interactive) computing to human-supervised (proactive) computing. The wireless connectivity will enable the development of virtual interfaces with experiments and fabrication facilities.

Forces Driving a Change in Research and Learning Environments (Cont'd.)

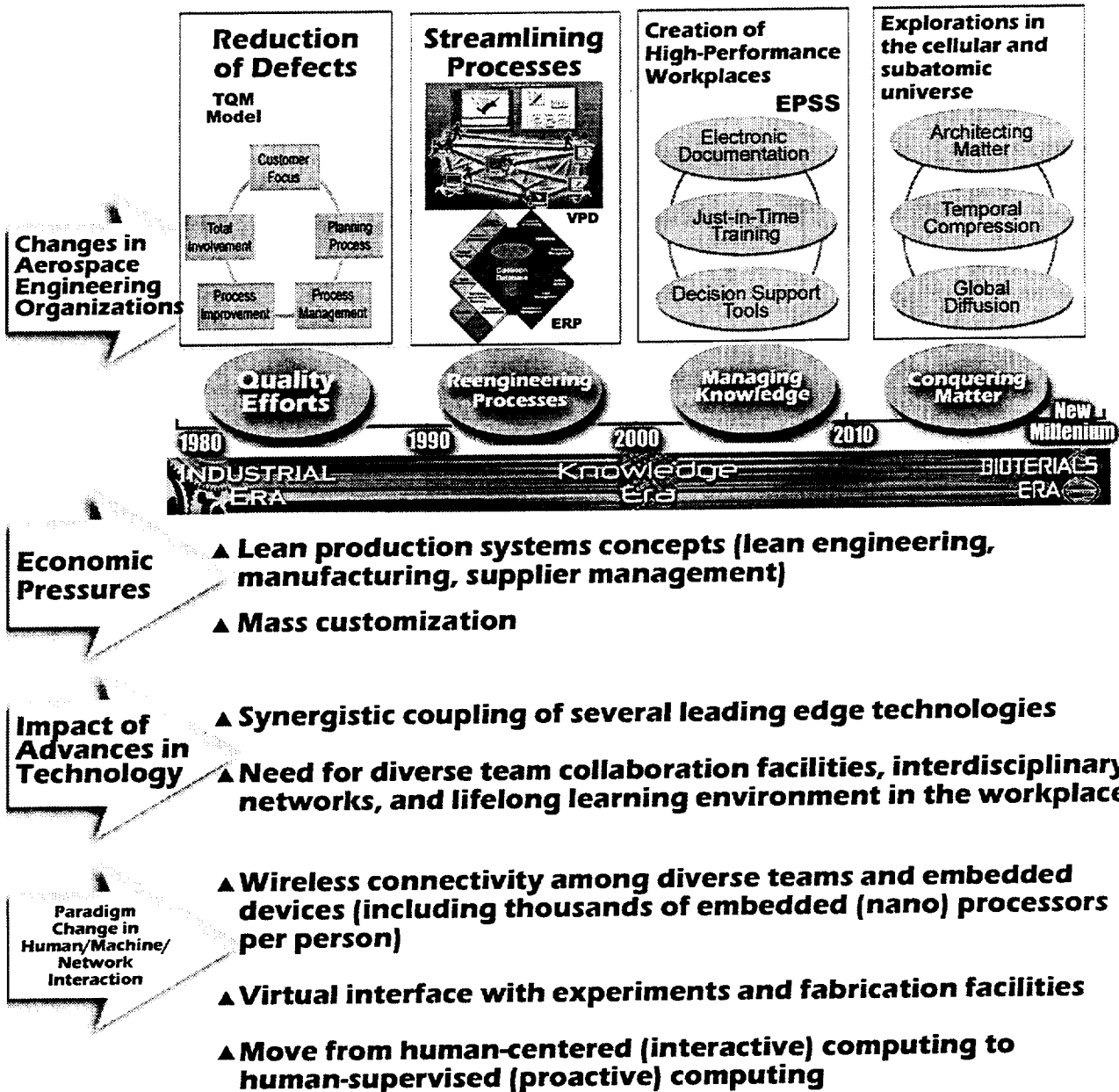


Figure 22

Key Components of Advanced Research Environment

The realization of the full potential of nanobiotechnology in aerospace and other engineering fields requires an advanced research environment that links diverse teams of scientists, engineers and technologists. The essential components of the environment can be grouped into three categories: intelligent tools and facilities, nontraditional methods, and advanced interfaces (Fig. 23).

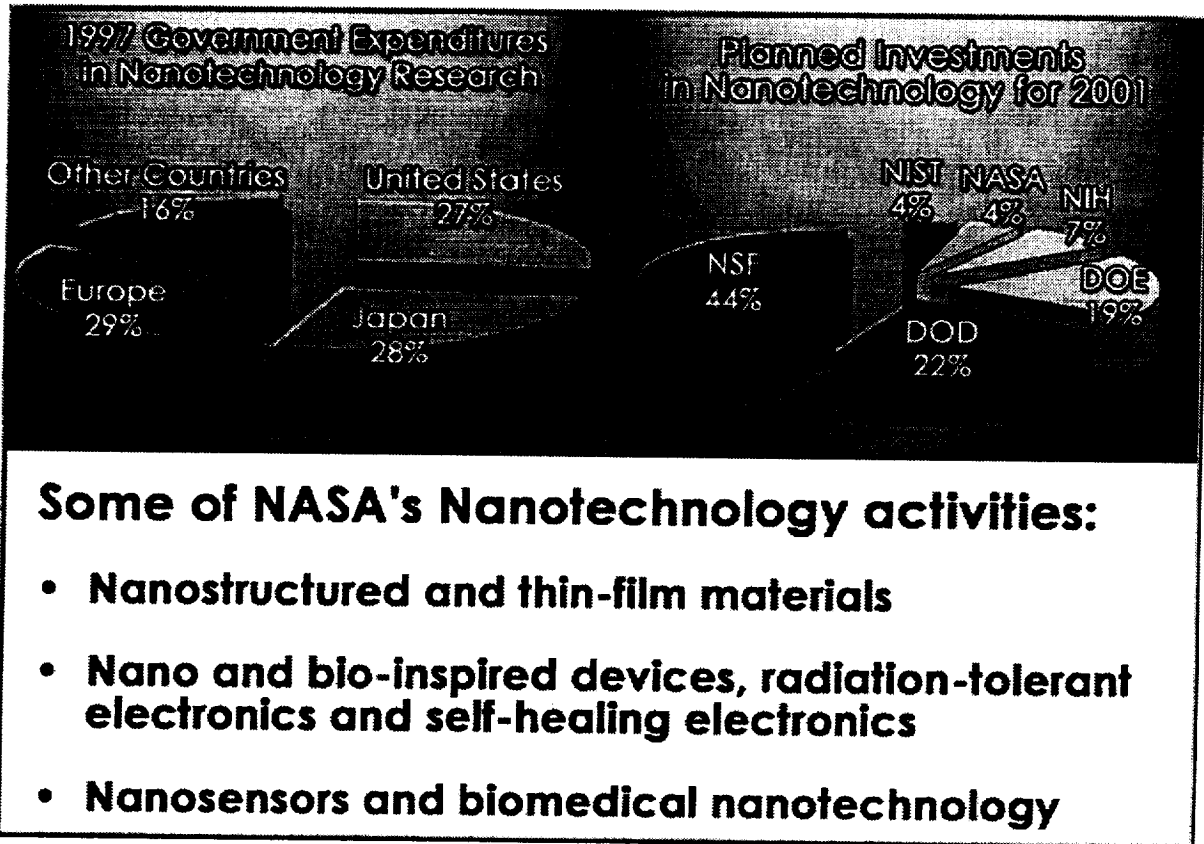


Figure 23

Intelligent Tools and Facilities

These include high fidelity rapid modeling and life cycle simulation and visualization tools; distributed high capacity computing, communications and networking facilities; synthetic immersive environment; automatic and semiautomatic selection of software and hardware platforms; collaborative group support and decision making facilities; computer simulation of physical experiments and remote control of these experiments. The life cycle simulation tools include tools for cost estimation, product assurance, safety analysis, risk management, virtual manufacturing and prototyping, testing for qualification, maintenance and operations, and life cycle optimizations. In all of these tools extensive use should be made of intelligent software agents and information technology (Fig. 24).

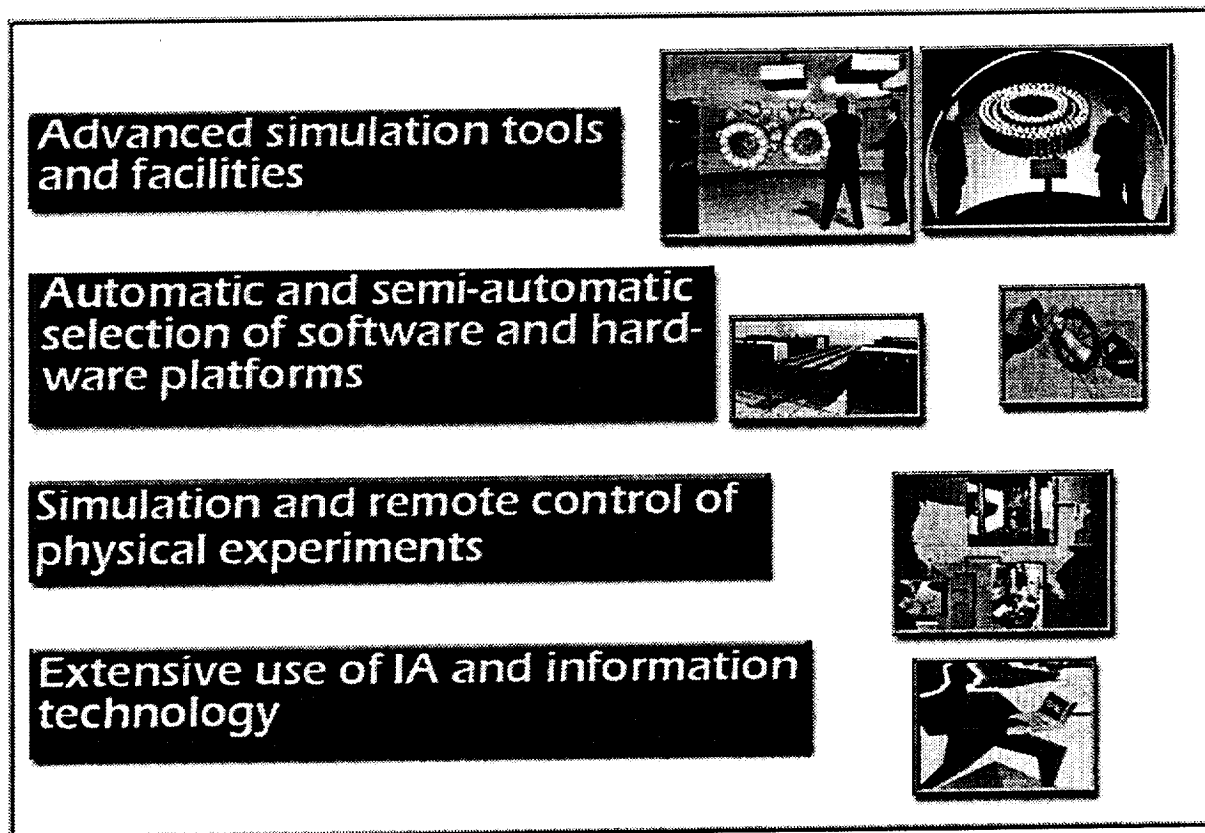


Figure 24

Advanced Human/Computer Interfaces

Although the WIMP (windows, icons, menus, pointer) paradigm has provided a stable and global interface, it will not scale to match the myriad form factors and uses of platforms in the future collaborative distributed environment. Perceptual user interfaces (PUIs) are likely to meet those needs. PUIs integrate perceptive, multimodal and multimedia interfaces to bring human capabilities to bear on creating more natural and intuitive interfaces. They enable multiple styles of interactions, such as speech only, speech and gesture, vision, and synthetic sound, each of which may be appropriate in different applications (Fig. 25). These new technologies will enable broad uses of computers as assistants, or agents, that will interact in more human-like ways.

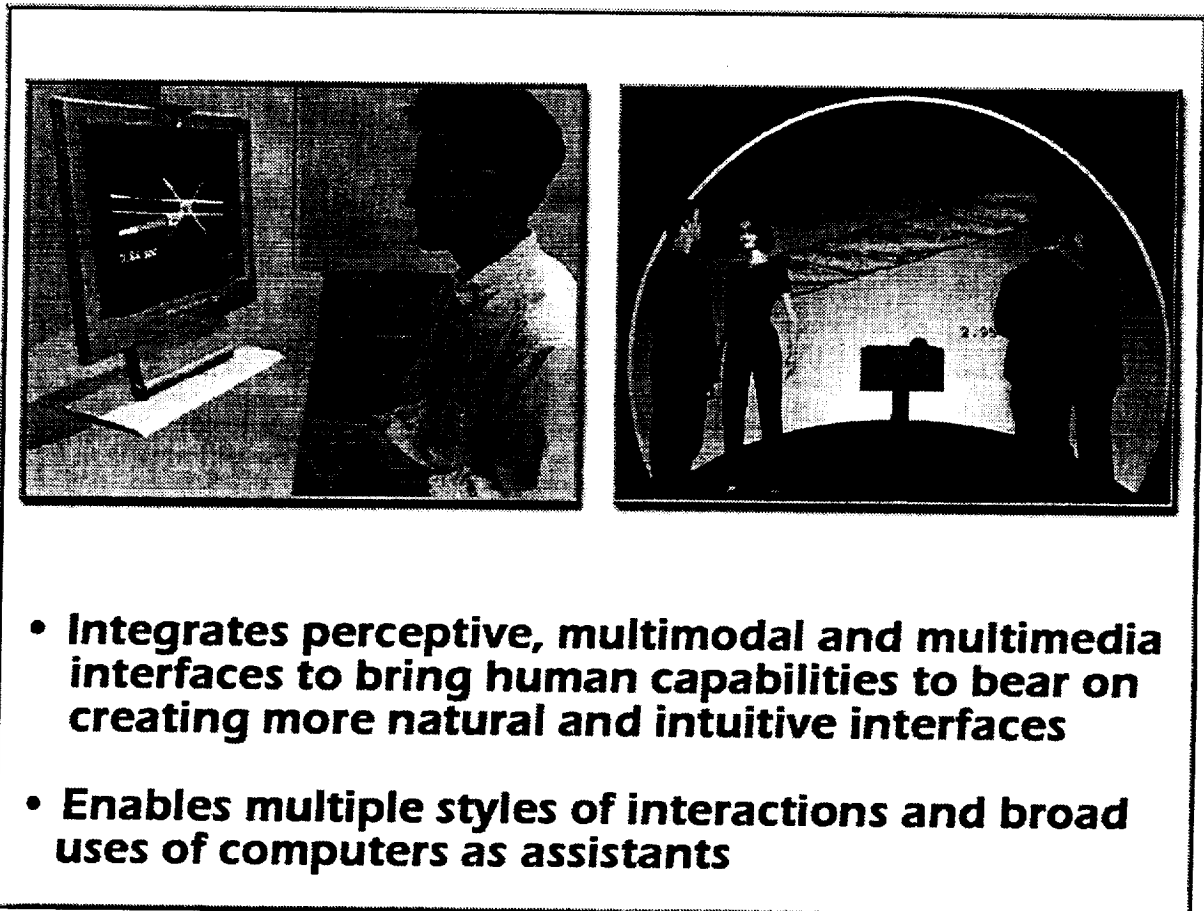


Figure 25

Nontraditional Methods

These include multiscale methods, strategies for highly coupled multiphysics problems, and nondeterministic approaches for handling uncertainty in geometry, material properties, boundary conditions, loading and operational environments (Fig. 26).

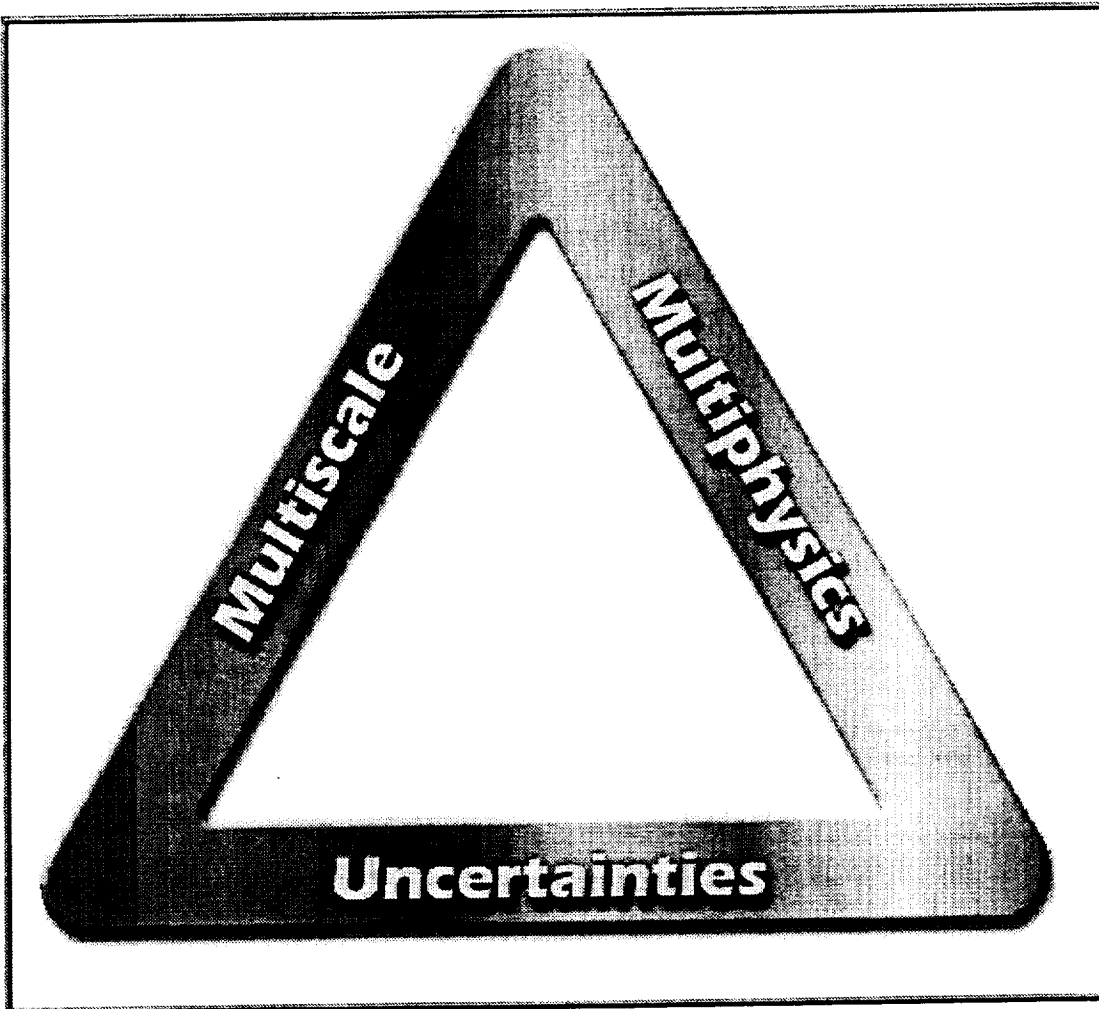


Figure 26

Multiscale Modeling

Multiscale methods integrate disciplinary approaches. Examples are quantum mechanics, molecular dynamics and continuum mechanics for the study of fracture phenomena and molecular robotics; and multiscale material modeling used in computationally driven material development. The hierarchy of material models that has developed is shown in Fig. 27. The models are arranged according to the phenomena they describe and the length scale at which the phenomena are studied (from 10^{-10} m to 1 m). The disciplines involved include computational chemistry (quantum mechanics and molecular dynamics), computational material science, and computational structural mechanics. However, many gaps still exist in the hierarchy of models, and to date no rational way exists to integrate these models and to couple them with experiments in order to relate the phenomena at the very small length scales with the macroscopic behavior. The central paradigm of the computationally driven material development activity is the sequence interrelation of processing, structure, properties, and performance of materials.

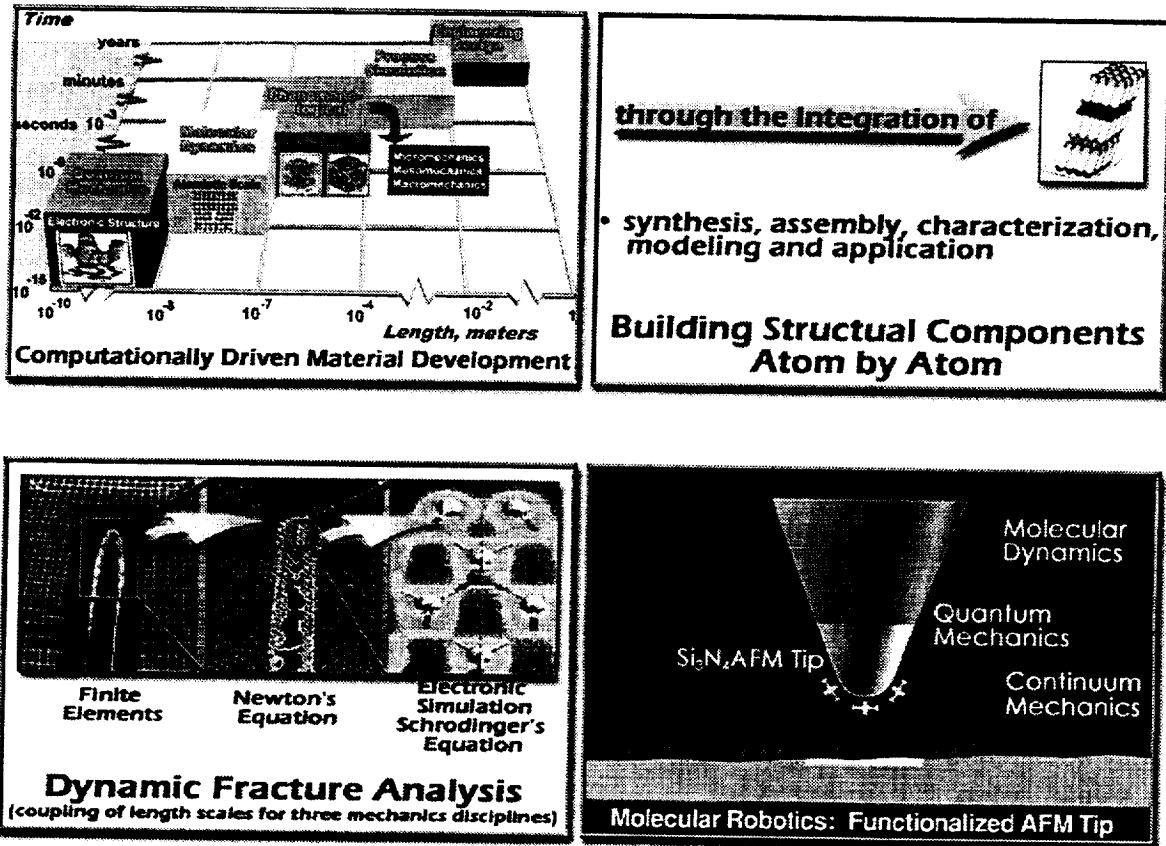


Figure 27

Highly Coupled Multiphysics Problems

Figure 28 shows an example of highly coupled multiphysics problems - the strong couplings between mechanical, electric, thermal and magnetic fields in smart materials. Two general strategies are used for solution of multi-physics problems: the staged solution strategy and the coupled solution strategy.

Staged Solution Strategy. The multiple fields are treated separately. The discrete models for each of the fields may be developed separately. Coupling effects are viewed as information that must be transferred between the discrete models of the different fields. A modification of this strategy is the multistagger solution strategy in which a partial decoupling is made of the full system. The full system of coupled equations is partitioned into smaller subsystems of equations. Each subsystem is solved separately under the assumption that the variables of the other subsystems are frozen (temporarily).

Coupled Solution Strategy. The multiple field problem is treated as an indivisible whole. The discrete models of the different fields are tightly coupled.

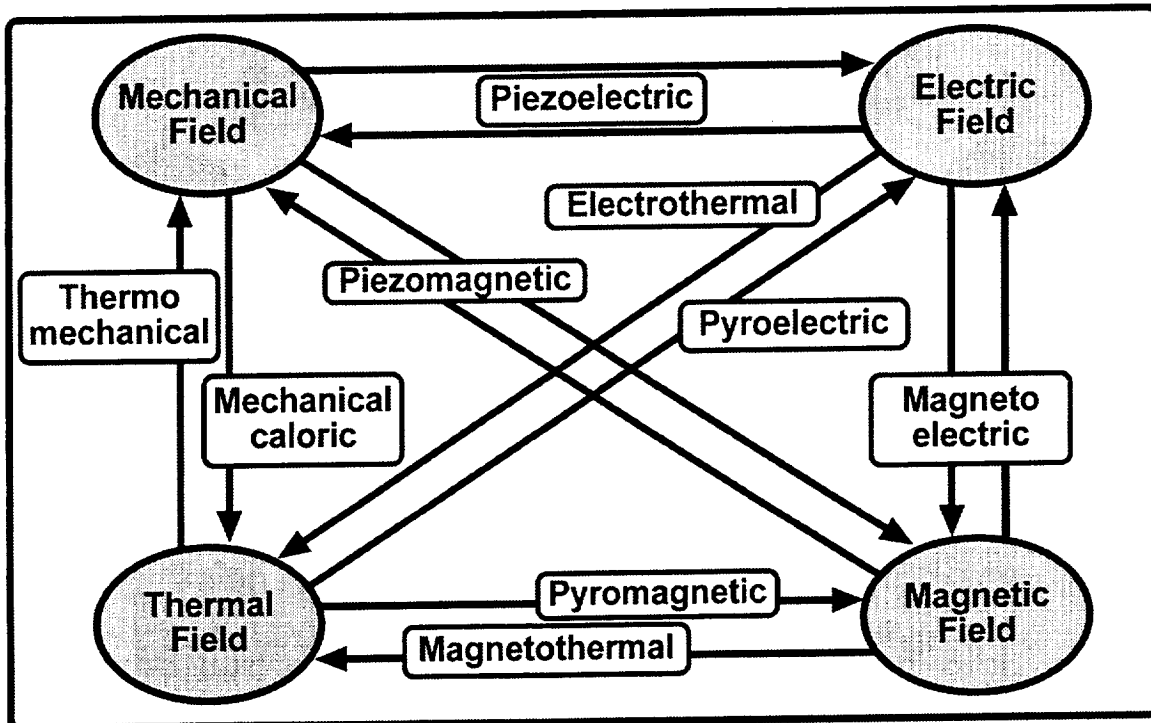


Figure 28

Types and Modeling of Uncertainties

Although it is difficult to list all the sources and kinds of uncertainties, the following five can be identified (Fig. 29):

- Probabilistic uncertainty, which arises due to chance or randomness;
- Resolutionary uncertainty, which is attributed to limitation of resolution (e.g., sensor resolution); and
- Fuzzy uncertainty, due to linguistic imprecision (e.g., set boundaries are not sharply defined).
- Uncertainty due to limited information available about the system (for example, in the early stages of the design process).
- Model uncertainty, which is attributed to lack of information about the model characteristics.

Some of the aspects of modeling uncertainty are listed in Fig. 29 below. The impact of these uncertainties on the reliability and certification of future systems are among important research areas.

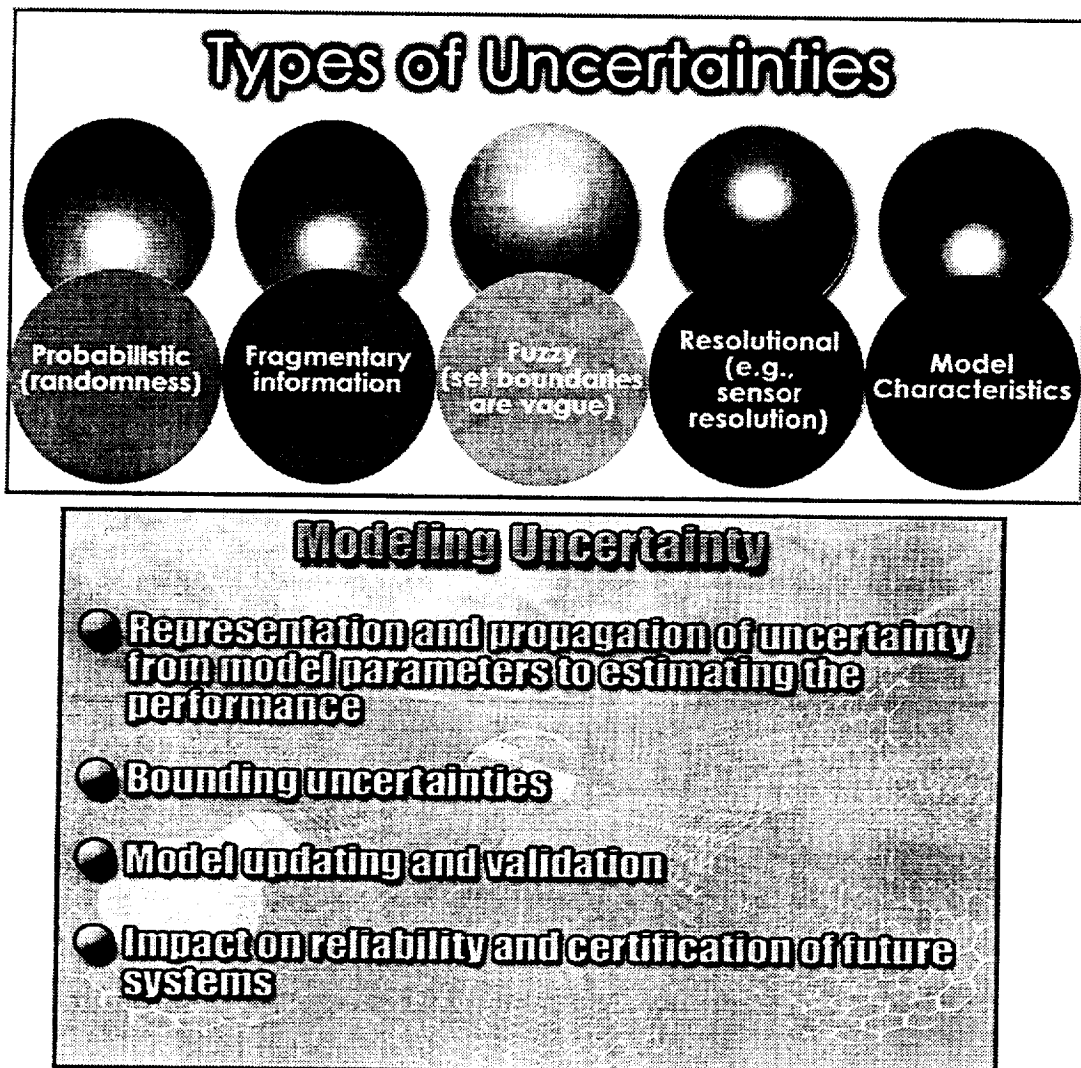


Figure 29

Principle of Complexity

One of the important consequences of uncertainty is its effect on precision. As the uncertainty and/or complexity of an engineering system increases, the ability to predict its response diminishes, until a threshold is reached beyond which precision and relevance become almost mutually exclusive. Consider, for example, numerical simulations in which sophisticated computational models are used for predicting the response, performance, and reliability of the engineering system, but the system parameters are little more than guesses. Such simulations can be characterized as Correct but Irrelevant Computations (CBIC); that is, forcing precision where it is not possible.

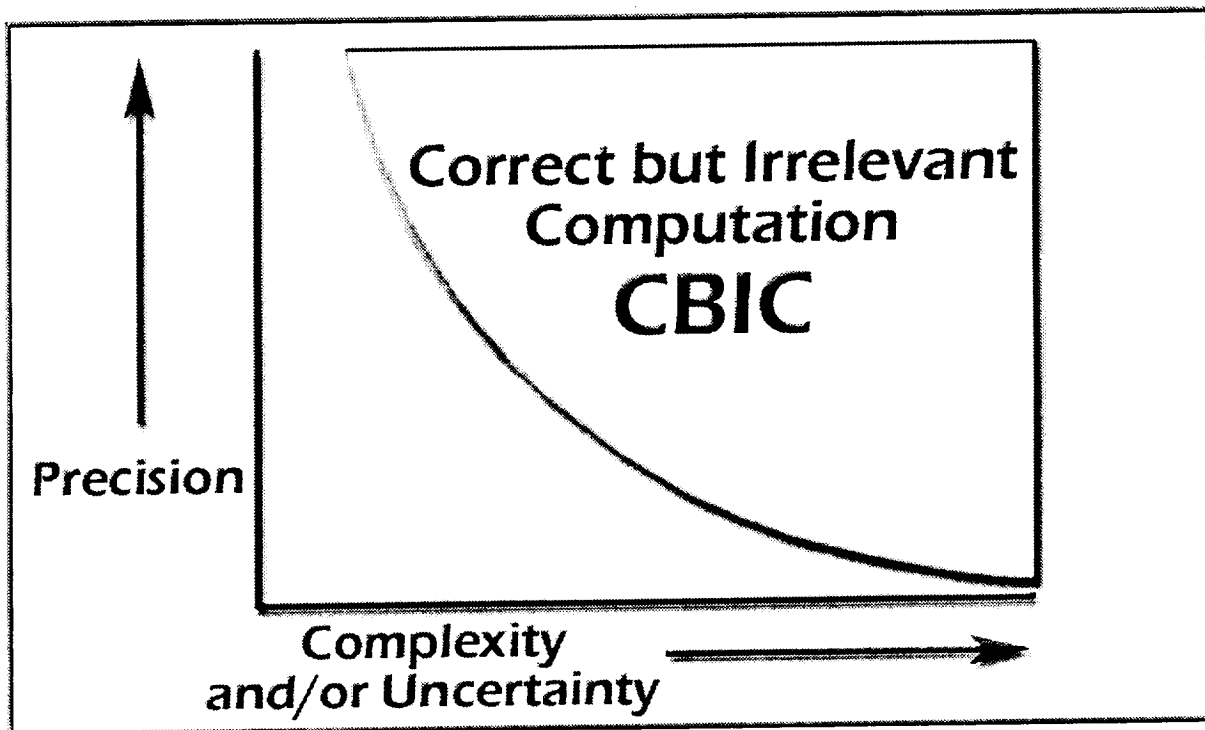


Figure 30

Nondeterministic Analysis Approaches

Three general approaches can be used for the analysis of systems with uncertainties; namely (Fig. 31): probabilistic methods for random processes; fuzzy sets; and set theoretical or anti-optimization methods. The domain of application of each of these techniques is identified in Fig. 31.

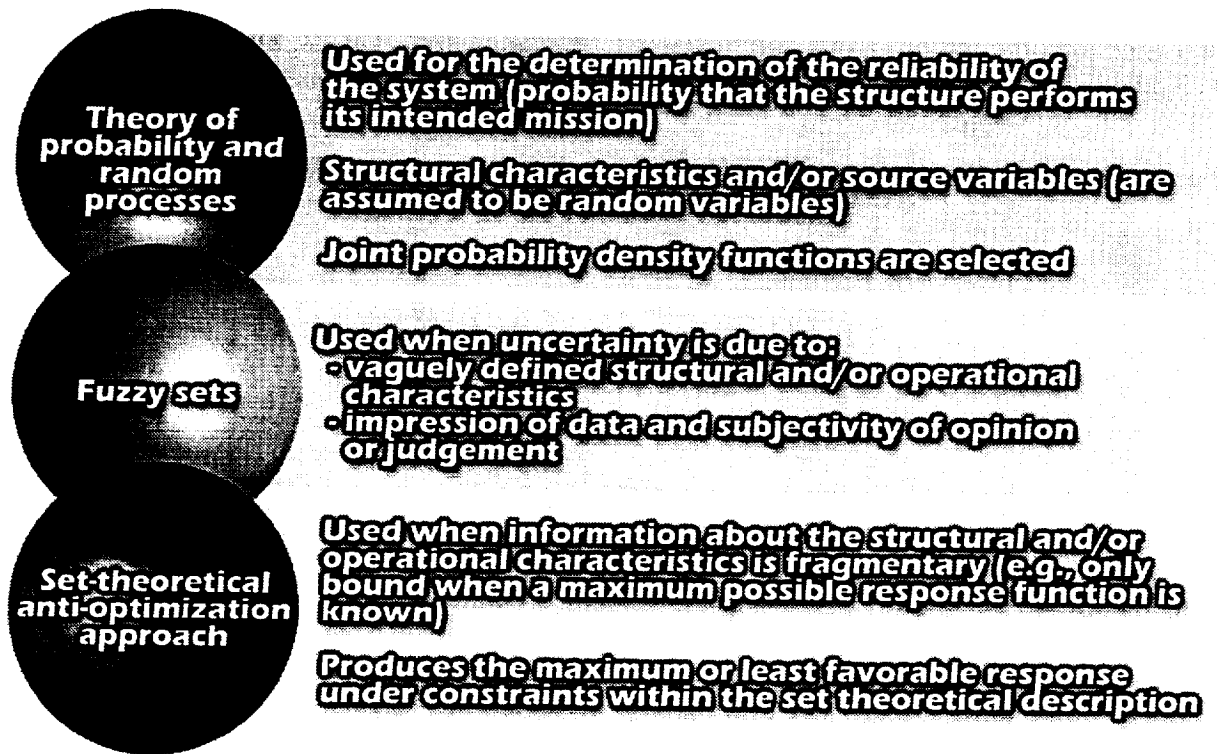


Figure 31

Advanced Learning Environments

In order to meet the life long learning demands of the future, three categories of learning environments are needed; namely, expert led group learning; self paced individual learning; and collaborative learning (Fig. 32). The three environments, in combination, can reduce the time and cost of learning, and sustain and increase worker competencies in high tech organizations.

The human instructors in these environments will serve many roles, including inspiring, motivating, observing, evaluating, and steering the learners, both individually and in distributed teams.



Figure 32

Expert Led Learning Environment

The human instructors in expert led distributed learning in a virtual environment serve as coaches, guides, facilitators, and course managers. Their presentations focus on a broad overview of the topic and its diverse applications (Fig. 33), and end with more penetrating, what-if questions that can enhance the critical thinking and creativity of the learners. Elaborate visualization and multimedia facilities are used in the presentations. Routine instructional and training tasks are relegated to the self-paced individual environment.

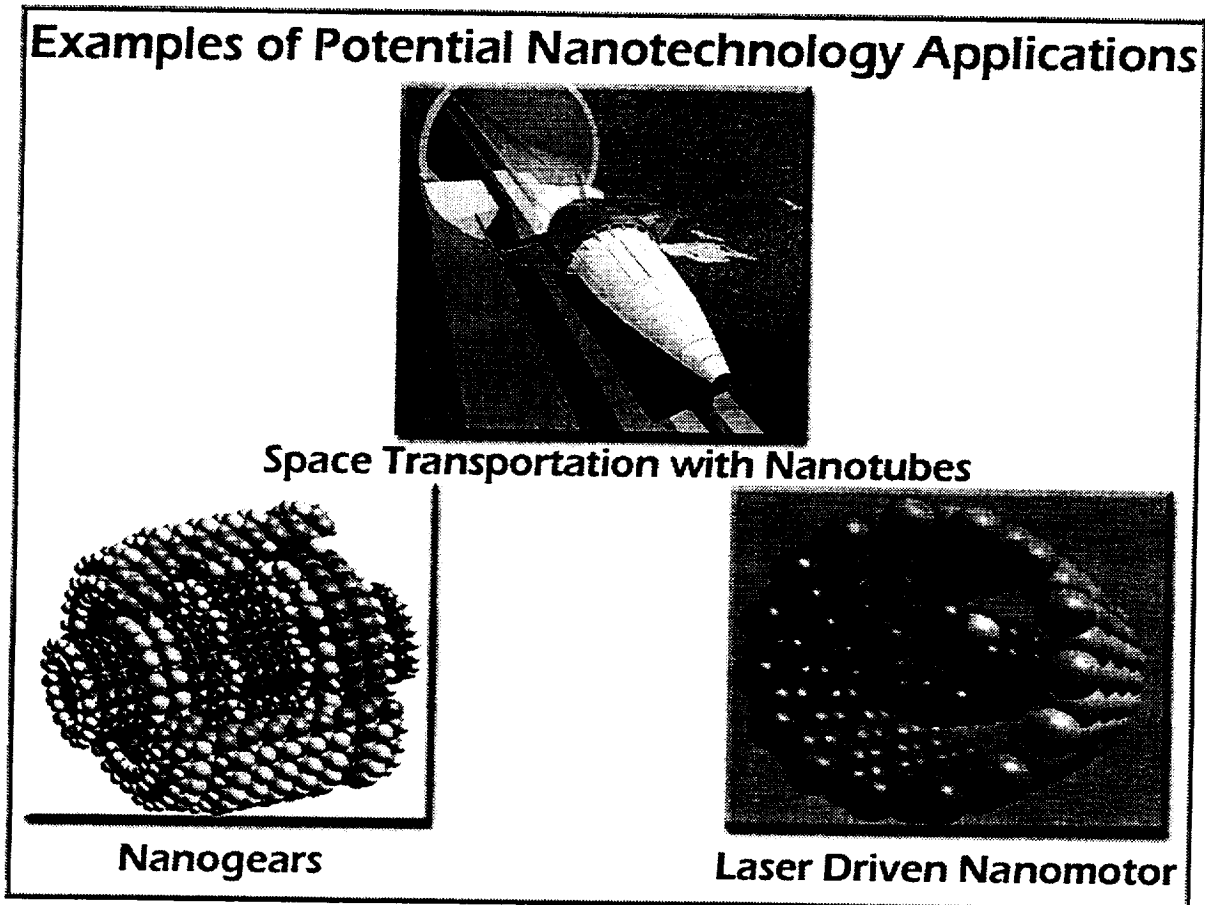


Figure 33

Self-Paced Learning Environment

The individual learning environment engages the learner and provides a high degree of tailored interactivity. It can be used for self-paced instruction of routine material not covered in the lecture. Using virtual instructors assigned by the human instructors can enhance such instruction. It can be used to study physical phenomena that can be coupled with biological processes using advanced visualization, multimedia and multisensory immersive facilities. The individual learning environment can serve to carry out virtual experiments - computer simulation of physical experiments (Fig. 34).



Figure 34

Collaborative / Distributed Learning Environment

Collaborative learning environments teach teamwork and group problem solving. Instructors and learners can be geographically dispersed. Eventually, they can be brought together through immersive telepresence facilities to share their experiences in highly heterogeneous environments involving different computing platforms, software and other facilities, and they will be able to work together to design complex engineering systems beyond what is traditionally done in academic settings. Because participants can be virtually collocated without leaving their industry and government laboratories, collaborative learning environments can enable the formation of new university, industry and government consortia. The ultimate goal of these learning facilities is to create an intellectual environment, where academic and experiential learning are effectively and efficiently co-mingled. In such an environment, academic rigor is learned in concert with professional job performance, and academic complexities are addressed within the industrial concern.

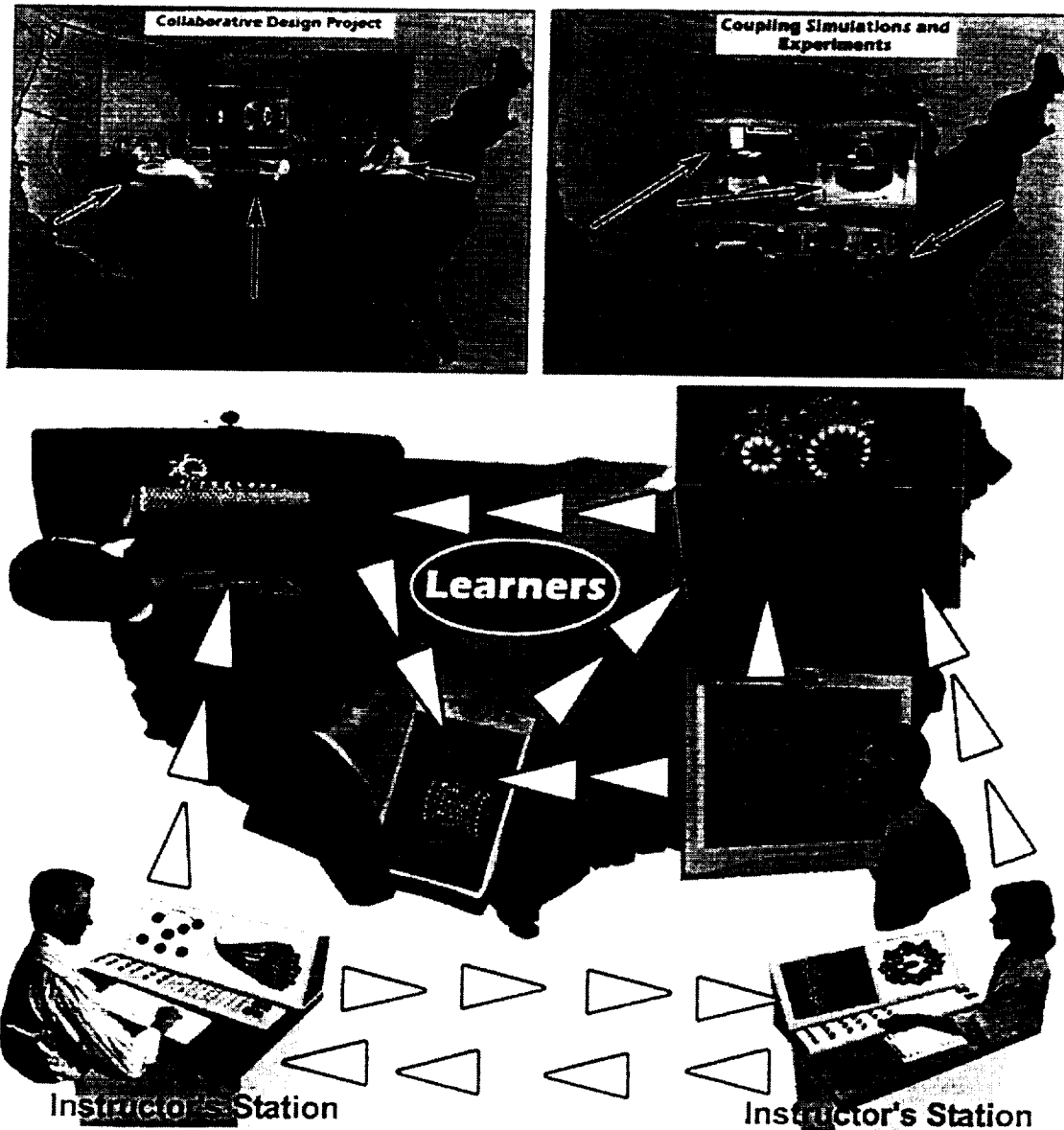


Figure 35

Virtual Classroom

Online training and virtual classrooms are typically used to provide learning environments with custom self-instruction, flexible tutorial support, and choice of both the place and time of learning. Three categories of facilities are used in these environments; namely: instruction, including multimedia lectures, links to other resources and tools for searching, browsing, and using archived knowledge; communication, including email, UseNet, chat centers, video and Internet conferencing; and course management and performance evaluation (Fig. 36).

The screenshot shows a virtual classroom interface for 'Carbon Nanotubes'. At the top, it says 'virtual classroom' and 'Carbon Nanotubes'. The interface is divided into several sections:

- Left Panel:** 'course material' (lectures, assignments), 'multimedia textbooks', 'links to other resources', and a search box with 'nanotubes' entered.
- Top Center:** 'Highlights' (Brief, Detailed), 'VRML', and 'email center'.
- Center:** A large 3D model of a carbon nanotube structure, labeled 'diode'.
- Right Panel:** 'email center', 'seminar', 'conference', and 'fabrication'.
- Bottom Left:** A text box with the following text: 'Carbon nanotubes are molecular-scale carbon fibers with structures related to those of the buckminster fullerene (a geodesic structure shaped like a geodesic sphere, constructed solely from sixty carbon atoms). Each carbon nanotube is a honey-comb lattice rolled into a cylinder. The diameter of the nanotube is of nanometer size and the length can be more than a nanometer.' Below this text are controls for 'SLOW', 'FAST', 'PLAY', and 'STOP'.
- Bottom Right:** A 'Nano-Fabrication' panel with 'Top View' and 'Side View' images.

Figure 36

Objectives and Format of Workshop

The objectives of the workshop are to a) provide an overview of the diverse activities in nanobiotechnology; and b) identify the potential of these technologies to future aerospace systems. The workshop, including eighteen presentations and three exhibits, illuminate some of the key issues in nanobiotechnology and provide fresh ideas for future research and development.

Objectives and Format of Workshop

Objectives

- **Overview of diverse activities in Nanobiotechnology**
- **Identify potential for aerospace systems**

Format

- **18 presentations, 7 sessions**
- **Exhibits**

Proceedings

- **Printed (NASA CP)**
- **Electronic**

Figure 37

Sources of Information on Nanobiotechnology

Extensive literature now exists on different aspects of nanobiotechnology. Several monographs, conference proceedings, and overview papers have been published on these subjects. In addition, a number of new journals are now devoted to the subject. Information on the research activities in these areas is also available on the Internet (Fig. 38).

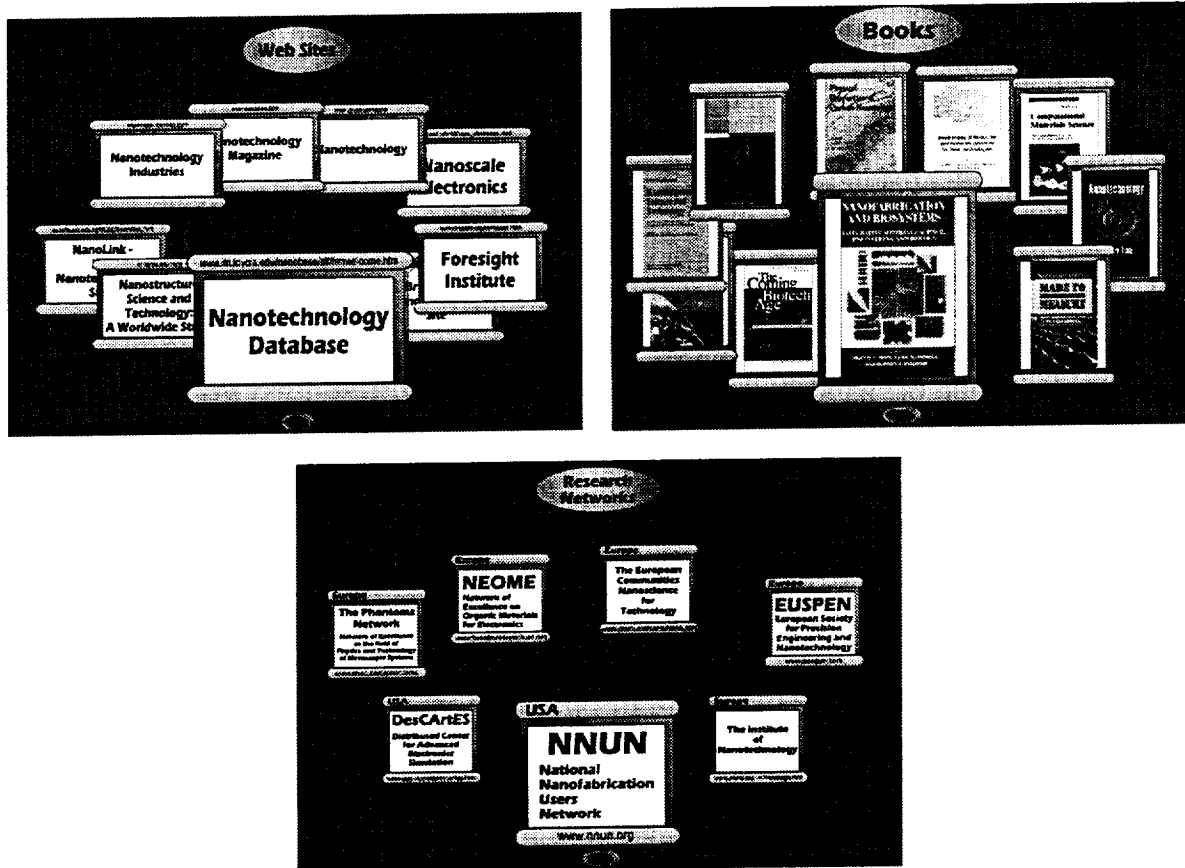


Figure 38

Web Sites for Information on Nanobiotechnology

- **Nanotechnology Research Directions: IWGN Workshop Report**
<http://itri.loyola.edu/nano/IWGN.Research.Directions/>
- **Nanostructure Science and Technology - A Worldwide Study**
<http://itri.loyola.edu/nano/toc.htm>
- **Nanotechnology Database**
<http://itri.loyola.edu/nanobase/alt/frmwelcome.htm>
- **The Nanotube Site**
<http://www.pa.msu.edu/cmp/csc/nanotube.html>
- **The National Biotechnology Information Facility (NBIF)**
<http://www.nbif.org/indxbd.html>
- **Internet Robotics Info**
<http://www.cs.indiana.edu/robotics/world.html>
- **Information Resources for Biotechnology**
<http://www.library.ucsb.edu/subj/biotech.html>
- **Internet Resources: Information Technology**
<http://bubl.ac.uk/link/i/informationtechnology.htm>
- **Internet Resources for Bioinformatics**
<http://www.science.gmu.edu/~ntongvic/Bioinformatics/index.html>
- **Bioinformatics and Computational Biology**
<http://www.unl.edu/stc-95/ResTools/biotools/biotools4.html>

Figure 39

32/70

16p

An Overview of Initiative on Biosystems At the Nanoscale

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Arlington, VA 22230
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An Overview of Initiative on Biosystems at the Nanoscale

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Acknowledgement: Mike Roco of NSF provided several slides for this presentation.

The National Nanotechnology Initiative

- The process
- Science and engineering research priorities
- Activities of the Interagency Working Group on Nanoscience, Engineering and Technology (IWGN)
- NSF Activities

History - NNI Timeline

- | | |
|-------------------|----------------------------------|
| ● November 1996 | Nanotechnology Group (bottom-up) |
| ● September 1998 | NSTC establishes IWGN |
| ● January 1999 | Workshop on research priorities |
| ● March 1999 | OSTP/CT presentation on NNI |
| ● May-June 1999 | Congress hearings |
| ● July-Sept. 1999 | Three background publications |
| ● August 1999 | First draft of the IWGN Plan |
| ● Oct.-Nov. 1999 | PCAST Nanotech Panel Review |
| ● December 1999 | PCAST Full Committee Consent |
| ● December 1999 | OMB Review |
| ● January 2000 | OSTP and WH Approval |
| ● February 2000 | Release of Initiative |

M.C. Roco, NSF

Nanotechnology R&D Funding by Agency

	FY 2000 (\$M)	FY 2001 (\$M)	% Increase
National Science Foundation	\$97M	\$217M	124%
Department of Defense	\$70M	\$110M	57%
Department of Energy	\$58M	\$94M	66%
NASA	\$5M	\$20M	300%
Department of Commerce	\$8M	\$18M	125%
<u>National Institutes of Health</u>	<u>\$32M</u>	<u>\$36M</u>	<u>13%</u>
TOTAL	\$270M	\$495M	83%

NNI Report, Feb. 2000

Funding by NNI Research Portfolio

	Fundamental Research	Grand Challenges	Centers & Networks of Excellence	Research Infrastr.	Societal Implications/ Workforce	Total
FY 2000	\$87M	\$71M	\$47M	\$50M	\$15M	\$270M
FY 2001	\$170M	\$140M	\$77M	\$80M	\$28M	\$495M

NNI Report, Feb. 2000

Neal Lane Testimony in Congress on April 1, 1998

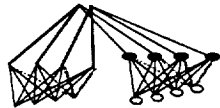
“If I were asked for an area of science and engineering that would most likely produce the breakthroughs of tomorrow, I would point to nanoscale science and engineering, often called simply, ‘nanotechnology,’ . . . only recently have scientists been able to glimpse Feynman’s vision by creating rudimentary nanostructures.”

Examples of Nanotechnology Applications

- Giant magnetoresistance in magnetic storage applications
- Nanostructured catalysts
- Drug delivery systems
- Nanocomposites: nanoparticle reinforced polymers
- Two examples of nanoelectronic devices
- LED lighting breakthroughs from nanotechnology
- National security: Bio detection
- Water purification and desalinization

Grand Challenges

- Nanostructured materials "by design" - stronger, lighter, harder, self-repairing, and safer
- Nanoelectronics, optoelectronics and magnetics
- Advanced healthcare, therapeutics and diagnostics
- Nanoscale processes for environmental improvement
- Efficient energy conversion and storage
- Microcraft space exploration and industrialization
- Bio-nanosensors for communicable disease and biological threat detection
- Application to economical and safe transportation
- National security



IWGN Publications

www.nano.gov

- *National Nanotechnology Initiative - Leading to the Next Industrial Revolution*
Supplement to the President's FY 2001 Budget, 2/2000
- *Nanotechnology - Shaping the World Atom by Atom*
Brochure for the Public
- *Nanostructure Science and Technology*
Worldwide Study
- *Nanotechnology Research Directions*
IWGN Workshop Report
- **15 Supporting Publications/Proceedings by Agencies for**
 - Specific scientific topics (modeling, selfassembling, macromolecules)
 - Technological issues (synthesis, processing, nanofabrication)
 - Areas of relevance (energy, space, biomedicine, biotech, chemicals)

Sampling the Programs at NSF

Mainly Seed Funds:

- Synthesis and Processing of Nanoparticles (since 1991)
- National Nanofabrication User Network (since 1994)
- Nanoscale Instrumentation (1995)

Larger Investments:

- Functional Nanostructures (1998)
- Biotechnology at Nanoscale (1999/00, exploratory), Nanoscale Modeling and Simulation Centers (2000)
- STTR and SBIR Solicitations on Nanotechnology (1999/00)

M.C. Roco, NSF

Nanoscale Science and Engineering NSF Areas of Focus in FY00 and FY01

- Nano-Biotechnology
- New Phenomena and Structures, Quantum Control

- Integration at the Nanoscale: Systems and Architectures

- Interfaces in Environment at Nanoscale
- Nanoscale Theory, Modeling and Simulations

- Education and Society Implications

NNI Interagency Collaborative Activities (Examples, to be Finalized After NNI Approval by Congress)

Agency	DOC	DOD	DOE	NASA	NIH	NSF
Fundamental research		x	x	x	x	x
Nanostructured materials	x	x	x	x	x	x
Molecular electronics		x (DARPA)		x		x
Spin Electronics		x		x		x
Lab-on-a-chip (nanocomponents)	x	x	x	x	x	x
Biosensors, bioinformatics (1)				x	x (NCI)	
Bioengineering		x (DARPA)	x		x	x
Quantum computing		x	x	x		x
Measurements and standards for tools	x	x	x		x	x
Nanoscale theory, modeling and simulation		x	x	x		x
Environmental monitoring			x	x		
Unmanned missions		x		x		
Nanofabrication user facilities	x		x	x		x

(1) NASA and National Cancer Institute (NCI) join effort to develop nano-explorers for the human body (MOU signed on 4/13/00)

From IWGN Implementation Plan

Biosystems at Nanoscale

- Principal Investigator: **Robert H. Austin**
- Institution: **Princeton University**
- Title:
**Cell Sorting Using Nanomagnetic
Nanofabricated Devices**
- Purpose:
**To fabricate nanomagnetic devices for cell
capture and sorting**

Examples of Exploratory Research on Biosystems at Nanoscale

Biosystems at Nanoscale

- Principal Investigator: **R. Bashir**
- Institution: **Purdue University**
- Title:
Hybridization Based Assembly of Silicon Electronic Devices
- Purpose:
To develop new approaches for fabrication and assembly of future hybrid bio-electronic devices based on the hybridization and specificity of DNA oligo-nucleotides.

Biosystems at Nanoscale

- Principal Investigator: **Elliot P. Douglas**
- Co-Principal Investigator: **Laurie B. Gower**
- Institution: **University of Florida**
- Title:
Nanostructured Composites via Biomimetic Processing
- Purpose:
Provide a new route to ceramic composites with controlled structure and properties by mimicking the structure of natural bone.

Biosystems at Nanoscale

- Principal Investigator: **Ashutosh Chilkoti**
- Institution: **Duke University**
- Title:
Elastin Nanobiosensors
- Purpose:
To design, fabricate, and characterize a genetically encodable protein nanobiosensor for *in vivo* intracellular real-time measurement of temperature, pH, or kinase activity.

Biosystems at Nanoscale

- Principal Investigator: **Vicki Colvin** (chemistry)
- Co-Principal Investigator: George Phillips (Biology)
- Institution: **Rice University**
- Title:
Protein Crystals as Templates for Nanoscale Materials
- Purpose:
To develop chemical methods for replicating the intricate nanoscale architecture of protein crystals into solid materials.

Biosystems at Nanoscale

- Principal Investigator: **Andrés J. García**
- Institution: **Georgia Institute of Technology**
- Title:
Structural Changes in Fibronectin Binding Domains upon Adsorption to Well-Defined Surface Chemistries
- Purpose:
Integration of experimental and computational approaches to model structural and functional changes in binding domains upon adsorption to model surfaces.

Biosystems at Nanoscale

- Principal Investigator: **Vladimir Hlady**
- Institution: **University of Utah**
- Title:
Creating Nanoscale Molecular Imprints Using 2-D Monolayer Templating
- Purpose:
Goal of the research is to create monolayer surfaces with a custom, nanoscale-imprinted 2-D structure-function relationship.

Biosystems at Nanoscale

- Principal Investigator: **Eric W. Kaler**
- Co-Principal Investigator: Orlin D. Velev
- Institution: **University of Delaware**
- Title:
Miniaturized On-chip Biosensors by In Situ Assembly of Colloidal Particles
- Purpose:
A new method is extended to assemble microscopic on-chip biosensors from widely available latex particles used in agglutination assays.

Biosystems at Nanoscale

- Principal Investigator: **Richard A. Kiehl**
- Institution: **University of Minnesota**
- Title:
Self-Assembly of Nanoparticle Arrays Using Two-Dimensional DNA Crystals
- Purpose:
To develop a revolutionary technology for the self-assembly of electronic circuitry at the nanoscale.

Biosystems at Nanoscale

- Principal Investigator: **Russell J. Mumper**
- Institution: **University of Kentucky**
- Title:
Pharmaceutically Engineered Nano-particles for the Targeted Delivery of Plasmid DNA
- Purpose:
To engineer nanoparticles containing DNA from micro-emulsion precursors that can spontaneously form without the use of expensive and/or damaging methods.

Biosystems at Nanoscale

- Principal Investigator: **W. Mark Saltzman**
- Co-Principal Investigator: **Dan Luo**
- Institution: **Cornell University**
- Title:
Modular Nanoscale DNA Delivery Systems
- Purpose:
To create novel DNA delivery systems that are totally synthetic, modeled after certain characteristics of viruses, produced at the nanoscale in modular fashion, and based entirely on biocompatible polymeric materials.

Biosystems at Nanoscale

- Principal Investigator: **Sandip Tiwari**
- Institution: **Cornell University**
- Title:
An Electronic Gain Cell for Monitoring Charge on Molecular Chains
- Purpose:
Demonstrate proof-of-principle of a miniature single-electron charge sensitive semiconductor device with gain that can rapidly profile charge at sub-nm resolution on molecules flowing in a channel.

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An Introduction and Overview of Interdisciplinary Nanoscience and Nanotechnology

James C. Ellenbogen
MITRE Nanosystems, Inc.
McLean, VA 22102

An Introduction and Overview of Interdisciplinary Nanoscience and Nanotechnology

James C. Ellenbogen, Ph.D.

MITRE Nanosystems Group
e-mail: ellenbgn@mitre.org

14 June 2000

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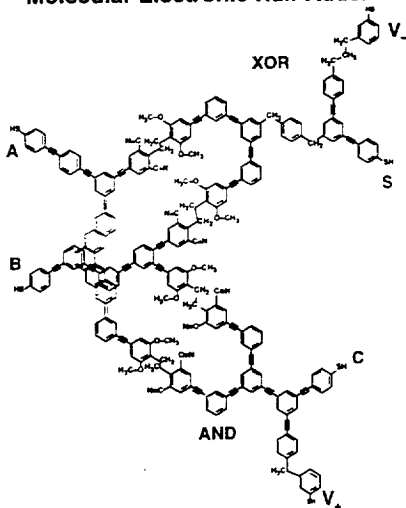
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14 June 2000

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Basis for this Presentation: MITRE's Broadly-Based R&D in Nanotechnology

**MITRE's Proposed
Molecular Electronic Half-Adder**



*1 million times smaller than
comparable circuit on Pentium II*

● **Present focus:** Investigate and develop architectures for electronic nanocomputers--*esp. molecular electronic computers*

● **Full Range of Tasks:**

- Nanocomputer technologies and designs investigations
- Applying nanocomputers to control micro-mechanisms
- Improved fabrication & modeling of nanosystems
- Bio-nanotechnology R&D
- Economic analysis of nanotechnology

More information at: <http://www.mitre.org/technology/nanotech>

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"Pink Book" Recently Published in March 2000 *Proceedings of the IEEE*

- Explains basic ideas of molecular electronics and shows what a molecular-scale computer might "look" like

Architectures for Molecular Electronic Computers: 1. Logic Structures and an Adder Designed from Molecular Electronic Diodes

JAMES C. ELLENBOGEN AND J. CHRISTOPHER LOVE

Recently, there have been significant advances in the fabrication and manipulation of individual molecular electronic wires and diode systems. This paper reviews these developments and shows how demonstrated molecular devices might be combined to design molecular-scale electronic digital computer logic. The design for the demonstrated resistive molecular diode switches is refined and

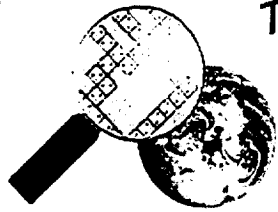
others. In addition, in the field of nanoelectronics, it might be possible to build and to demonstrate somewhat more complex molecular electronic structures that would include two or three molecular electronic diodes and that would perform as digital logic circuits.

- Reviews recent experimental and theoretical results in molecular electronics
- Proposes designs for molecular logic circuits and functions

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More Nanotech Information on the Internet: Nanoelectronics & Nanocomputing Home Page



MITRE
The
Nanoelectronics
&
Nanocomputing
Home Page

The BIG picture for a small world

Overview articles available on Web site

Architectures for Molecular Electronic Computers
1. Logic Structures and an Adder Built from Individual Molecular Diodes

James C. Ellenbogen
J. Christopher Love

Overview of Nanoelectronics

David C. Greiner, David H. Hamel, S. Manassis, J. Christopher Love, Gregory T. Oberer, James C. Ellenbogen

- 🔍 What are Nanotechnology and Nanoelectronics?
- 🔍 Top 10 Recent
- 🔍 Basic References on Nanoelectronics and Nanocomputing
- 🔍 Top 10 Hard Pro for Nanoelectr
- 🔍 Who's Who in Nanoelectronics and Nanocomputing
- 🔍 Status and Prospects for the Future
- 🔍 Links to other WWW Sites Relevant to Nanoelectronics
- 🔍 and much more!

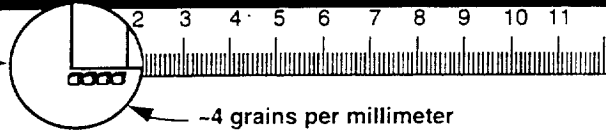
On the Internet at <http://www.mitre.org/technology/nanotech>

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Objectives of this Presentation

Start by focusing on a grain of salt...



...To address the questions:

- What are nanotechnology and bio-nanotechnology?
- What are some key applications of bio-nanotechnology?
- Why is it of particular importance to NASA?
- What are some key challenges to fulfilling the promise of nanotechnology?



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Enter the Nanocosm: Range of Length Scales for Bio-Nanotechnology

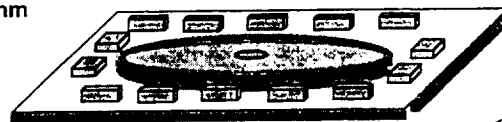
Cells are the micron-scale building blocks of life, but their function relies on complex *nanometer-scale* mechanisms

Grain of Salt
 ~0.25 mm
 250 μm
 250,000 nm

Micro-machine
 ~100 μm
 100,000 nm

Cell
 ~15 μm
 15,000 nm

Micro-electronic Transistor
 ~1 μm
 1000 nm



Molecule (e.g., in cell membrane)
 ~10 nm

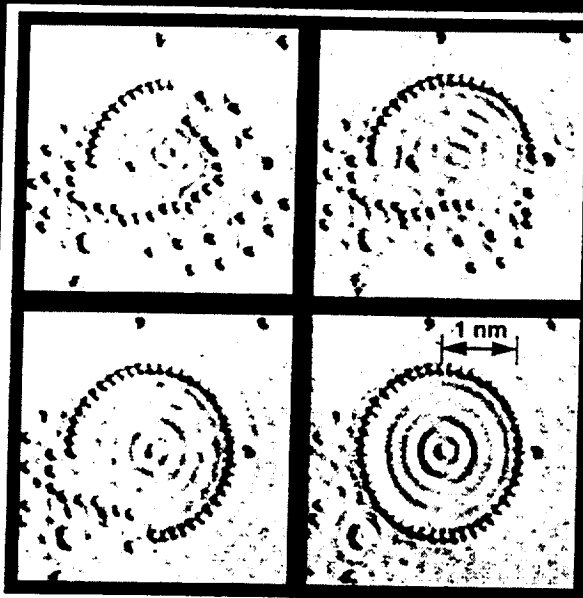
Molecules are at least 10,000 times shorter than cells and 50,000 to 100,000 times shorter than a salt grain

1 micron (μm) = 1 millionth of a meter
 1 nanometer (nm) = 1 billionth of a meter = 10 atomic diameters



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This is Nanotechnology: Engineering on the Atomic & Molecular Scale



Work of Eigler *et al.* Source: IBM Almaden Rsch. Labs

- Sequence at right shows the assembly of a 2 nanometer (nm) circle of iron atoms on a copper surface
- 1 nm \approx 10 atomic diameters
- Quantum effects are ubiquitous
- "Quantum corral" is assembled arduously, atom-by-atom at very low temperatures, using a "nanoprobe"
- Nanoprobe both manipulates and images the atoms

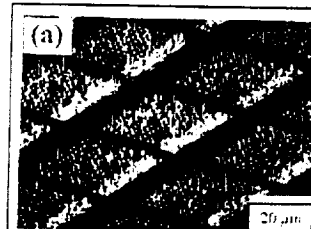
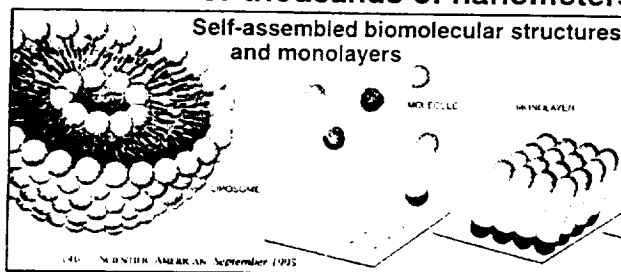
Reference: Crommie, Lutz, & Eigler, *Science*, 8 Oct. 1993, pp. 218-220.

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This is Nanotechnology: Molecular Self-Assembly

- Putting molecules where you want them by clever use of the "natural" physico-chemical properties of atoms, molecules, and nanometer-scale metal clusters
- Highly parallel processes effective for organizing many, many atoms or molecules all at once
- Create structures much larger than molecules with extended order over hundreds or thousands of nanometers



Multi-wall carbon nanotubes grown on nickel nano-dots

LH graphic from: G. Whitesides, *Sci. Am.*, Sept. 1995, pp. 145-146.

RH graphic from: Ren *et al.*, *Appl. Phys. Lett.*, v. 75, pp. 1086-1088, 1999.

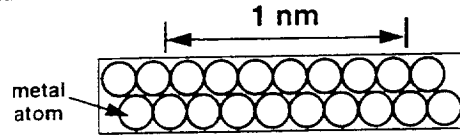
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As requested by S. Venneri at NanoSpace 2000 Conference:

Nanotechnology: A More Formal Definition

- A *nanometer* is a billionth of a meter (10^{-9} m) and spans approximately 10 atomic diameters



- **Nanotechnology is:**

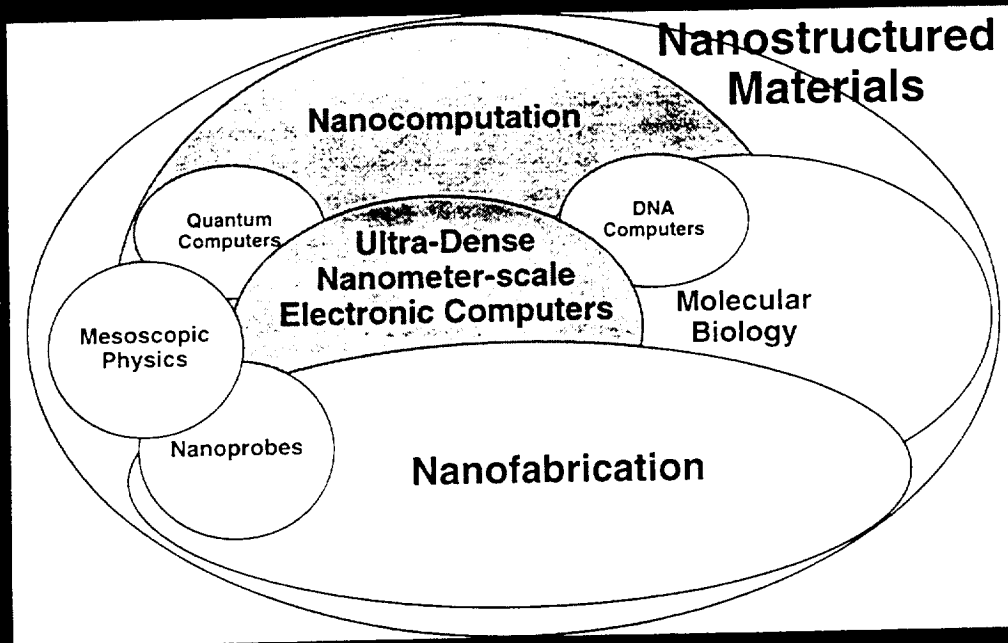
- Technology for designing, fabricating, and applying nanometer-scale devices or systems ("nanosystems")
 - Entire systems having dimensions < 100 nanometers
 - Interdisciplinary technology (a synthesis of electrical engineering, physics, chemistry, and biotechnology)
- Engineering on the nanometer scale
 - Involving the exploration or integration of nanometer-scale components in/into a nanometer-scale device or system
 - Involving nanostructured materials, devices, or systems "with every atom or molecule in its place" by design*

* Last definition on bottom adapted from comments of R. Merkel of Zyvex Corp.

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Domains of Nanotechnology: An Interdisciplinary Field



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National Nanotechnology Initiative Proposed by the President in January

- Interdisciplinary effort--“Grand Challenges” to include tinier computers, as well as dramatic advances in medicine

The screenshot shows a web browser window displaying a New York Times article. The page title is "Technology" and the source is "The New York Times ON THE WEB". Navigation links include Home, Site Index, Site Search, Forums, Archives, and Marketplace. The date is "January 21, 2000". The main headline is "A Clinton Initiative in Science of Smallness" with a large black arrow pointing to it from the right. The byline is "BY JOHN MARKOFF". The article text begins with "The Clinton administration plans today to announce ambitious plans to accelerate basic research in the field of nanotechnology, the design and fabrication of devices of atomic-scale size." A sub-headline reads "Nanotechnology is widely considered an extremely promising area of science and engineering, but it has realized only limited commercial success to date." The main text continues: "Today, in a speech at the California Institute of Technology in Pasadena, President Clinton will stress the importance of expanding basic research in both the physical and biological sciences. As part of the speech, he will announce plans to ask Congress to finance a National Nanotechnology Initiative." A "Related Articles" section lists "Computer Scientists Are Bored" and "For Revolution in Chip Size" with a date of "November 11, 1999".

- Explicit mention of “molecular computers” in State of Union speech implicitly referred to R&D at MITRE and elsewhere

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Trends and Potential for Nanotechnology

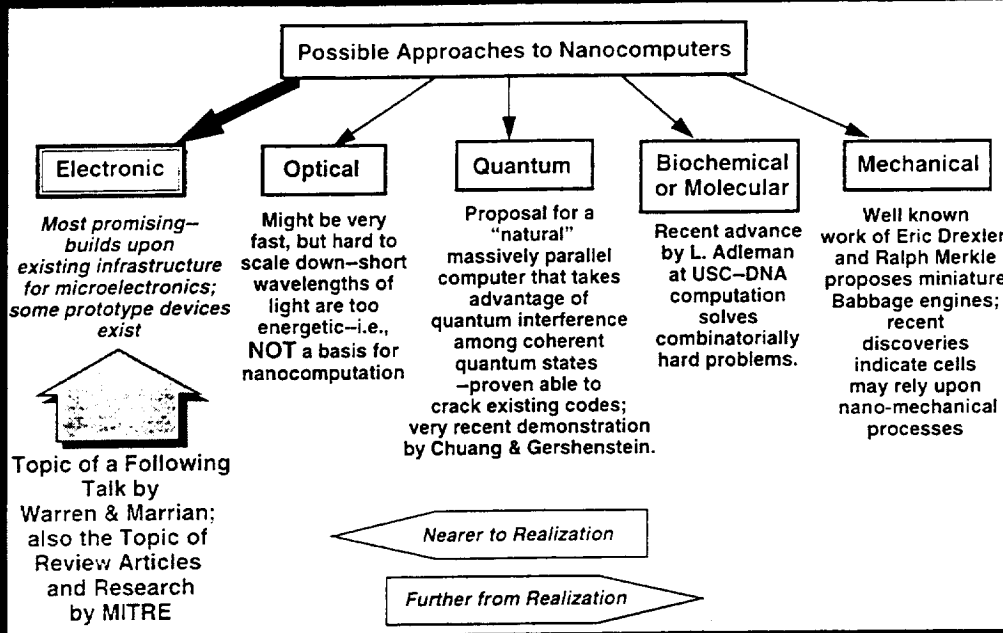
- *Over the next decade: Ascent of nanotechnology and nanocomputers--esp., molecular electronic computers*
 - Investment essential to maintain the vigor of the present information technology revolution*
- *Over the next 20 years: Ascent of bio-nanotechnology*
 - Powerful combination of molecular biology with physical methods for nanofabrication
 - New vistas for both medicine and engineering--harness mechanisms of the cell for medicine & manufacturing
- *Ultimately: Matter as software*
 - e.g., distributed desktop manufacturing to make objects “downloadable” from the Internet
 - Bring the “information economy” to material goods--desirable physical & economic properties like software

* Issue highlighted in 1996 & 1997 MITRE review articles and in recent article by P. Packan, Science, 23 Sept. 1999, pp. 2079-2080.

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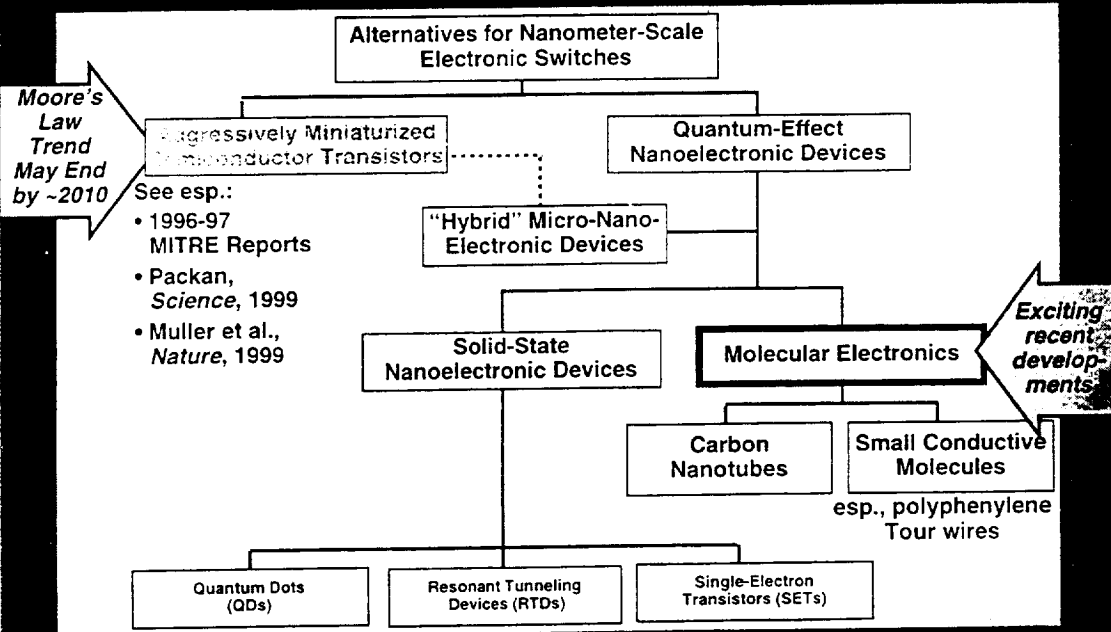
Range of Proposed Approaches for Building Future Nanocomputers



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Approaches to Nanometer-Scale Switches: “Overview of Nanoelectronic Devices”*



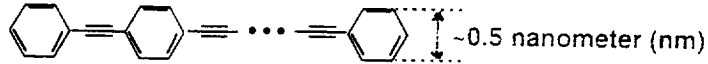
* Title of MITRE-written paper that appeared in April 1997 issue of the *Proceedings of IEEE*, which is dedicated entirely to nanoelectronics.

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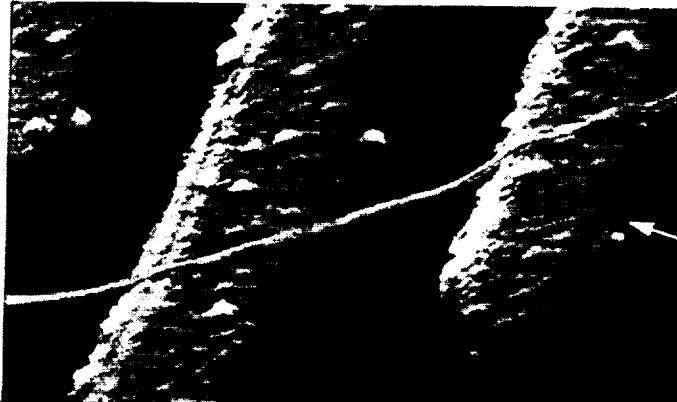
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Molecular Wires and Switches Already Have Been Demonstrated (1996-97)

- Individual small molecules: polyphenylene "Tour wires"



- Also, carbon nanotubes (CNTs) have been interfaced with nanofabricated metal & silicon to make wires and switches



Single Carbon Nanotube with 1.5 nm diameter

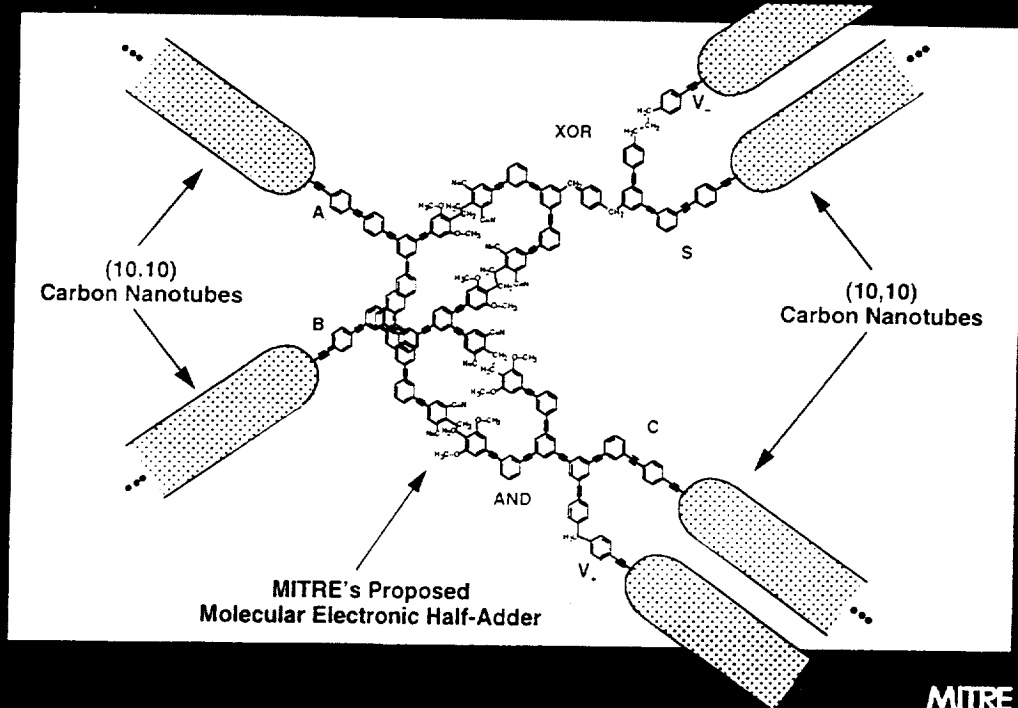
Gold contact 100 nm wide

NOTE: Graphic extracted from the work of S. Tans and C. Dekker, TU Delft, The Netherlands. Published in Nature, 1997.

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Might Use Nanotubes and Tour Wires Together in Molecular Computer Circuits

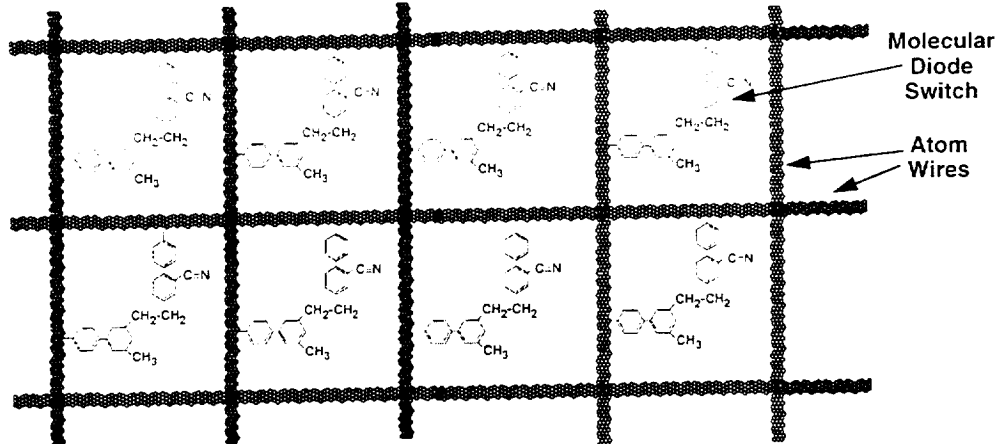


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Higher-Level Nanocomputer Architectures: Molecular Switches in Grids of Atom Wires

- Stanley Williams & Phil Kuekes of H-P envision grid of atom wires linking array of molecular diode switches



- Above, MITRE-designed molecular diodes are made from substituted backbone of polyphenylene-based Tour wires

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Future Miniaturization of Electronic Switches: Industry's Roadmap and Beyond

<p>1997 e.g., transistor on Pentium II Chip</p> <p>← 1000 nanometers (nm) →</p> <p>250 nm</p> <p>SIDE VIEW</p> <p>TOP VIEW</p>		<p>2011 or 2012 Projected by 1997-98 SIA Roadmap, if scaling can continue</p> <p>200 nanometer transistor</p> <p>100 nm</p> <p>based upon 50 nm linewidth</p> <p><i>Beyond</i></p> <p>Reed-Tour Molecular Switch (Demonstrated in 1997)</p> <p>MITRE Molecular Electronic Adder (Proposed for 2003-2005)</p>
Memory Chips	256 Megabit	64 Gigabit
CPUs	3.7 M devices/cm ²	180 M devices/cm ²

SIA = Semiconductor Industry Association

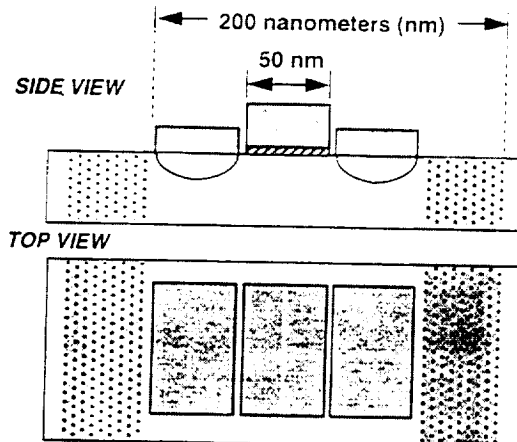
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Future Molecular Electronics: Outpacing the Semiconductor Industry Roadmap

Transistor in 2011 or 2012 ??

Projected by 1997-98 SIA Roadmap,
if scaling can continue



Before 2010

Beyond the Roadmap

~3 nm

Reed-Tour Molecular Switch
(Demonstrated in 1997)

MITRE Molecular Electronic
Adder

(Proposed for ~2003)

~10 nm

*Potential: A simple molecular
computer where the Roadmap
would place only one switch*

Memory Chips

64 Gigabit

CPUs

180 M devices/cm²

>10 Terabit Memory Chip*

1 PC on a grain of salt

* Based on only 2-dimensional tiling of devices;
Note also: SIA = Semiconductor Industry Association

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Challenges Posed by Nanoelectronics and Nanotechnology

- Development of nanoelectronics
 - Design, development, and fabrication of nanometer-scale switches and wires
 - Devising new designs and architectures for ultra-dense nanoelectronic computers with trillions of components
 - Fabrication and packaging
 - Arranging trillions of nanometer-scale components
 - Protecting tiny components
 - Interface to micron-scale/macroscopic worlds
- Discovery, exploration, refinement, and mass production of other nanostructured materials with novel, useful properties
- Application and integration of nanoelectronics and nanotechnology--esp., into Space Systems

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Implications of Nanotechnology/Nanoelectronics for Aerospace Information Systems

- **Much more densely integrated, faster computers**
 - *More powerful computers, computationally*
 - *Smaller, lighter computers integrated with smaller electrical & mechanical devices*
- Lower power consumption
- Denser memory--Terabyte mass storage with no moving parts
- Nanocomputers integrated with micro-electromechanical systems (MEMS) and devices--e.g., focal plane arrays (FPAs)

Nanometer-Scale Electronics

Micron-Scale Machines & Sensors

Next-Generation, Light-weight, Low-Power Aerospace Systems

- Higher redundancy, more reliability in the vehicle
- "Smart", instrumented, self-repairing aerospace materials and life-support systems
- Nano- & pico-scale robotic planetary explorers
- etc.

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Space Nanoscience & Nanotech Are The Keys To Planetary Exploration

- **Improved Platforms: Lower launch costs & more capability**
 - Nanostructured materials--lighter, stronger, self-healing
 - Lower Power Electronics
 - New Fuels & Novel Fuel Storage
- **Enhanced Endurance of Crew: Nanomedicine**
 - The 21st Century is/will be the "Biotech Century"
 - Explosion of knowledge about life processes at the molecular level
 - Building a better human & keeping him/her well longer
- **Maintenance of Crew and Systems in Space & On Planets**
 - Distributed manufacturing of necessities & luxuries
 - "Downloading" spare parts, food, and medicine
- **Conceptual blockbusting--e.g., the elevator to orbit??**

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**Biomaterials, Biomimetics and Biological
Interfaces Research at the Oak Ridge
National Laboratory**

Mark E. Reeves
Biological and Environmental Sciences Directorate
Oak Ridge National Laboratory
Oak Ridge, TN 37831

Biomaterials, Biomimetics and Biological Interfaces Research at the Oak Ridge National Laboratory

Mark Reeves

Biological and Environmental Sciences Directorate

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY



Outline

- **Biomaterials**
 - **Biocompatible Materials**
 - **Materials Science Approach to Characterizing Biological Materials**
 - **“Hybrid” Biomaterials**
 - **Biologically Produced Materials**
- **Biomimetics**
 - **Mimicking Biological Processes**
 - **Mimicking Biological Function**
- **Biological Interfaces Research**
 - **Interfaces with Materials (Signal Processing/Propagation)**
 - **Interfaces with Computing (Modeling Biological Function)**

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY



Outline

- **Biomaterials**
 - **Biocompatible Materials**
 - Bio-ceramics (synthetic bone and implant materials)
 - **Materials Science Approach to Characterizing Biological Materials**
 - Residual stress analysis of bone
 - **“Hybrid” Biomaterials**
 - Bio-ligand-grafted polymers
 - **Biologically Produced Materials**
 - Bacterial magnetite crystals

OAK RIDGE NATIONAL LABORATORY
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Outline

- **Biomimetics**
 - **Mimicking Biological Processes**
 - Biomimetic process for inorganic thin-film growth
 - **Mimicking Biological Function**
 - Virtual human

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Outline

- **Biological Interfaces Research**
 - **Interfaces with Materials (Signal Processing/Propagation)**
 - “Critters on a chip”
 - **Interfaces with Computing (Modeling Biological Function)**
 - Critters on a chip example
 - Virtual human

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Biomaterials

- **Biocompatible Materials**
 - **Bio-ceramics (Synthetic Bone and Implant Materials)**
 - Better biocompatible materials and composites
 - Formation of synthetic bone and dental materials using ceramic microsphere technology
 - Mimics natural porosity
 - Encourages vascularization and osteogenesis
 - Appropriate materials properties (strength, density, etc.)

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Biomaterials

• Biocompatible Materials

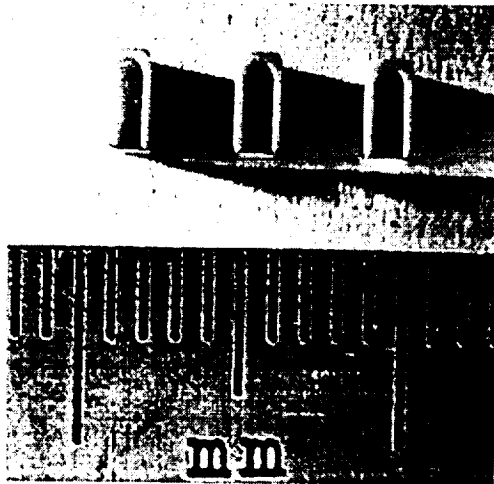
– Bio-ceramics (Synthetic Bone and Implant Materials)

- Better biocompatible materials and composites
- Net-shape forming of prosthetic devices, including rapid manufacturing
- Gelcasting of ceramic mimics of bone for implants
 - Hydroxyapatite, alumina, zirconia, tricalcium phosphate, etc.
 - Can be cast to near net shape
 - Can control porosity
 - Very rugged process
 - Meets FDA requirements for implantation (phase content: $\geq 95\%$ HA;
 - $\leq 5\%$ beta-tricalcium phosphate)

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Ceramic Gelcasting of Bone Mimics



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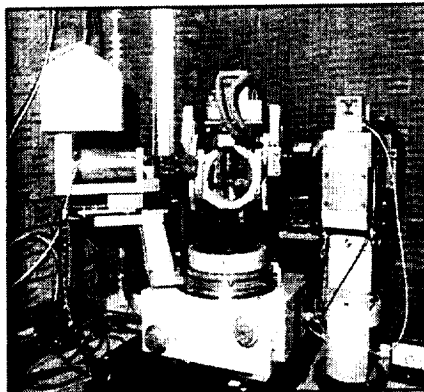
Biomaterials

- **Materials Characterization—Residual Stress Analysis**
 - Abalone as a Model System
 - Watch change in lattice parameters in mineral phase
 - Neutrons allow one to surmise what is going on in the proteins
 - Natural Bone

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Biomaterials Characterization



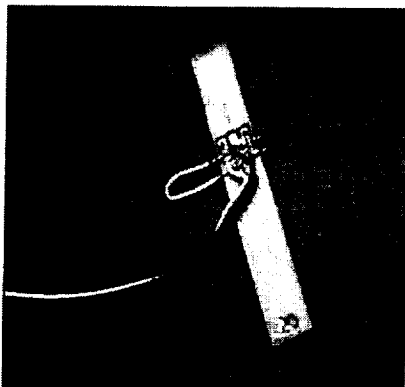
#2003-05 University of Alabama-Birmingham,
RSUC User Center

COMPACT
- 4-8

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Biomaterials Characterization



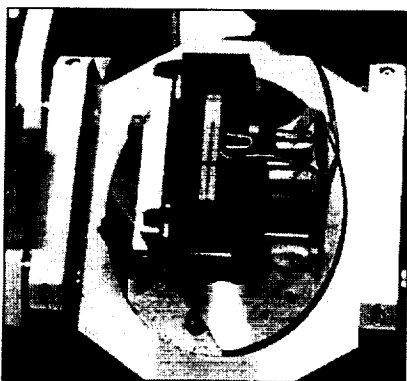
#2009-05 University Of Alabama-Birmingham
RSUC User Center

CPWET-04
1/2/05

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Biomaterials Characterization



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1/2/05

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Biomaterials

- **“Hybrid” Biomaterials**

- **Biochemical Ligands Covalently Grafted to Polymer Structure of Polyurethane**
- **Gel or Foam Structure of Final Materials**
 - **Ability to create high-specificity materials for chemical separations involving metal cations, radionuclides**
 - **Mimics natural biomolecular recognition properties of ligands from biochemical sources**

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Biomimetics

- **Mimicking Biological Processes**

- **Biomimetic process for inorganic thin-film growth**

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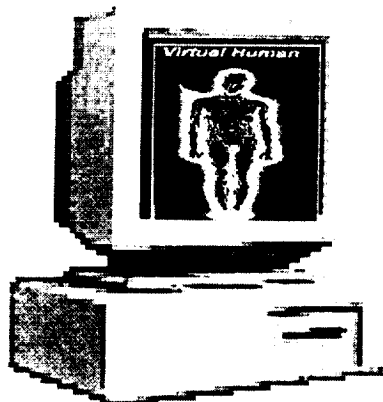
Biomimetics

- **Mimicking Biological Function**
 - The virtual human (the ultimate biomimetic!)

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Vision



- **Model the Human**
- **Link Biology with Physics and Chemistry**
- **Structure and Function**

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Vision (Cont'd.)

- **Complete System Consistent with Current Science (Physiological and Cognitive)**
- **Collaborators Retain Ownership of Work**
- **Contribution From Oak Ridge National Laboratory**
 - **Catalyze idea**
 - **Integration**
 - **Specific modeling**
 - **Instrumentation/data**

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Functional Goals of Virtual Human Year 0+ 5 to 10

- **Scalable by Age and Gender**
- **All Organs, Full Anatomy and Physiology**
- **Limited Pharmacokinetic Capability**
- **Radiation and Chemical Risk**
- **Biophysical Constants (Tissue Properties)**
- **Blood Flow, Breathing, Endocrine, GI, Renal, Sensory, Thermo-regulation, Shock, Limited Brain Function**

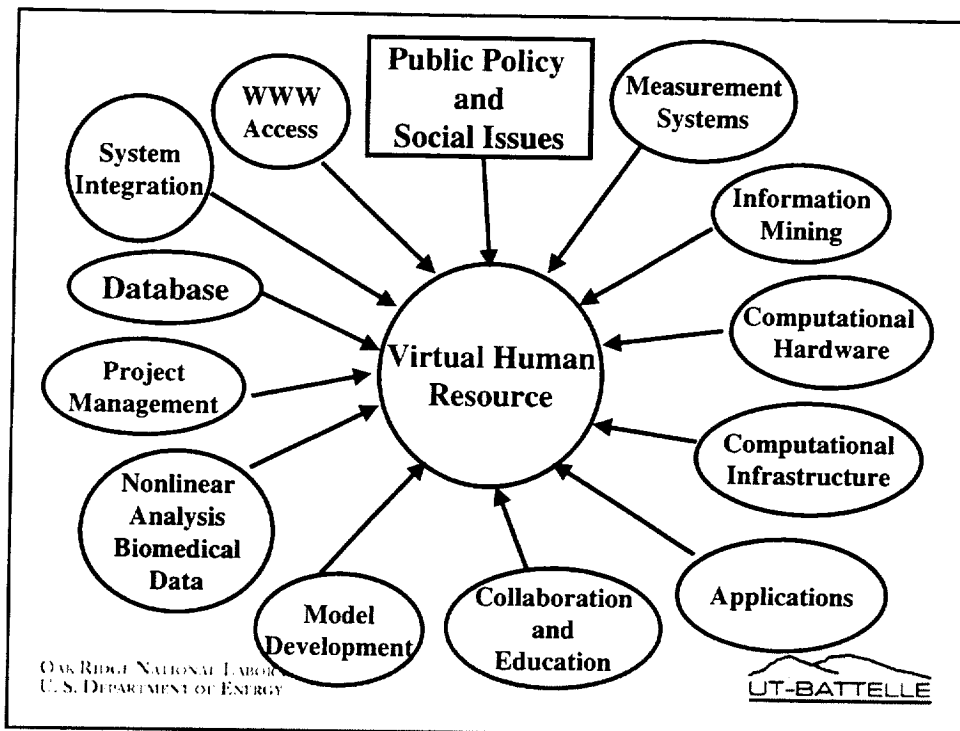
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Functional Goals (Cont.'d)

- **Specific Disease Information**
- **Duplicates Physiology Tests**
- **Incorporates Certain Patient-Specific Data**
- **Emphasize Diagnostic Assistance**
- **Patient Education and Teaching Tool**
- **Fast Forward Capability**

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ORNL's Vision of Virtual Human Initiative

**Simulate Human Biology to Advance Our
Understanding of Complex Biological Systems**

- **Infrastructure (National Resource)**
**Computational Infrastructure to Facilitate Use of
Data and Models**
- **Integration**
Data and Models

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Virtual Human Initiative Meeting National Academy, 28 Oct 1999

- **45 Attendees**
- **Presentations of Vision by Scientific Panel**
- **Responses by Agency Representatives**
- **Conclusion: To request that a report on the Virtual
Human Initiative be prepared by the National
Academy.**

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What's Coming in the Near-Term?

- **Focused Workshops**
- **Kinetic Energy Effects**
 - **Current models**
 - **Active sources of data**
 - **Legacy models and data**
 - **Workshop designed to build database**
 - **Develop links between disparate data**
- **Series of Gordon-Like Conferences**

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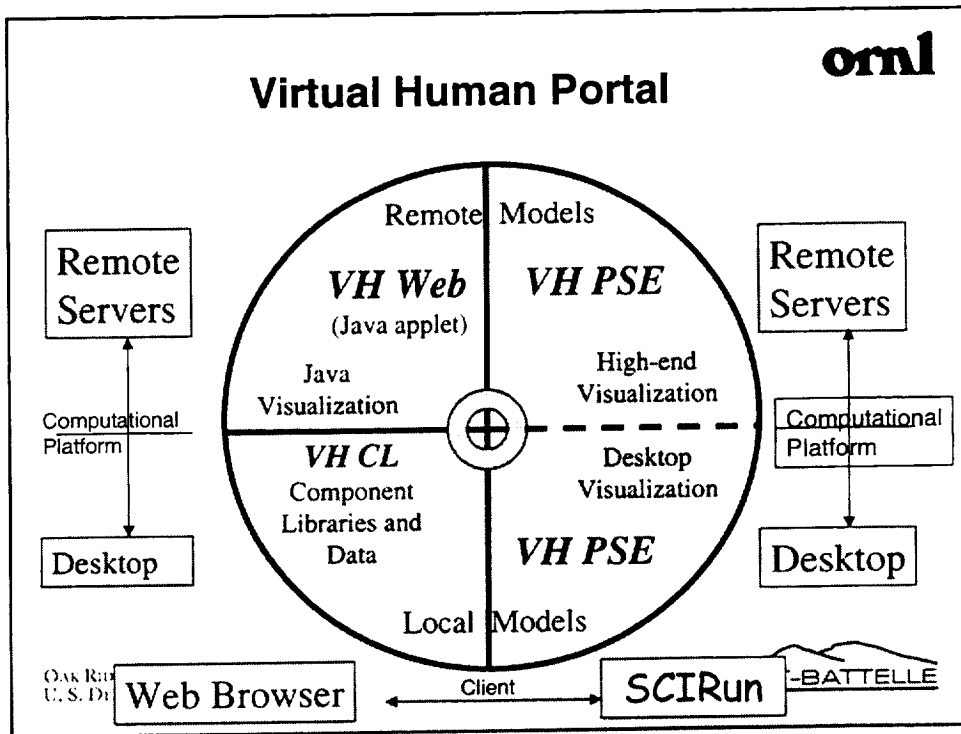
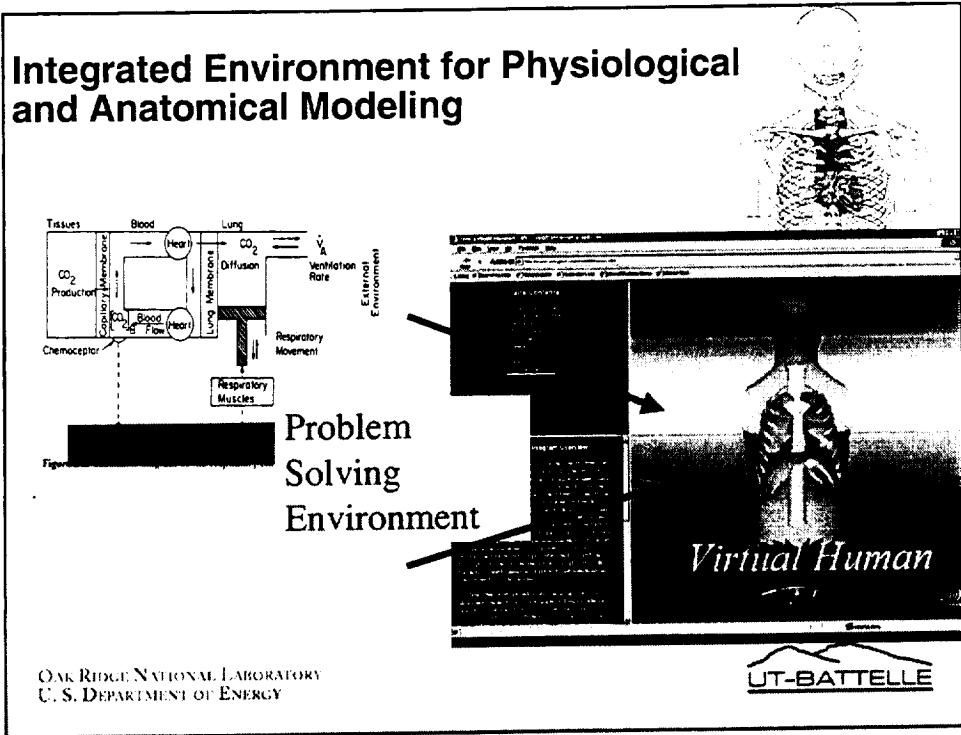
Brief Glimpse of Work On-Going at ORNL

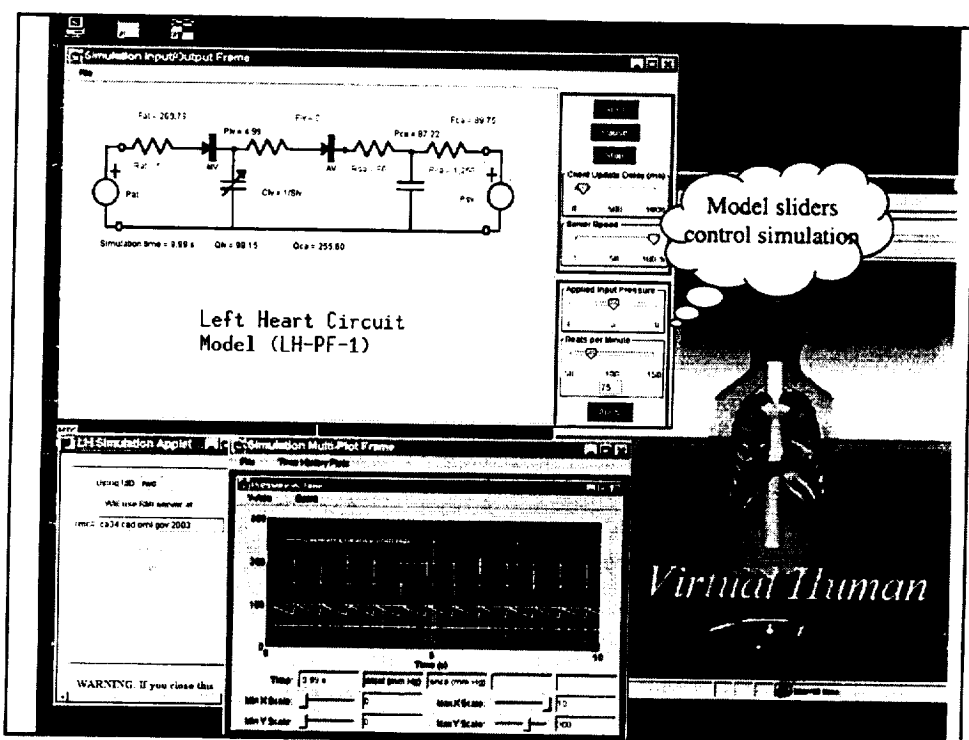
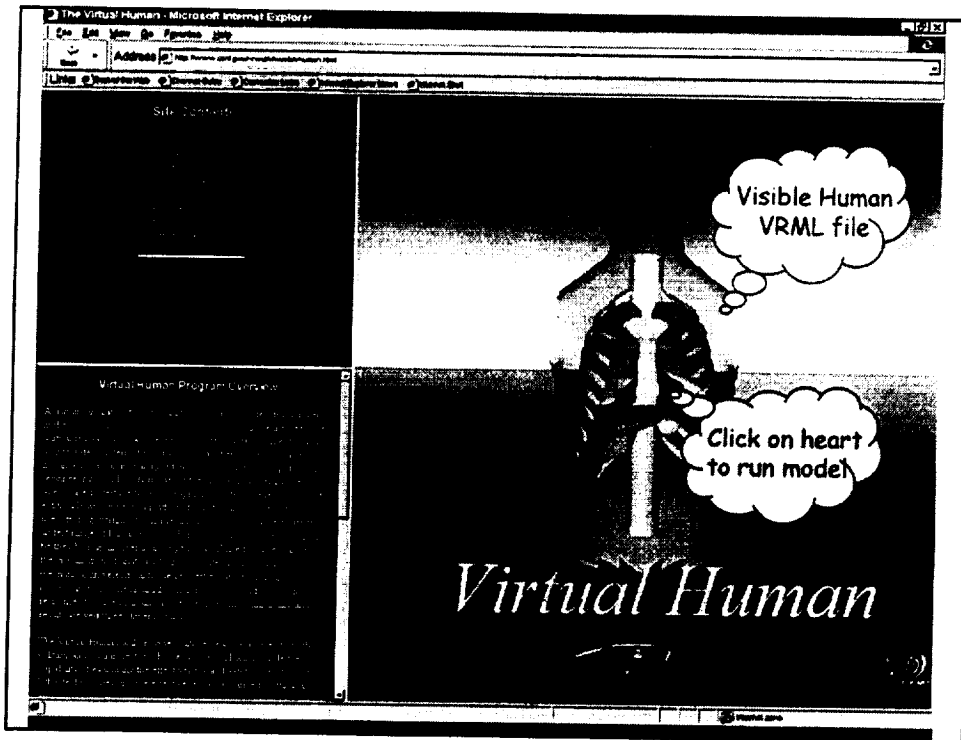
Three General Options Present Themselves:

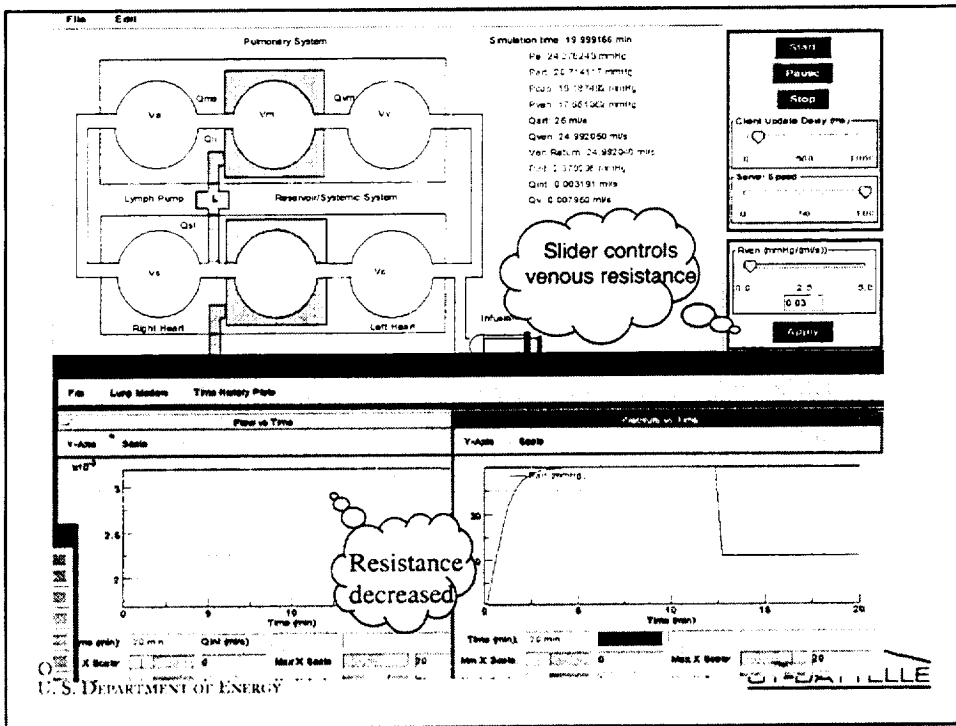
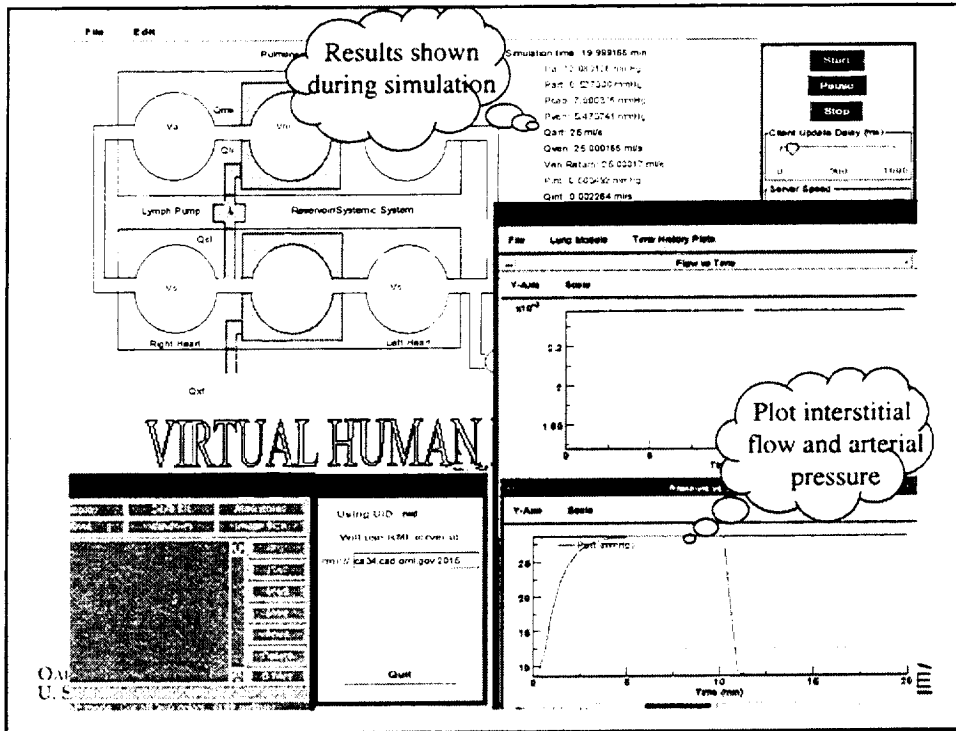
- 1. Develop infrastructure that allows communication between models**
- 2. Attempt to directly link existing models**
- 3. Develop infrastructure that serves as unifying feature for future models**

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Why Now?

- **Confluence of Complementary Technologies**
- **Faster Networks and Communications**
- **Network Software Technologies such as CORBA, Java, XML, etc.**
- **“Big Science” is inherently distributed and collaborative, and needs to migrate to the Internet to progress.**

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Is the Type of Mathematical Approach Important to the Application?

- **Application determines degree of complexity.**
- **Blunt trauma, testing military gear, forensic,... applications not requiring time series data... may not benefit significantly.**
- **Biomedical data... many types of data require chaos analysis to move beyond interpretation available 30 years ago.**
- **Applicability will change as understanding of human system matures.**

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Biomaterials

- **Biologically Produced Materials**
 - **Magnetic nano-particle formation by bacteria from the deep subsurface**
 - **Extracellular metal reduction/precipitation/crystallization**
 - **Iron reduction results in highly ordered nanocrystalline magnetite, maghemite, and siderite**
 - **Culture conditions affect phase mixture**
 - **Doping magnetite crystals with other metals (e.g., Ni, Co, Zn) is possible by adding them as soluble minerals in growth medium.**

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Biological Interfaces Research

- **Interfaces with Materials (Signal Processing/ Propagation)**
 - **Whole-cell sensing and bio-computing in a microelectronic format (“critters on a chip”)**

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Bioluminescent Bioreporter Integrated Circuits (BBICs)

CMOS IC-based whole-cell biosensors that detect chemical and biological agents.

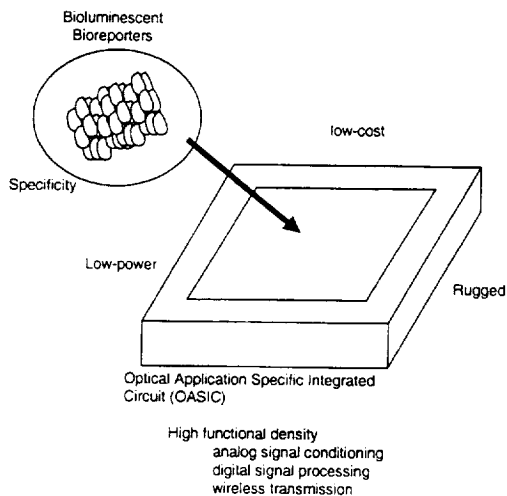
- *Environmental monitoring*
- *Chem/bio hazard detection*
- *Therapeutic drug discovery*
- *Medical diagnostics*
- *Disease control/management*



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BBIC Concept



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~~Device Physics~~ Biochemistry

Note: no exogenous addition of substrate

Membrane
↑
Lipids
↑
Myristol-ACP
↑
Acetyl-CoA

ATP → AMP+PP_i → Synthetase
Myristol-ACP → Myristic Acid (via Transferase, H₂O)
Myristic Acid → Myristyl Aldehyde (via Reductase, NADPH → NADP)
Myristyl Aldehyde → Light (via Luciferase, FMN, FMNH₂, O₂, H₂O)

Upper Pathway: A B F C D E
Lower Pathway: G Lux Cassette

Naphthalene → Salicylate (accumulating metabolite) → 2-oxo-4-hydroxypentanoate

Legend:
 ■ Promoter
 ▨ NahR Regulatory Protein
 ◇ Salicylate

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First Microluminometer Prototype

"Macroluminometer"
BG-250 LUMINOMETER

1.2- μ m bulk CMOS process

Signal processing

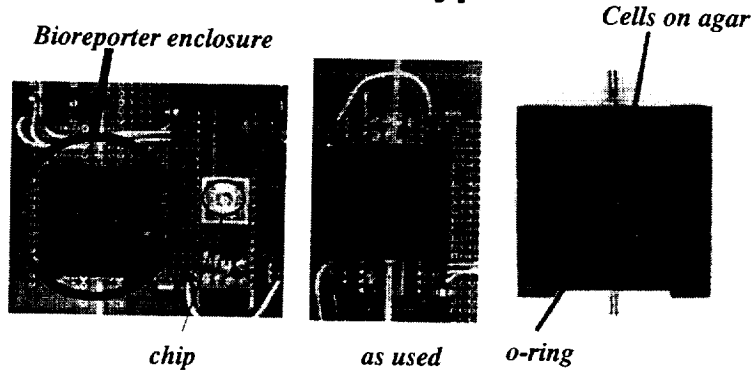
p-diff/n-well photo-detector

2.2 mm

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BBIC Prototype



Reference

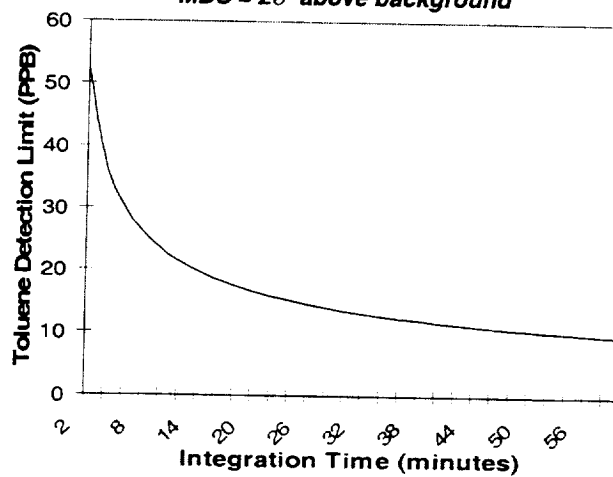
Simpson, Michael L., Saylor, Gary S., Ripp, Steven, Nivens, David E., Applegate, Bruce M., Paulus, Michael J. and Jellison, Jr., Gerald E., "Bioluminescent-Bioreporter Integrated Circuits Form Novel Whole-Cell Biosensors." (invited) *Trends in Biotechnology*, Vol. 16, August 1998, pp. 332-338.

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Toluene Sensing: Pseudomonas Putida TVA8

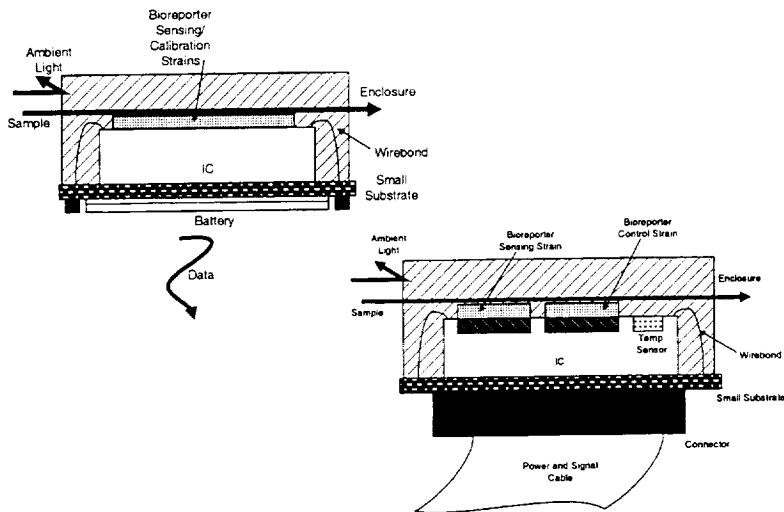
-1ppm toluene signal = 12 counts/minute
MDS = 2σ above background



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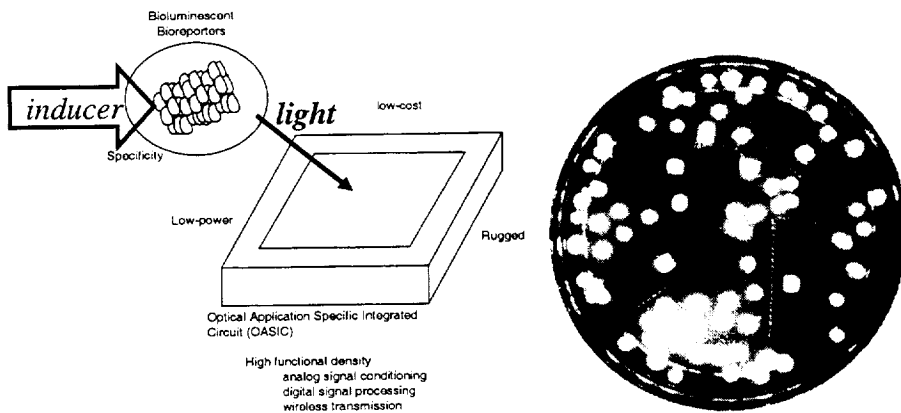
Possible Embodiments



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Bioluminescent Bioreporter Integrated Circuit (BBIC) Operates by Observing Single Gene Regulation

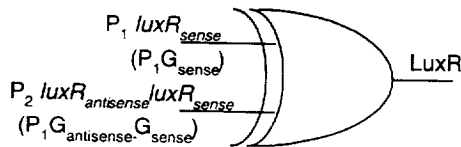
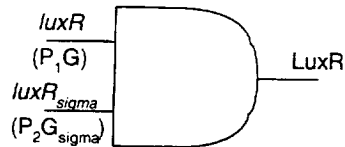
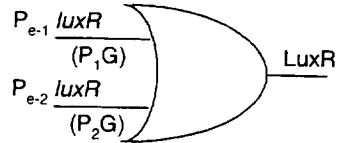


Can we do more?

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UT-BATTELLE

Engineered Information Processing in Whole Cells: *in vivo* Combinatorial Logic



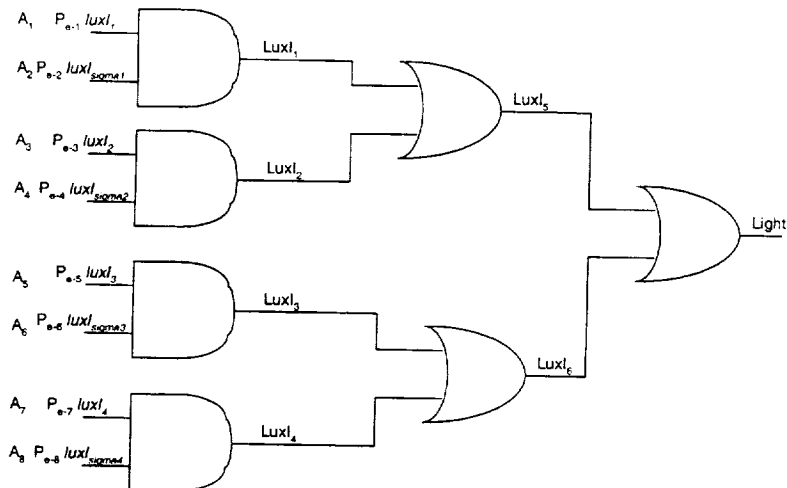
We can realize any combinatorial logic function with these three gates.

Latched devices can be made by adding feedback to these gates.

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A Reporter Gene Multiplexer Made with *in vivo* Logic Devices



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Communication to Cells

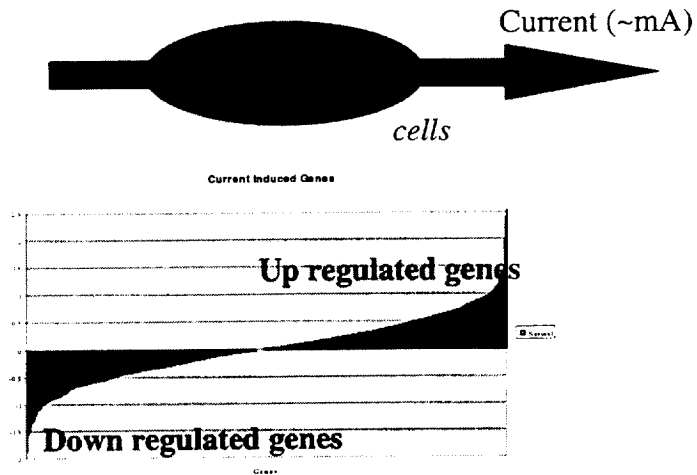
- *Chemical induction*
- *Thermal control of gene expression or enzyme activity*
- *Physical inducers (e.g., UV light)*

Question: Could we control gene expression from a microelectronic chip?

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Electrically-Inducible Promoters?



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Summary—Critters on a Chip

- *BBICs are novel whole-cell biosensors that combine the specificity of engineered bioluminescent bioreporters with the functionality, flexibility, and low cost of CMOS integrated sensor/circuit.*
- *We have developed a large number of bacterial and yeast bioluminescent bioreporters for BBIC sensing applications.*
- *We are now working to combine in vivo computing capabilities with the sensing functionality -- flexible, configurable, sensing devices.*

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Biological Interfaces Research

- **Interfaces with Materials (Signal Processing/ Propagation)**
 - Photon Bridging Between Biotic and Abiotic Components
 - Critters on a chip
 - Electron Bridging Between Biotic and Abiotic Components
 - Platinized Photosystem I particles
 - Hydrogen evolution
 - Sensing/biomolecular electronics applications
- **Interfaces with Computing**
 - Critters on a Chip Example: Biologically Based Logic Components
 - Virtual Human Example: Modeling Biological Function

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Biomorphic Systems and Biomorphic Missions

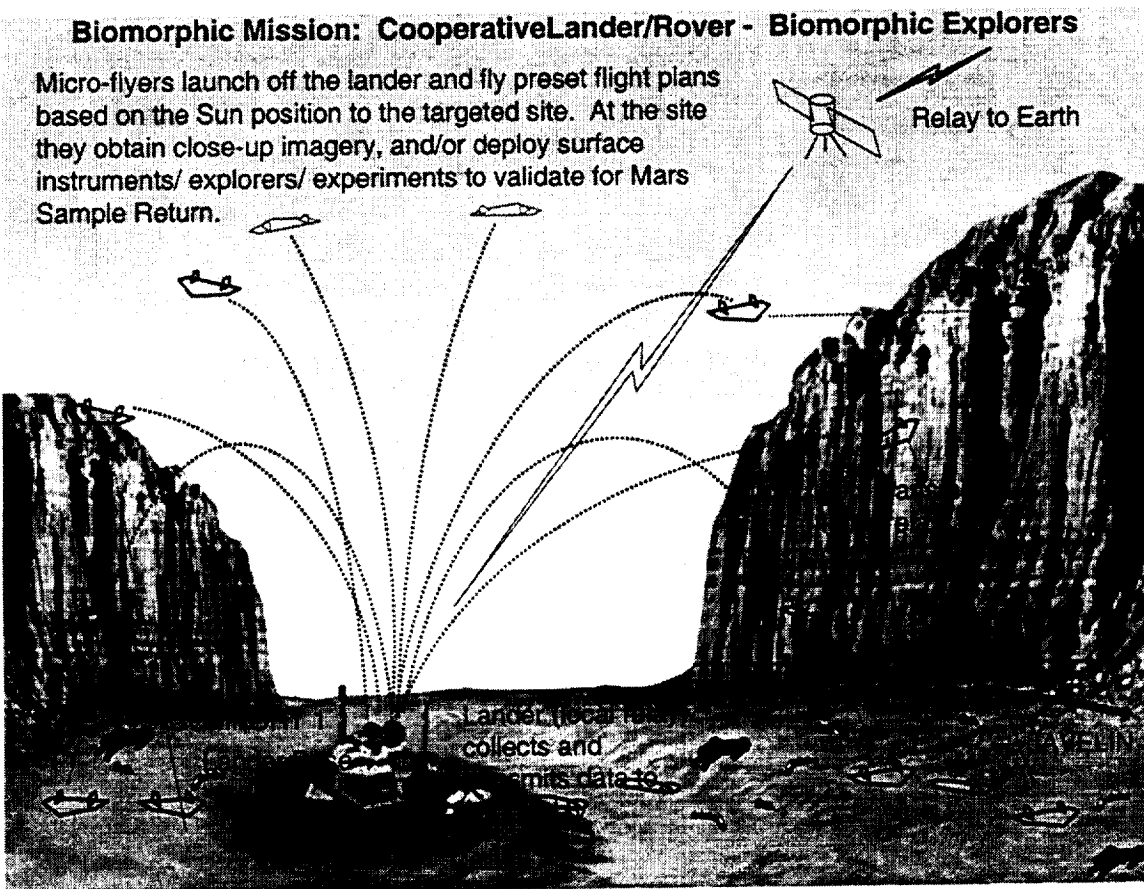
Sarita Thakoor
Jet Propulsion Laboratory
Pasadena, CA 91109

Biomorphic Systems and Biomorphic Missions

Sarita Thakoor

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, CA 91109-8099
(818) 354-3991
Email: sarita.thakoor@jpl.nasa.gov

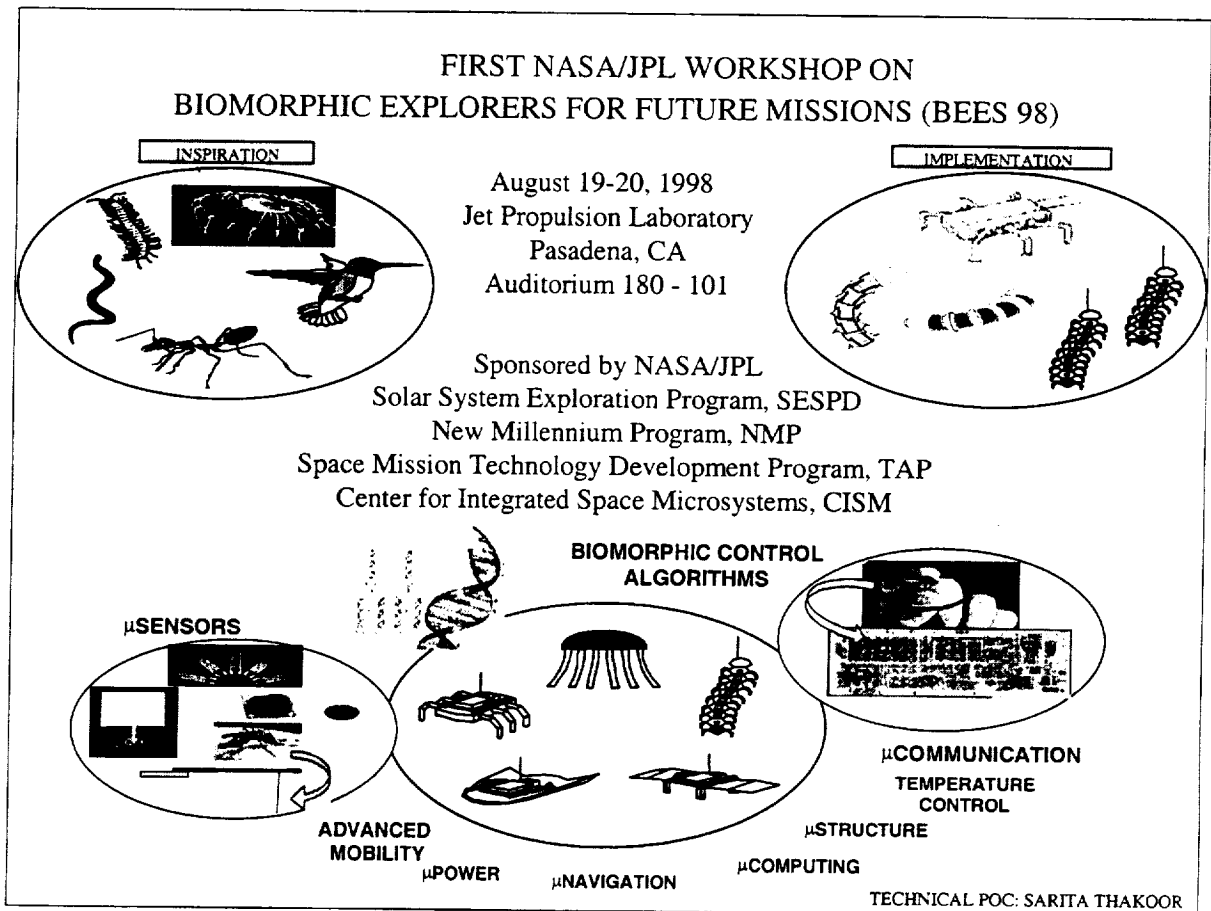
Training Workshop on Nano-biotechnology
NASA Langley Research Center, Hampton, VA
June 14-15, 2000



Biomorphic Explorers

- A multidisciplinary system concept for small, dedicated, low-cost explorers that capture some of the key features of biological organisms
 - Small... 100-1000g (useful space/terrestrial exploration functions are implementable* using this mass).
- Conducted workshop, Aug 19-20, 1998
 - Sponsored by NASA/JPL
 - WEBSITE: <http://nmp.jpl.nasa.gov/bees/>
 - An enthusiastic response: over 150 participants

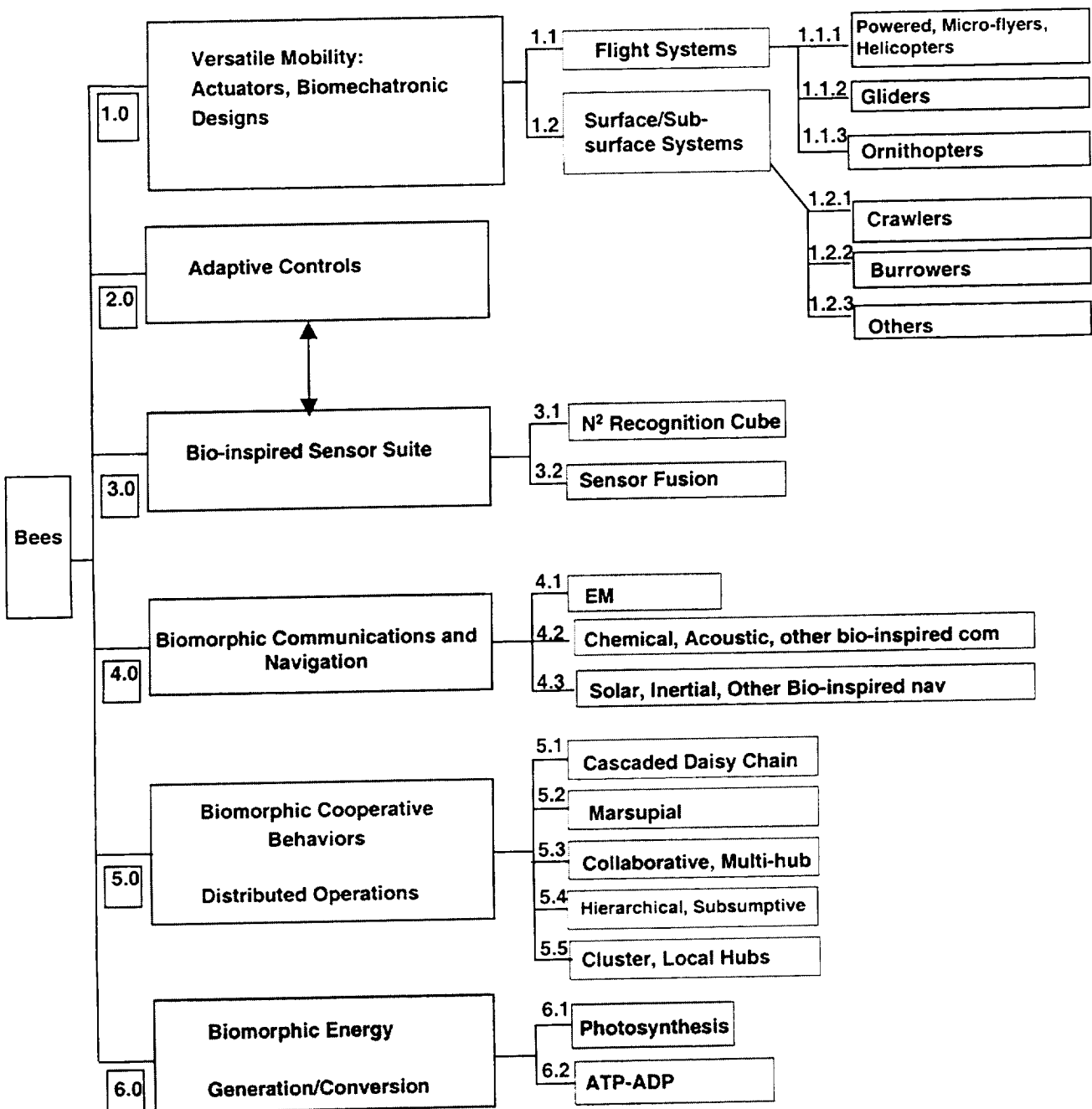
* JPL document D-14879A, JPL document D-16300A
 JPL document D-16500, Author: Sarita Thakoor



Bio-inspired Engineering of Exploration Systems (Bees) Subsystems Breakdown

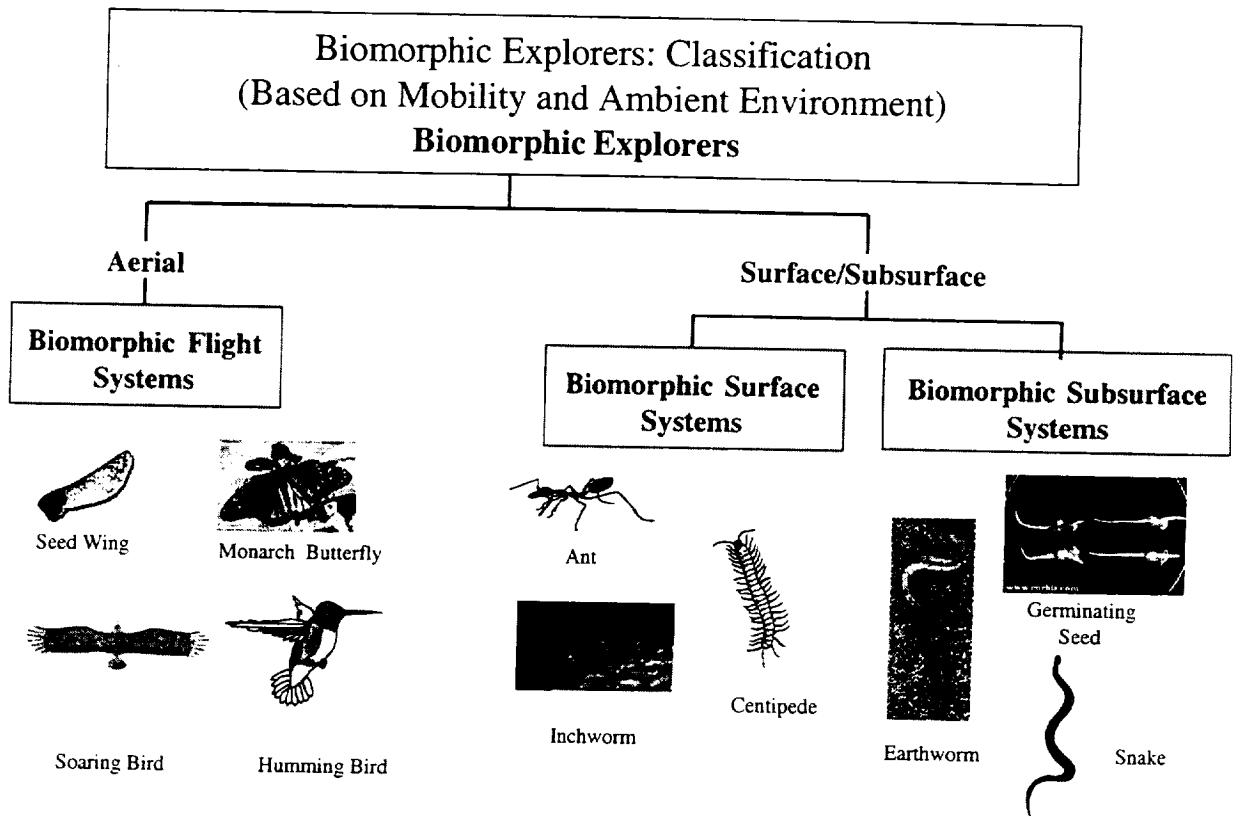
The following slide shows the sub-categories within the subject of bio-inspired engineering of exploration systems. This talk will focus mainly on the versatile mobility area and will briefly mention the highlights on the other sub-categories.

Bio-inspired Engineering of Exploration Systems (Bees) Subsystems Breakdown



Biomorphic Explorers: Classification

Examples of biological systems that serve as inspiration for designing the biomorphic explorers are illustrated. Choose a feature, say soaring. The intent is to make an explorer that combines the different attributes seen in nature in diverse species and capture them all in one artificial entity. In that sense the explorer goes beyond biology to provide us the adaptability that we need in encountering and exploring what is yet unknown.



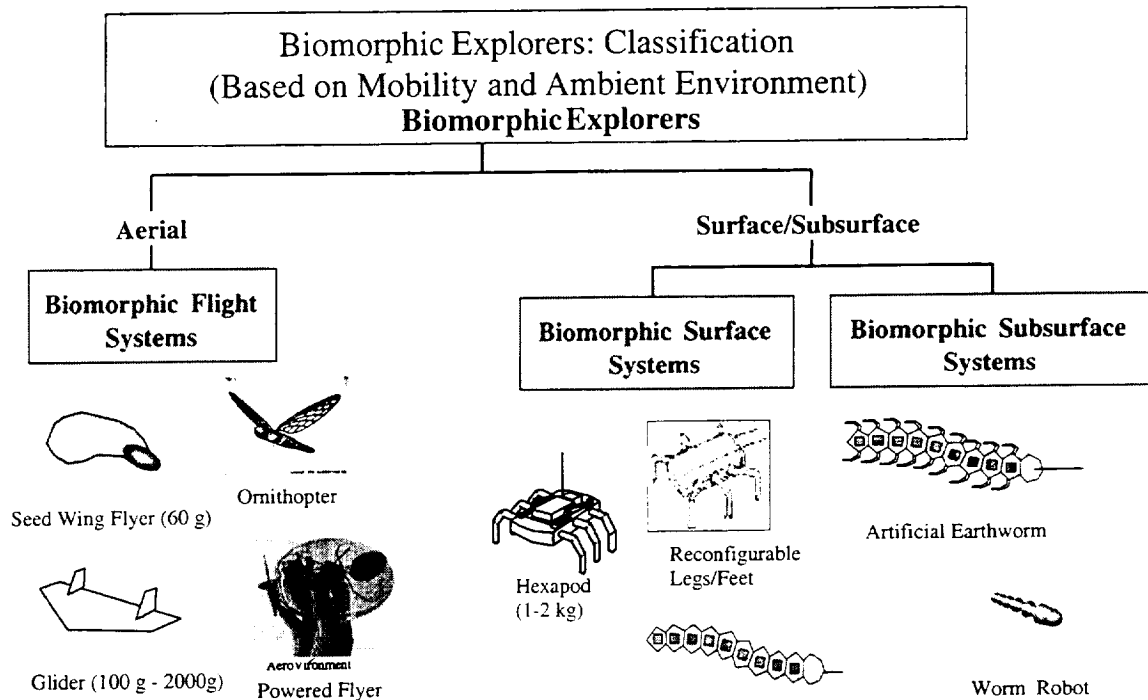
The Challenge to Obtain A Biomorphic Robot

Nature's Creations

- Primarily organics based.
- Evolution led surviving design and minimalist operational principles are inherent.
- Geological time scale has been used for evolution.

Bio-morphic Robot

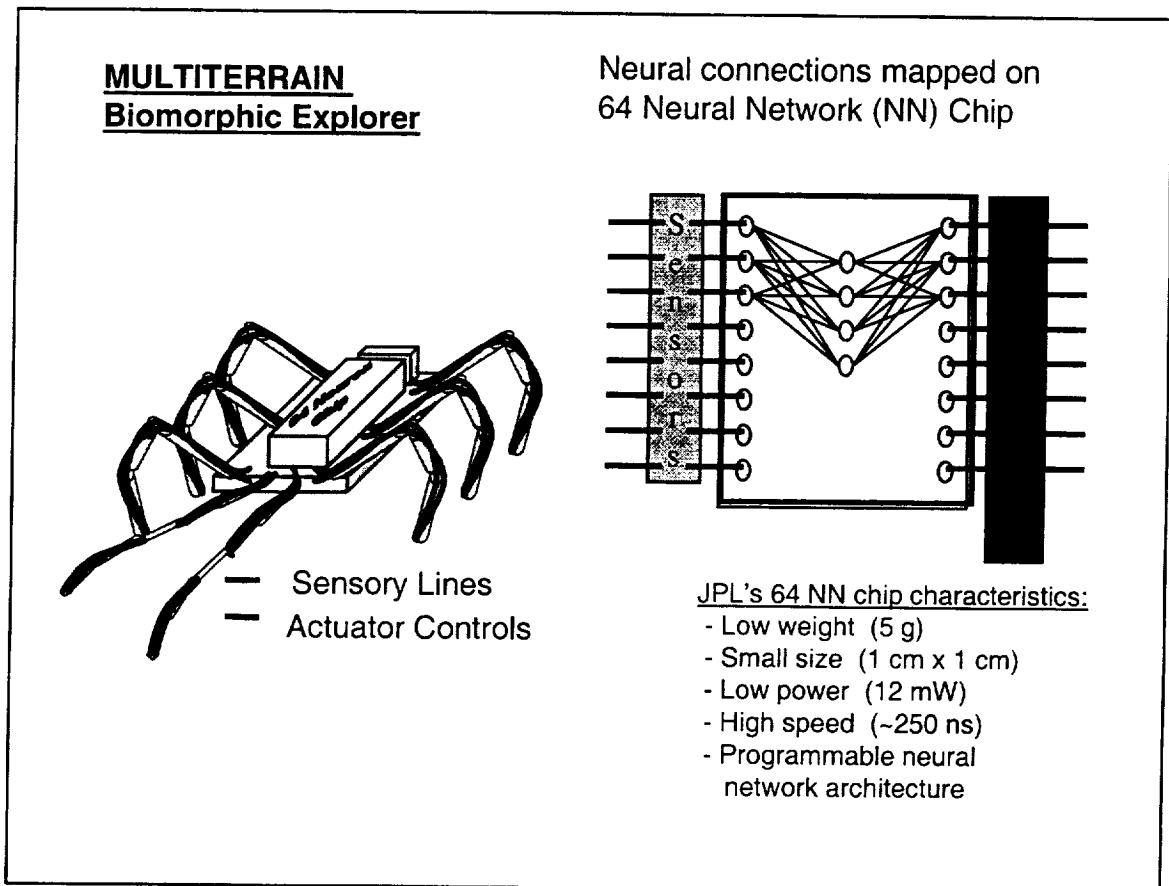
- Primarily inorganics based, the ingredients/materials are available to us.
- Needs to be created by distilling the principles offered by natural mechanisms.
- Capturing the bio-mechatronic designs and minimalist operation principles from nature's success strategies.
- Do it within a lifetime.



Candidate biomorphic explorers on the drawing board, with mass of design under study in parentheses

Multi-terrain Biomorphic Explorer

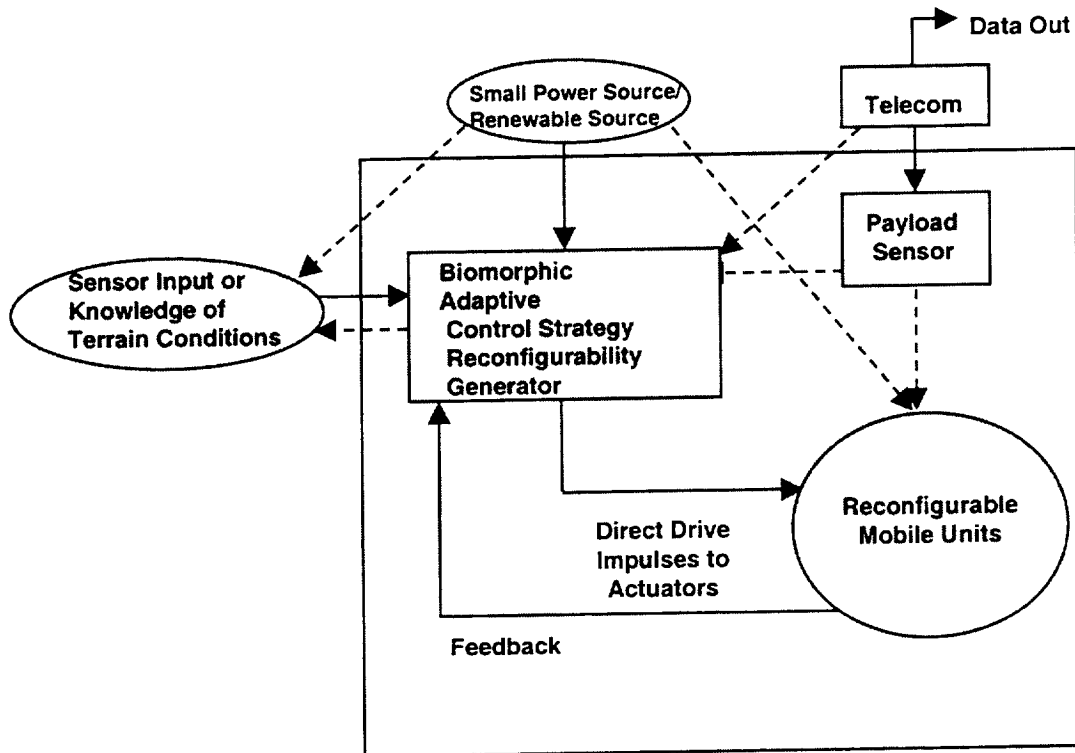
This development is geared toward the creation of an explorer that is capable of identifying its environmental condition/situation and adaptively change its mobility mode to suit the prevailing/impending situation. For example, if the terrain changes from hard and rocky to swampy slushy ground, then the explorer changes from a small footprint pogo stick type mode to a duck foot like wide footprint mode.



Distributed Control Operational Schematic

The following slide shows the operational schematic of the biomorphic strategy controller that utilizes multiple sensory inputs and generates the most suited output choice of mobility mode both in terms of the reconfigurable unit that is used and the mobility parameters that need to be used.

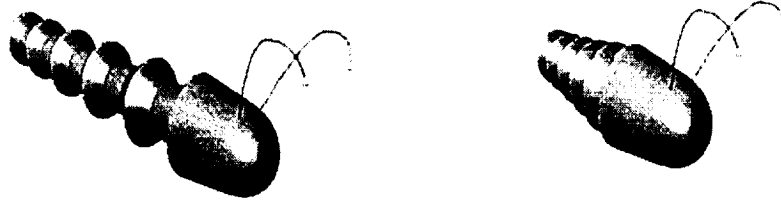
Distributed Control Operational Schematic



Worm Robot for In-situ Exploration

The worm robot conceptual design illustrated in the following slide, and shown in animation, is inspired by the technique used by earthworms and inchworms. The mobile entity is composed of a series of modules in which each module is capable of contracting or expanding and has anchors at each end. It anchors at one end and expands fully, then it de-anchors the back end and anchors the front end and contracts again and re-anchors the back end. This wave of contraction/expansion and anchoring/ de-anchoring proceeds continuously to achieve the forward motion. The animation shows how such a worm would be capable of burrowing in sandy soil and entering narrow cracks in rocks for obtaining pristine samples from such hard to reach places.

Worm Robot for In-Situ Exploration



Extended Configuration

Contracted Configuration

Z. Gorjian and S. Thakoor, "Biomorphic Explorers Animation Video," First NASA/JPL Workshop on Biomorphing Explorers for Future Missions, August 19-20, 1998, Jet Propulsion Laboratory, Pasadena, CA

Biomorphic Explorers: Versatile Mobility

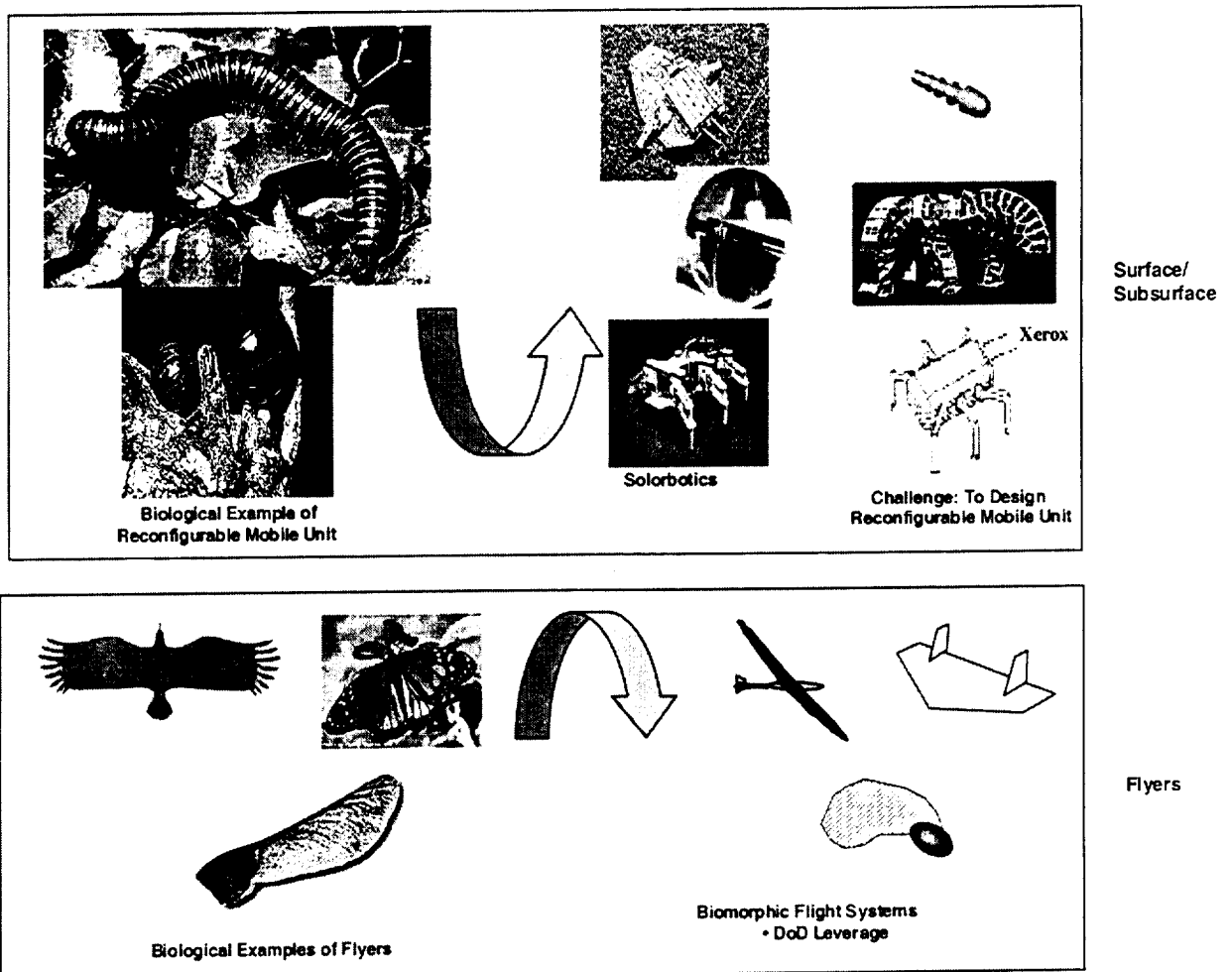
The surface/subsurface examples of versatile mobility discussed thus far are summarized in the top section of this slide. The bottom section of the slide shows examples of biomorphic flight systems and their respective inspirations.

Biomorphic flight systems are attractive because they provide:

- Extended reach over all kinds of terrain.
- Unique perspective for IMAGING, SPECTRAL SIGNATURE.
- Ability to perform distributed ATMOSPHERIC MEASUREMENTS.
- Ability to deploy/distribute payloads.

Many biomorphic explorers (seed wing flyers, crawlers, burrowers, gliders, etc.) can work in cooperation with large UXV's to enable new missions and achieve successfully (currently) UNATTAINABLE MISSIONS.

Biomorphic Explorers: Versatile Mobility

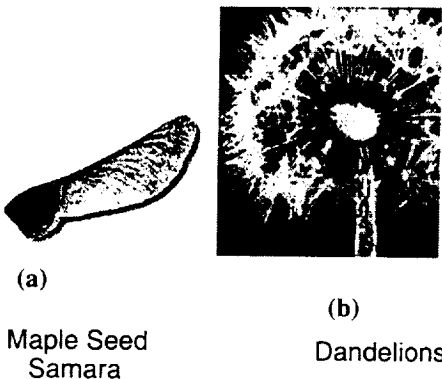


Biomorphic Controls in Seed Wing Flyers

Active control of seed wing descent is a significant concept for further development to impact the usefulness of seed wing flyers. This is an effort to influence the direction of descent, by periodic movement of a control surface on the wing portion. For example, a simple wing structural element made of advanced piezo-polymeric composite actuators could play a dual role as a structural member as well as an active control element when activated, altering the lift characteristics for a fraction of one rotation. The signal to drive the structural element would be generated by the measurement of sunlight on the upper payload surface. That signal would normally vary with rotation due to changing sun angle. Detection of a certain part of that periodic signal would be programmed to activate the change in wing shape. Thus, the seed wing would tend to move in a consistent pattern relative to the sun's direction. Individual seed wings in an ensemble could be programmed to have varying solar response patterns, ensuring that the group travels away from each other, for maximum dispersion in the landing location.

Plant World Inspired Payload Distribution Methods

- **Simpler and smaller than parachute on small scale for dispersion of sensors and small surveillance instruments.**
- **Controlled Descent Rate ~ 15 m/s (on surface of Mars)**



Design Goals:

- Small total mass, ~100 g.
- High payload mass fraction > 80%.
- Captures key features of controlled and stable descent as observed in Samaras, such as maple seeds.
- Reliable, minimal infrastructure.
- Unobstructed view overhead for atmospheric measurements.
- Simple construction, few constituent parts.

Biomorphic Explorers

- Bio-morphic explorers constitute a new paradigm in mobile systems that capture key features and mobility attributes of biological systems to enable new scientific endeavors.
- The general premise of biomorphic systems is to distill the principles offered by natural mechanisms to obtain the selected features/functional traits and capture the biomechatronic designs and minimalist operation principles from nature's success strategies.
- Bio-morphic explorers are a unique combination of versatile mobility controlled by adaptive, fault tolerant biomorphic algorithms to autonomously match with the changing ambient/terrain conditions.
- Significant scientific payoff at a low cost is realizable by using the potential of a large number of such cooperatively operating biomorphic systems.
- Biomorphic explorers can empower the human to obtain extended reach and sensory acquisition capability from locations otherwise hazardous/inaccessible.

Biomorphic Missions

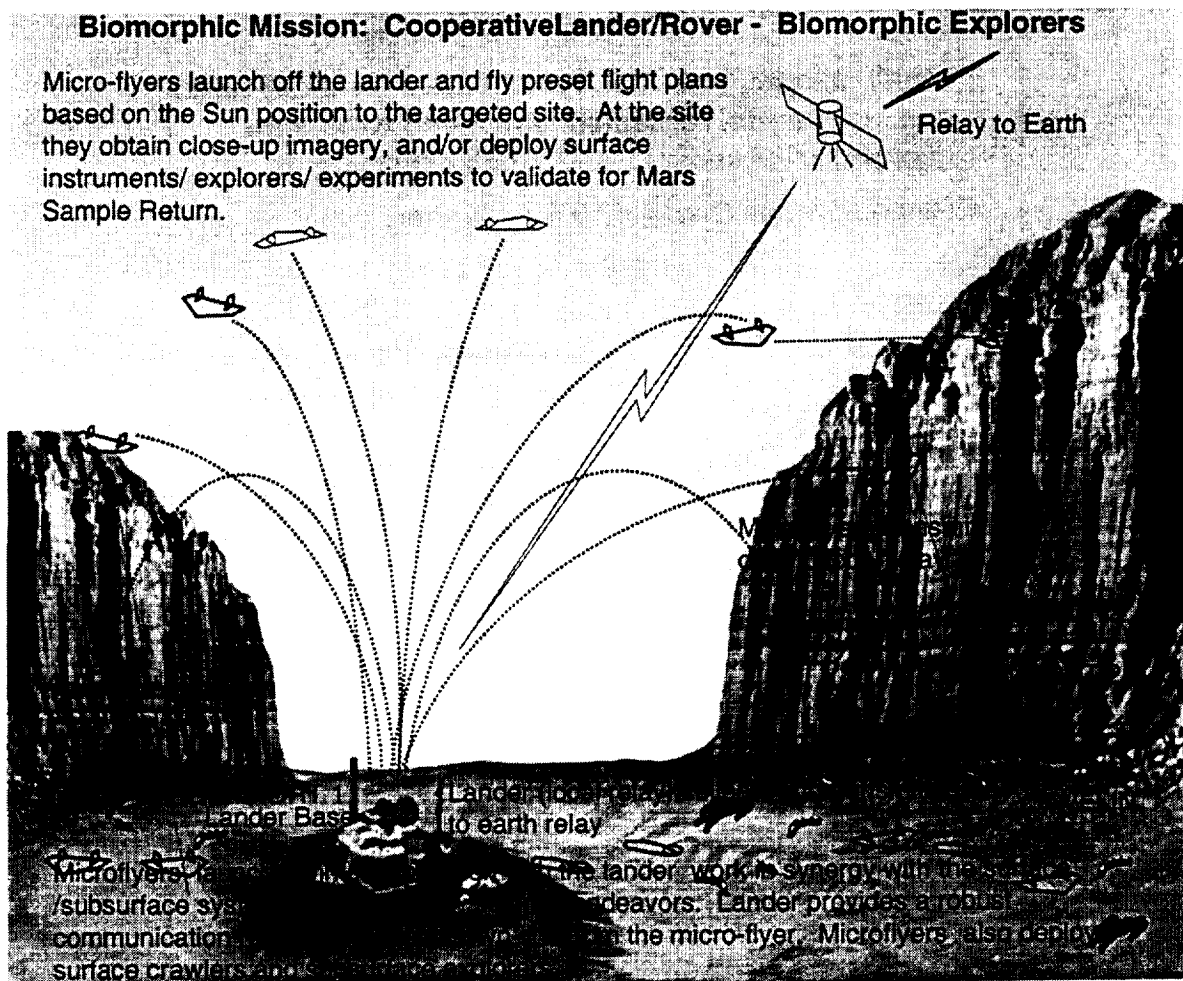
- Biomorphic missions are cooperative missions that make synergistic use of existing/conventional surface and aerial assets along with biomorphic robots.
- Just as in nature, biological systems offer a proof of concept of symbiotic co-existence. The intent is to capture/imbibe some of the key principles/success strategies utilized by nature and capture them in our biomorphic mission implementations.
- Specific science objectives targeted for these missions include:
 - Close-up imaging for identifying hazards and slopes;
 - Assessing sample return potential of target geological sites;
 - Atmospheric information gathering by distributed multiple site measurements; and
 - Deployment of surface payloads such as instruments/biomorphic surface systems or surface experiments.

Science Requirements

- Orbiter provides imaging perspective from ~ 400 Km height with resolution ~ 60cm to 1 m/pixel; lander mast imagery is viewed from ~ 1-2 m height. *The essential mid range 50m-1000m altitude perspective is as yet uncovered and is an essential science need. Imaging from this mid-range is required to obtain details of surface features/topography, particularly to identify hazards and slopes for a successful mission).*
 - Close-up imagery of sites of interest (~ 5 - 10 cm resolution).
 - 1-10 Km range, wide area coverage.
 - Distributed measurements across the entire range.
 - In-situ surface mineralogy.
- Candidate instruments include:
 - Camera (hazard and slope identification by close-up imagery).
 - Meteorological suite (in-flight atmospheric measurements).
 - Microphone to hear surface sounds, wind and particle impact noises.
 - Electrical measurement of surface conductivity.
 - Accelerometer measurement of surface hardness.
 - Seismic measurement (accelerometers).

Biomorphic Mission: Cooperative Lander/Rover - Biomorphic Explorers

- An auxiliary payload of a Mars Lander (2-10kg).
- Micro-gliders (4 - 20) launched/deployed from the Lander.
- Lander serves as a local relay for imagery/data downlink.
- Micro-glider provides:
 - Close-up imagery of sites of interest (~ 5-10 cm resolution).
 - Deploys surface payload/experiments (20g - 500 g).
 - In-flight atmospheric measurements.
 - Candidate instruments:
 - Camera (hazard and slope identification by close-up imagery).
 - Meteorological suite (in-flight atmospheric measurements).
 - Microphone to hear surface sounds, wind and particle impact noises.
 - Electrical measurement of surface conductivity.
 - Accelerometer measurement of surface hardness.
 - Seismic measurement (accelerometers).
- 50m-500m height, unique and essential perspective for imaging.
- 1-10 Km range, wide area coverage very quickly.
- Useful close-up imagery and surface payload deployment.
- 2005 Missions: Scout Missions, Sample Return Missions 2007 and beyond.

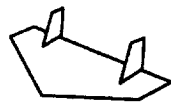
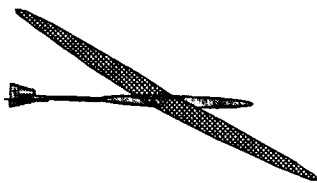


Surface Launched Microflyers: Options Comparison

- Contamination free launch options:
 - Spring launched (massive, KE leftover, complex possibly damaging recoil).
 - Electric launch options (power hungry):
 - Electrically driven propeller (Mars atmosphere is too thin).
 - Electromagnetic gun.
 - Inflate and release a balloon (complicated mechanism, thin atmosphere a challenge, susceptible to winds).
 - Pneumatic, compressed gas launch (simple mechanism, simple recoil, leading candidate).
- Rocket boosted launch (contaminants, HCl, nitrates, etc.) a good option for application such as scouting where contamination is not an issue.

Biomorphic Microflyers

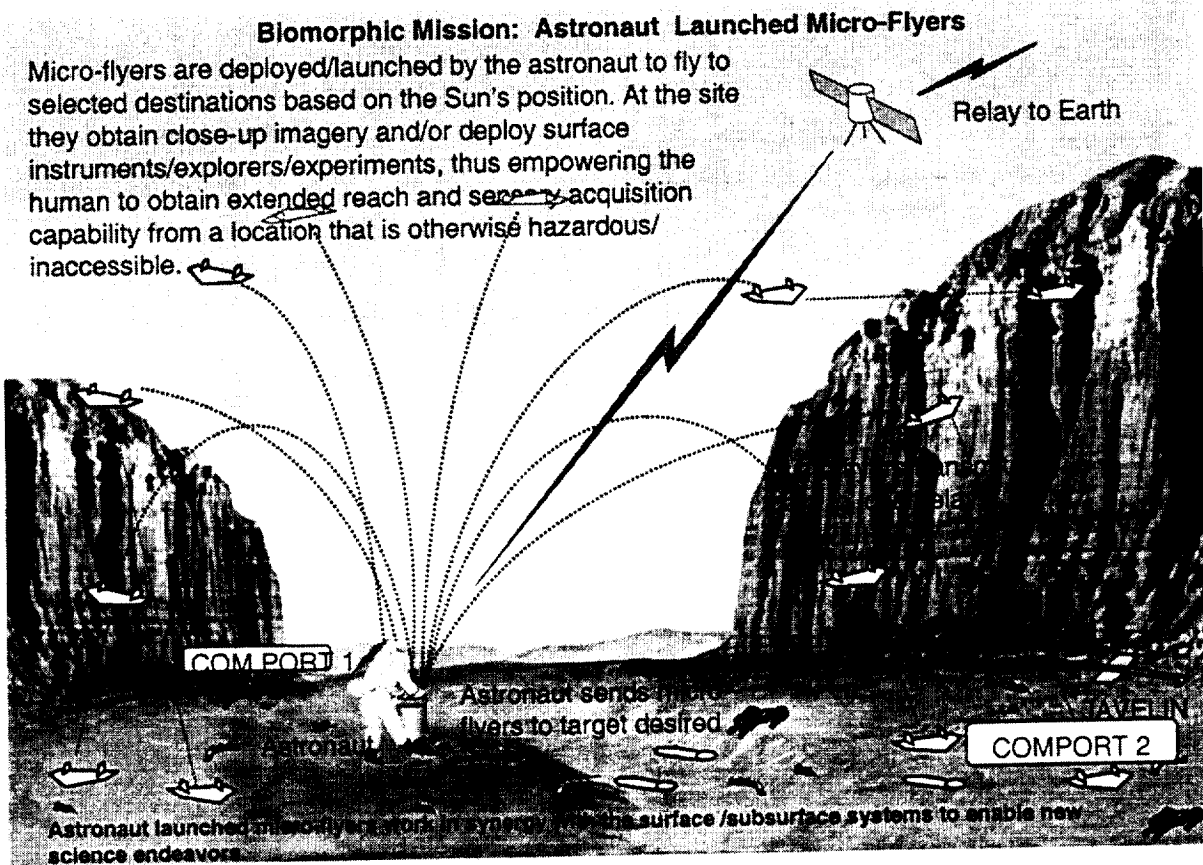
- **Small, simple, low-cost system ideal for distributed measurements, reconnaissance and wide-area dispersion of sensors and small experiments.**
- **Payload mass fraction 50% or higher.**



- **Small mass (100 g - 1000 g)**
- **Low radar cross section**
- **Larger numbers for given payload due to low mass**
- **Precision targeting to destination**
- **Amenable to cooperative behaviors**
- **Missions can use potential energy by deploying from existing craft at high altitude**
- **Captures features of soaring birds, utilizing rising currents in the environment**
- ***Adaptive behavior***
- ***Self repair features***

Science Objectives

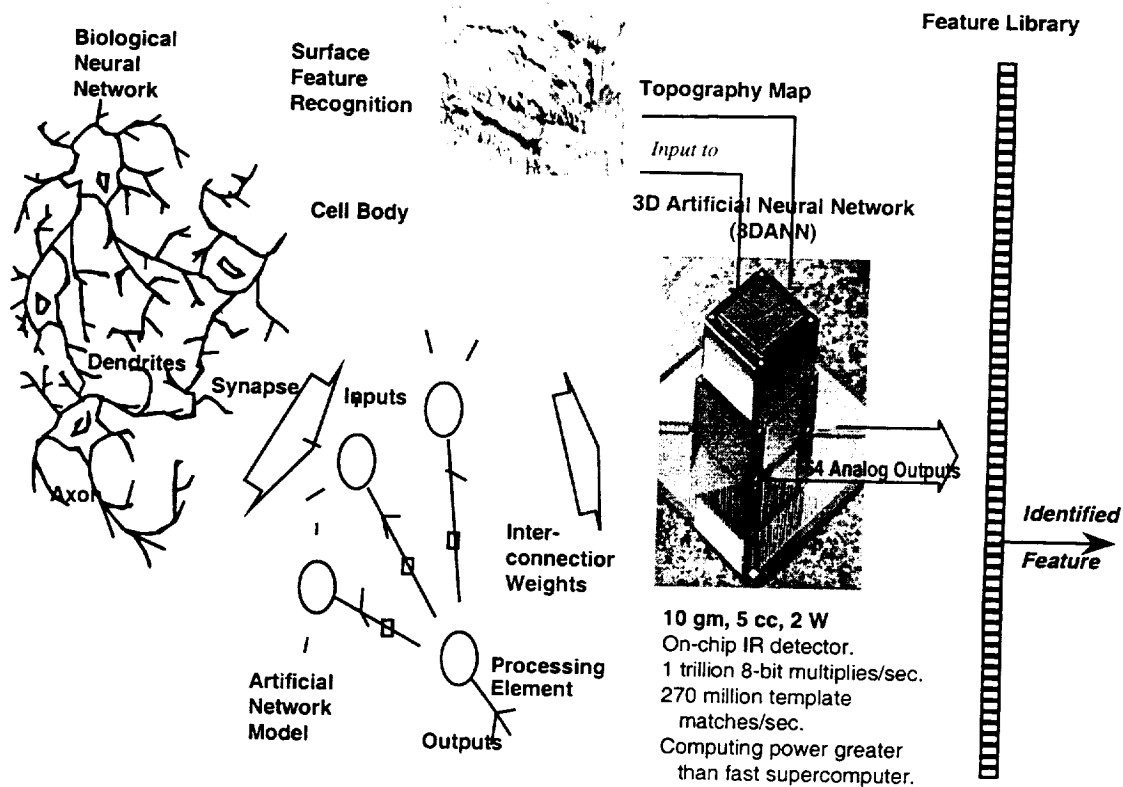
- Near Term 2005
 - Image surface topography.
 - Characterize terrain around lander.
 - Identify rocks of interest for rover.
 - Distribution of instruments/experiments/surface explorers to targeted sites.
- 2007-2009
 - Enable sample return by allowing scouting and long range maps of areas of interest.
- Long Term 2011 and Beyond
 - Cooperative operation of a multitude of explorers together to obtain imagery and deploy surface payloads.
 - Astronaut launched micro-flyers: Empowering the human to obtain extended reach and sensory acquisition capability from locations that are otherwise hazardous/inaccessible.



Enabling Processor for Surface Feature Recognition

Modeled after the massively parallel neural networks in the human brain, 3DANN is a low-power, analog computing device capable of achieving human-like target recognition capability. The sugar-cube sized 3DANN processor has achieved an overall computing speed of ~ 1 trillion operations per second, consuming only ~ 8 watts of power. This is ~ 3 orders of magnitude higher than the state-of-the-art image-processing on conventional digital machines (e.g., Apple's recently introduced G4 computer which delivers ~ 1 billion operations per second, consuming ~ 200 watts of power). The N3 processor can be trained to recognize geological features of interest and used to obtain real time processing of camera input imagery to identify surface features of interest. As a compact, low-power, intelligent processor on-board a space system, it would enable for the first time, real-time functions such as in-situ landing site selection with hazard avoidance, visual navigation, precision rendezvous and docking, and visually intelligent planetary robots/rovers capable of autonomous selection of scientifically interesting spots for maximum science return.

Enabling Processor for Surface Feature Recognition



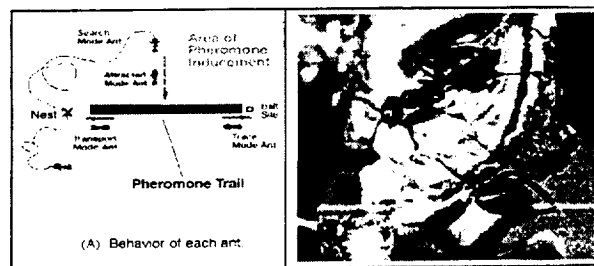
Biomorphic Cooperative Behaviors

The behavior of ant colonies, specifically, how the ants coordinate complex activities like foraging and nest building, has fascinated researchers in ethology and animal behavior for a long time. Several behavioral models have been proposed to explain these capabilities. Algorithms inspired by the behavior of ant colonies have already entered the mathematical field of multi-parameter optimization. Solar system exploration, particularly of Mars and certain planet/satellites, could be substantially enhanced through the use of a multitude of simple, small, somewhat autonomous explorers that as a group would be capable of "covering" large areas. A fleet of such explorers would have some form of limited communication with a mother ship (a larger lander/rover or an orbiter). In many cases, cooperation among all the "fleet-mates" could greatly enhance group effectiveness. Our program is geared to identify potential useful cooperative behaviors for such explorers by surveying emerging multi-robot multi-agent techniques and by assessing some of the uniquely powerful examples of cooperative behavior and self-organization observed in nature, specifically in the insect kingdom.

Biomorphic Communication and Navigation

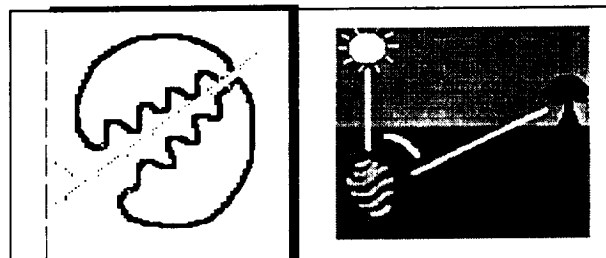
Honeybees are impressive in their ability to communicate precise navigational information. They use a recruitment dance and the sun as a celestial reference to communicate the location of a food source. Such principles related to planetary exploration could be utilized in a new class of small, dedicated, low cost biomorphic explorers.

Insects Operating Cooperatively:



Nakamura and Kurumatani, 1995
Kubo, 1996

Ants' elaborate communication method with pheromone trails.



Karl von Frisch, 1965,
Wehner and Rossel, 1985,
Barbara Shipman, 1997

Honeybee's recruitment dance with the sun as a celestial reference.

Science Applications

....which would be enabled/enhanced by such explorers.....

- Valles Marineris' Exploration
 - One single site rich in geologic units
 - Study strati-graphic column top to bottom along the canyon wall
 - Optimum science sample site
 -imager, temperature sensor, pressure sensor, sniffer: e-nose, individual gases, elements, etc.
- Scouting for conditions compatible with life to lead us to the spots that may hold samples of extinct/extant life
 - Wide-area search with inexpensive explorers executing dedicated sensing functions: close-up imaging!!!!
 -individual gases, sniffer: e-nose, chemical reactions, pyrotechnic test, elements, specific amino acids, signatures of prebiotic chemistry, etc.
- Geological data gathering:
 - Distributed temperature sensing
 - Seismic activity monitoring
 - Volcanic site
 -multitude of explorers working in a cascade or daisy-chain fashion cooperatively to fulfill task.

Applications (Dual Use NASA and DoD)

- Close-up Imaging, Site Selection
- Meteorological Events: Storm Watch
- Reconnaissance
- Biological Chemical Warfare
- Search and Rescue, etc.
- Surveillance
- Jamming
- Distributed Aerial Measurements
 - Ephemeral Phenomena
 - Extended Duration Using Soaring
- Delivery and Lateral Distribution of Agents (Sensors, Surface/Subsurface Crawlers, Clean-up Agents)

Acknowledgements

JPL

Matt Golombek: Mars Geology
Brett Kennedy: Mechanical Design
Gerhard Klose: Structure
Ken Klassen: Camera
Terry Martin/Tim Schofield: Atmospheric Science
John Michael Morookian: Electrical Design and System Integration
Frank Palluconi: Science Imagery
Satish Krishnan/Robert Manning: Lander/Rover
Dara Sabahi: Entry and Landing
Anil Thakoor: Image Processing
Ken Nealson: Astrobiology

CALTECH:

Ali Hajimiri and Dave Rutledge: Telecom

RAYTHEON:

Jim Small: Aerodynamics and Navigation

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JET PROPULSION LABORATORY

INDUSTRY: RAYTHEON, AEROVIRONMENT, SONY, XEROX,
PIONEER

NATIONAL LABS: LANL, SRI, ORNL, SANDIA

ACADEMIA: MINNESOTA, BERKELEY, CALTECH, PENN STATE,
VANDERBILT, USC, UCLA, ARIZONA, ROCHESTER, MONTANA,
CORNELL, NAGOYA, JAPAN, AUSTRALIA

OTHER NASA CENTERS: GSFC, AMES, LANGLEY, JSC

12/12

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Nanomaterials in Biotechnology

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Nanomaterials in Biotechnology

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NASA Workshop on NanoBiotechnology

June 15, 2000

NASA Langley Research Center, Hampton, VA

Nanotechnology in Biotechnology

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Robert W. Hunt Professor
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The past decade has seen an explosive growth worldwide in the synthesis and study of a wide range of nanostructured materials. A brief overview of this field, and its relationship to nanotechnology in general, will be presented with respect to possible applications in biotechnology. Results from our recent investigations of a variety of nanocomposites and cellular interactions with nanoscale ceramics will be presented, along with some considerations of novel future directions.



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**NATIONAL
NANOTECHNOLOGY
INITIATIVE**

<http://www.nano.gov/>

WTEC Panel Report on:

**Nanostructure
Science and
Technology**

R & D Status and Trends in Nanoparticles,
Nanostructured Materials, and Nanodevices

Edited by
Richard W. Siegel, Evelyn Hu and M.C. Hoo

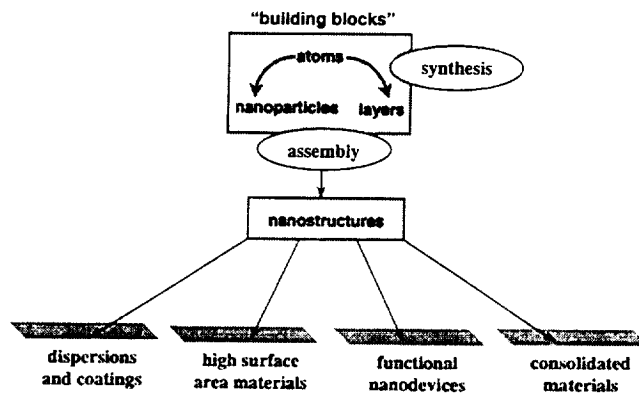
Kluwer Academic Publishers
Dordrecht / Boston / London



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Nanotechnology Organization Chart



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Characteristics of Nanostructures (Materials and Assemblies)

- ◆ Small
- ◆ Lightweight
- ◆ Novel properties
- ◆ Multifunctional
- ◆ Hierarchical
- ◆ Smart



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What Are Some Opportunities?

- ◆ **Nanocomposite materials and coatings:**
 - Thermal and environmental barriers
 - Wear resistant coatings and parts
 - Tailored optical and chemical barriers
 - Flame retardant plastics (packaging)
- ◆ **High surface area nanostructures:**
 - Fillers and catalysts
 - Energy storage media (batteries, fuel cells)
 - Drug or food supplement delivery vehicles



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◆ Hierarchical Nanostructures

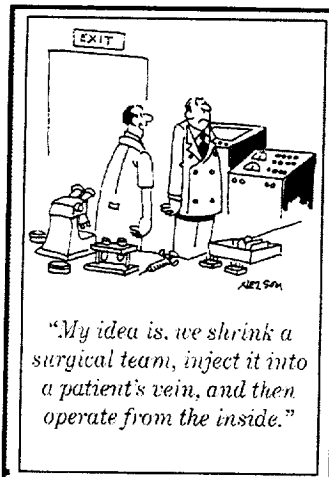
- Ultrahigh-strength, tough structural materials
- Ductile and strong cements
- Net-shape formed ceramic parts (wear, cutting)
- Magnetic/thermoelectric thermal management
- New materials for MEMS and sensors
- Smart materials with embedded sensors and actuators



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The Ultimate Biomedical Goal of Nanotechnology:



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Issues in Nanostructuring:

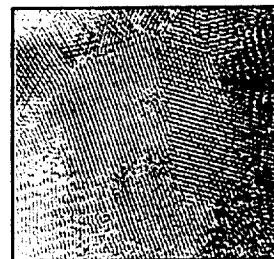
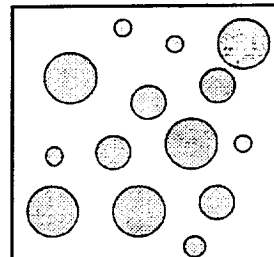
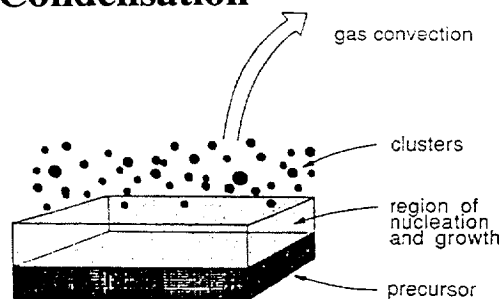
- ◆ **Building Blocks**
 - Scale
 - Composition
- ◆ **Assembly**
 - Interaction (interfaces)
 - Modulation dimensionality
 - Architecture (hierarchy)
- ◆ **Function**
 - Properties



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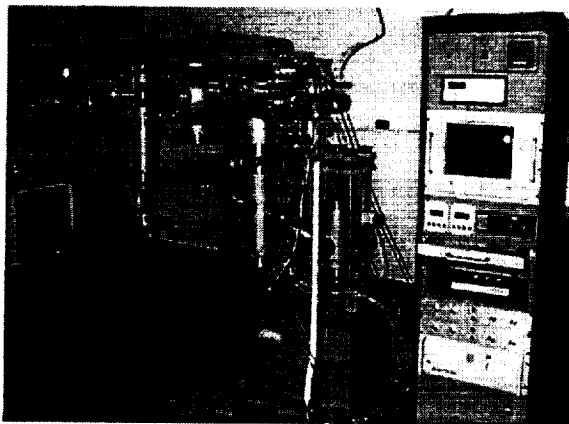
Cluster Synthesis by Gas Condensation



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Nanoparticle Synthesis System at Rensselaer



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Nature:

Scaffold or
template



fill with
“nanoparticles”

Nanostructuring:

“Nanoparticle”
building blocks



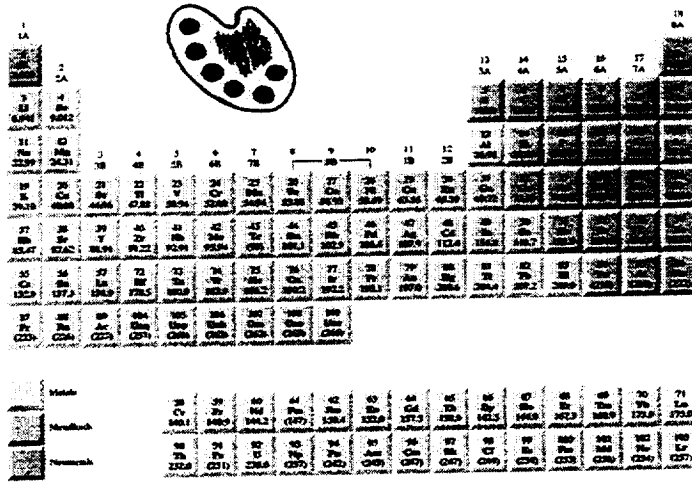
assembly



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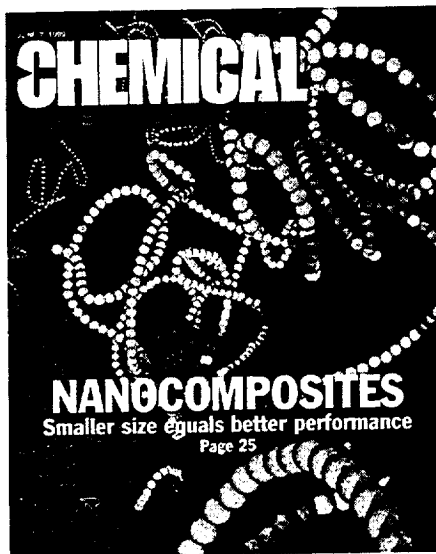
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Palette for Nanostructuring



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- ◆ matrix
- ◆ filler
- ◆ interface

Schadler, Ajayan et al. (1999)



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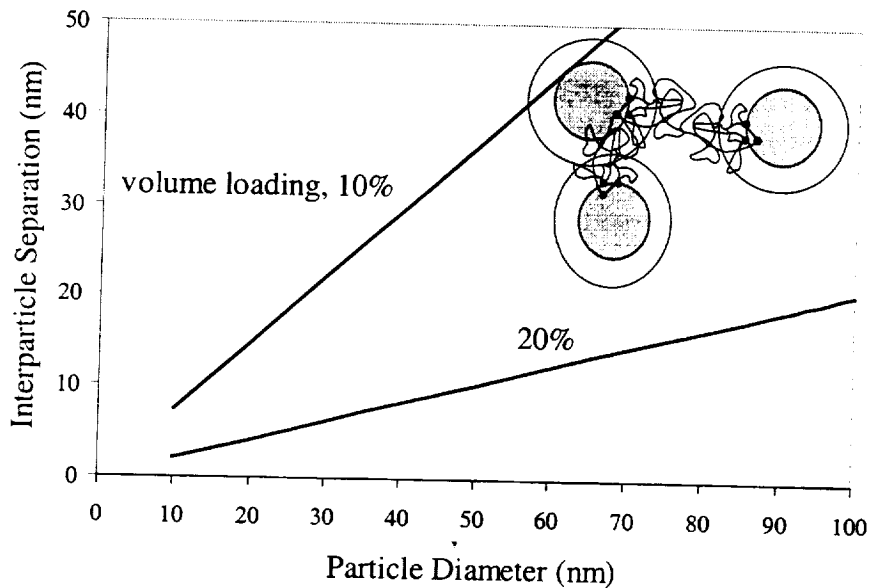
Nanocomposites: Opportunities

- ◆ **Fillers: Inorganic Nanoparticles, Carbon Nanotubes**
- ◆ **Matrices: Polymers, Ceramics**
 - Large Interface Area
 - Light Weight
 - Variable Conductivity (Electrical, Thermal)
 - High Strength/Stiffness
 - (Modulus of Nanotubes ~ 1 TPa)



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Composite Systems Investigated

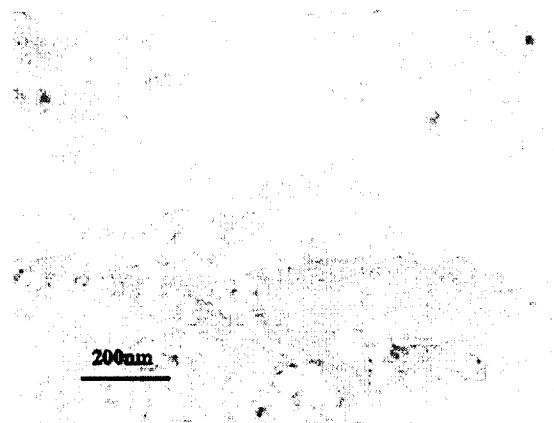
- ◆ Ceramic nanoparticles/polymer
- ◆ Carbon nanotubes/polymer
- ◆ Carbon nanotubes/nanophase ceramic



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Titania/Epoxy Nanocomposite

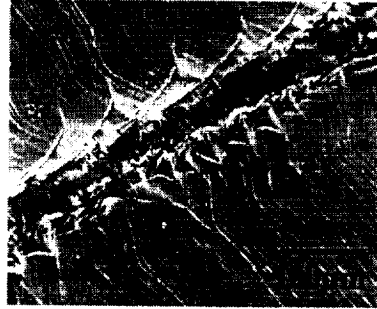


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Scratch Testing

The damage surrounding the scratch is reduced for 10 wt% *nano*-TiO₂ filled epoxy, compared to 10 wt% micron-TiO₂ filled epoxy. (Scratch depth in parentheses.)



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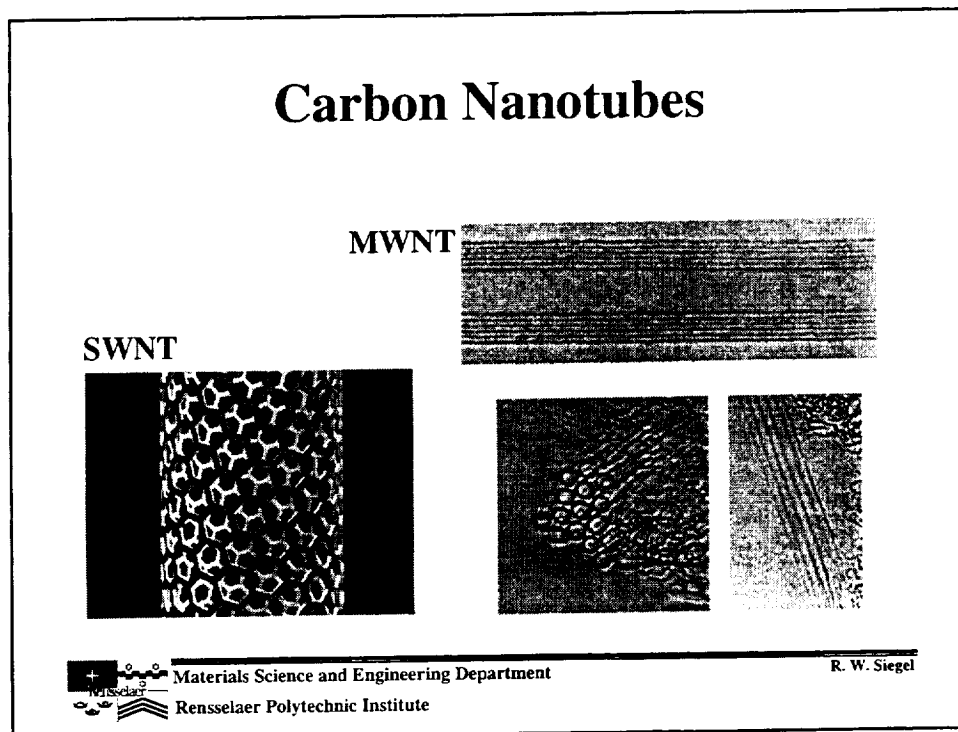
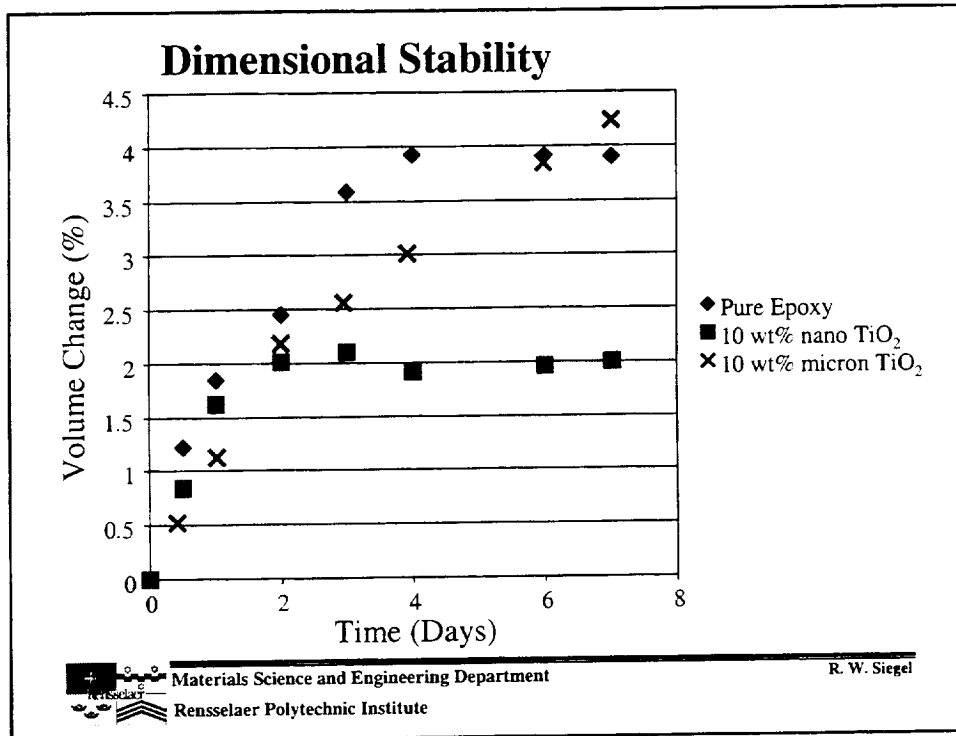
Results of Tensile Testing

Materials	Modulus (GPa)	Strain to failure(%)
Epoxy	3.0	4.9 ± 0.9
5 wt% nano TiO ₂ / Epoxy	3.4	N/A
10 wt% nano TiO ₂ /Epoxy	3.3	5.6 ± 0.9
10 wt% micron TiO ₂ / Epoxy	3.3	4.1 ± 1.5
20 wt% nano TiO ₂ /Epoxy	3.5	3.0 ± 0.8

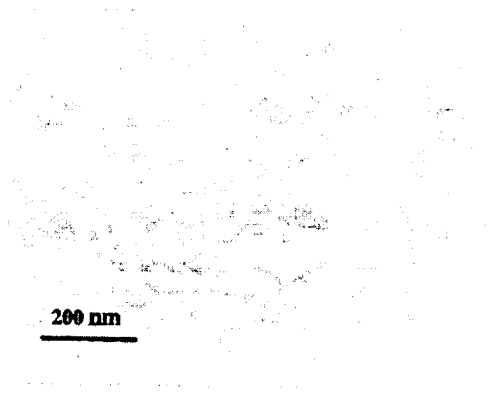


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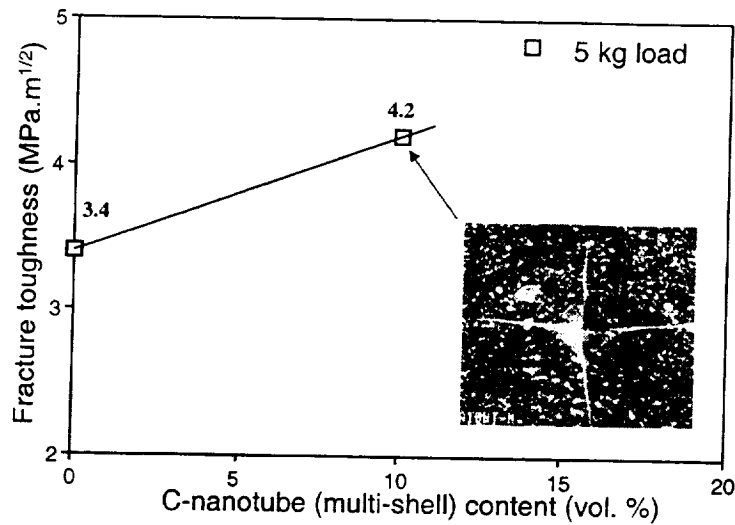
Carbon Nanotube/Alumina Nanocomposite



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Fracture Toughness



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**Nanophase TiO₂ Before and After
Compression at 810°C for 15 h**



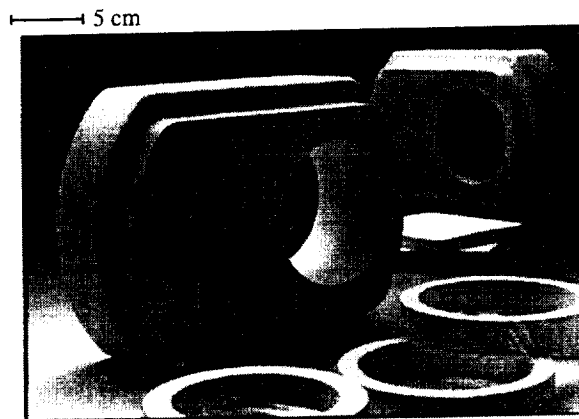
Hahn et al. (1990)



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Net-shape Formed Ceramic (Al₂O₃) Parts



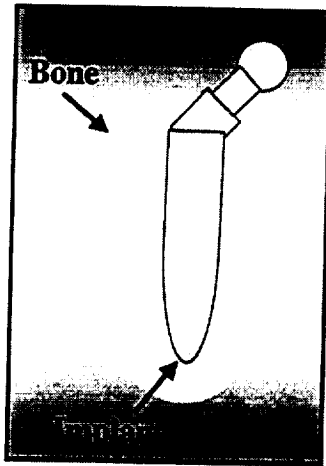
Nanophase Technologies Corporation (1997)



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Consolidated Nanophase Ceramics as Biomaterials



- ◆ Formation and maintenance of viable bone closely apposed to the surface of biomaterials is essential for the clinical success of orthopaedic/dental implants.
- ◆ Insufficient bonding of juxtaposed bone to an implant could be caused by either surface properties that do not support new bone growth and/or mechanical properties that do not duplicate those of surrounding tissue.

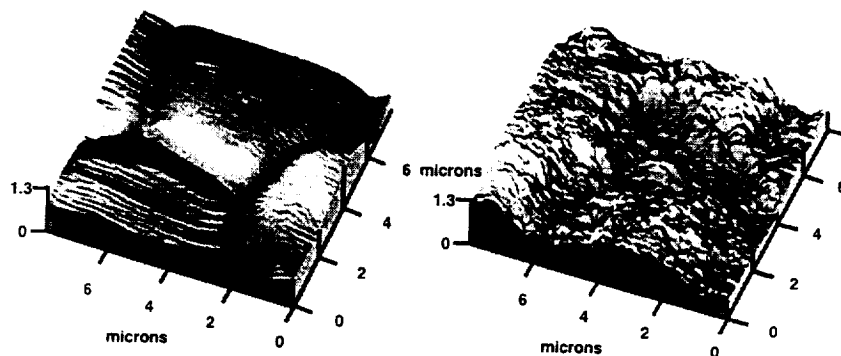
Webster, Bizios et al. (2000)



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Atomic Force Micrographs of Nanophase and Conventional Titania



4.5 μm (conventional)
Titania

39 nm (nanophase)
Titania



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Bending Stiffness of Nanophase and Conventional Ceramics

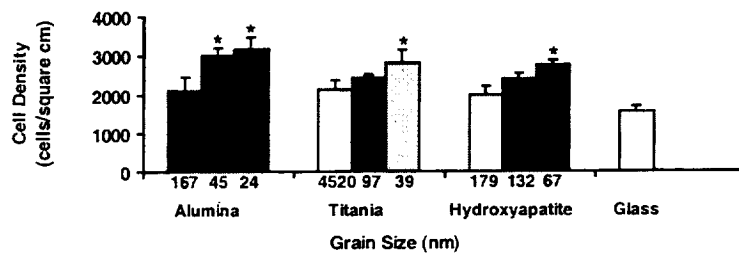
Ceramic Grain Size (nm)		Bending Stiffness (GPa)
Alumina	24 (nanophase)	35.1 ± 2.8
	167 (conventional)	52.0 ± 6.8
Titania	39 (nanophase)	38.0 ± 7.6
	4,520 (conventional)	56.2 ± 8.9
Hydroxyapatite	67 (nanophase)	50.9 ± 4.5
	179 (conventional)	71.1 ± 8.2
Human Femur Bone		19.4 ± 2.4



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Enhanced Osteoblast Adhesion on Nanophase Ceramics



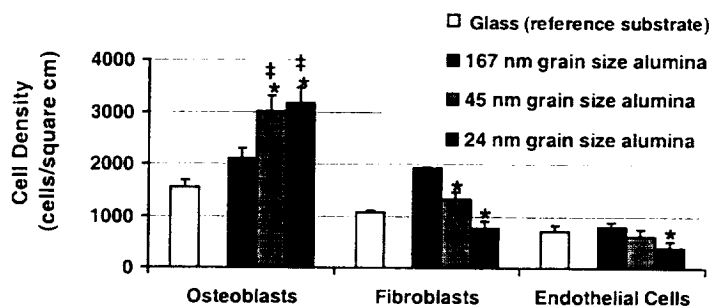
Culture media = DMEM supplemented with 10% fetal bovine serum. Adhesion time = 4 hours. Values are mean ± SEM; n = 3; * $p < 0.01$ (student t-tests compared to respective conventional grain size ceramic).



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Comparison of Cell Adhesion on Nanophase Al₂O₃



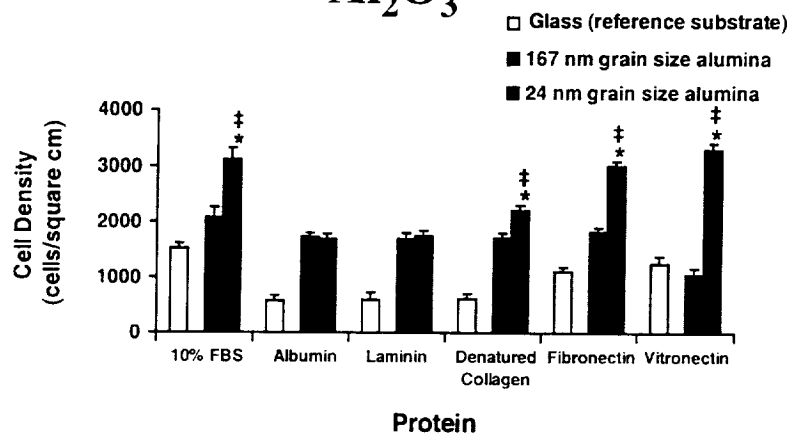
Culture medium = DMEM supplemented with 10% fetal bovine serum. Adhesion time = 4 hours. Values are mean +/- SEM; n = 3; * p < 0.01 (student t-tests compared to 167 nm grain size alumina); ‡ p < 0.01 (student t-tests compared to fibroblast and endothelial cell adhesion on respective grain size alumina).



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Osteoblast Adhesion on Nanophase Al₂O₃



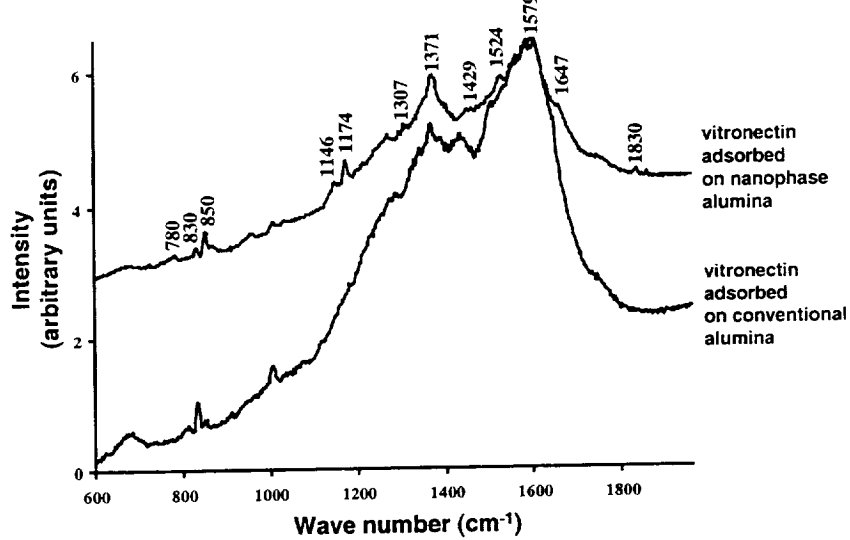
Culture medium = DMEM without serum. Adhesion time = 4 hours. Values are mean +/- SEM; n = 3; * p < 0.01 (student t-tests compared to 167 nm grain size alumina); ‡ p < 0.01 (student t-tests compared to respective grain size alumina pretreated with albumin).



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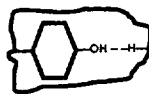
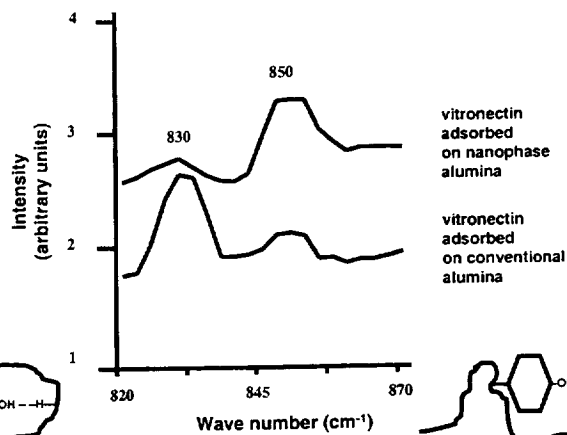
Surface Enhanced Raman Spectroscopy of Vitronectin Adsorbed on Al₂O₃



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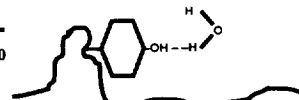
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Tyrosine Doublet Ratio of Vitronectin Adsorbed on Alumina



Protein Folding

$$I_{830} > I_{850}$$



Protein Unfolding

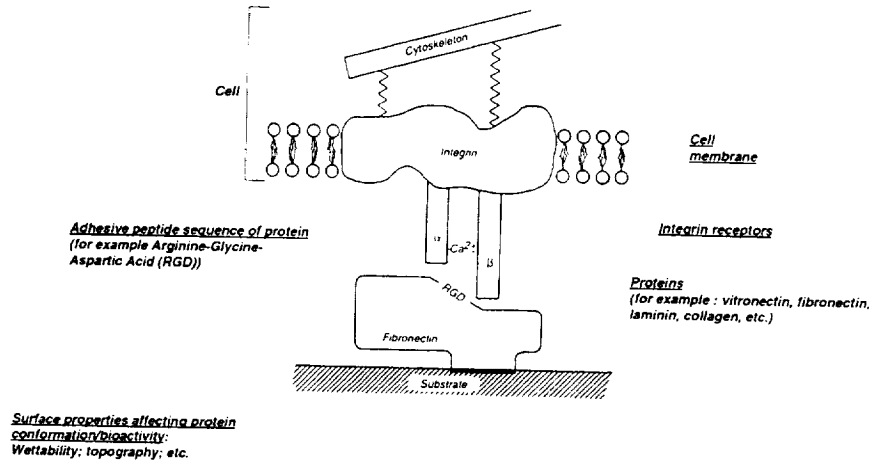
$$I_{850} > I_{830}$$



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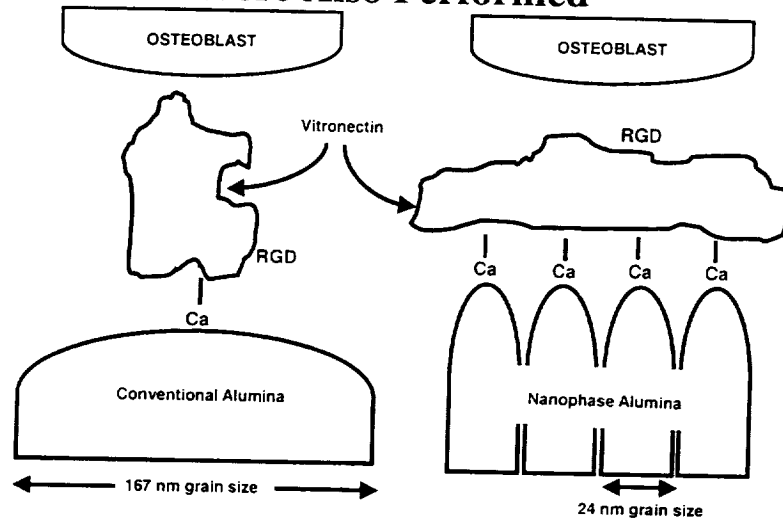
Cell-Biomaterial Interactions



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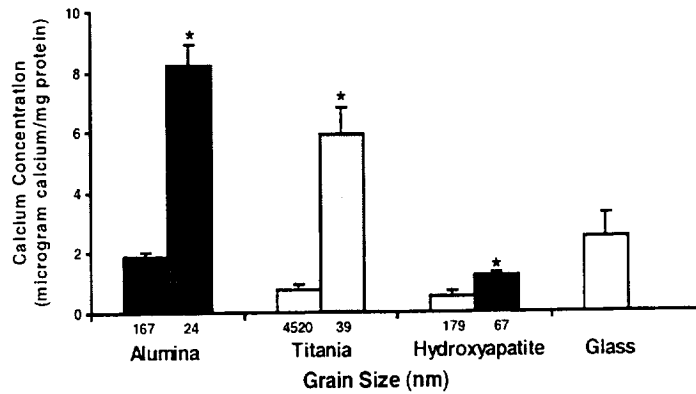
Competitive Inhibition Experiments Were Also Performed



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Enhanced Calcium Mineralization on Nanophase Ceramics



Culture medium = DMEM supplemented with 10% fetal bovine serum, 50 micrograms/mL L-ascorbate and 10 mM b-glycerophosphate. Culture time = 28 days. Values are mean +/- SEM; n = 3; * $p < 0.01$ (compared to respective conventional grain size ceramic).



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Bending Moduli of Nanophase and Conventional Alumina Composites with PLA

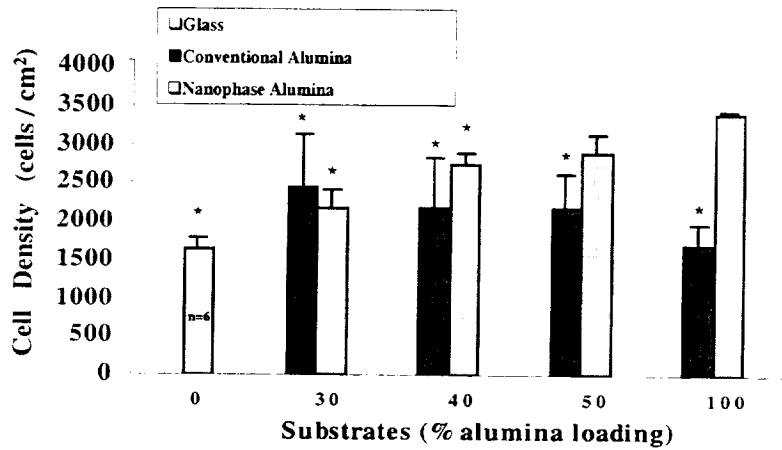
Bending Modulus (MPa)					
Pure PLA	Weight % alumina	30	40	50	100
324 ± 200	Nanophase	1,950 ± 510	977 ± 200	1,430 ± 800	3.7 ± 0.5
	Conventional	14.6 ± 2.0	1.7 ± 0.9	1.0 ± 0.7	2.6 ± 0.5



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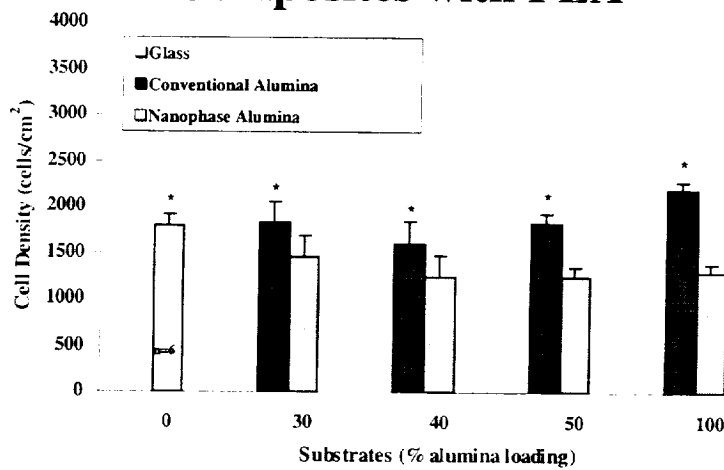
Osteoblast Adhesion on Nanophase Al_2O_3 and on Conventional Al_2O_3 Composites with PLA



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Fibroblast Adhesion on Nanophase Al_2O_3 and on Conventional Al_2O_3 Composites with PLA



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Technological Impact: Present and Potential

Technology	Present	Potential
Dispersions and Coatings	<ul style="list-style-type: none"> ◆ Thermal barriers ◆ Optical barriers (visible and UV) ◆ Imaging enhancement ◆ Ink-jet materials ◆ Coated abrasive slurries ◆ Information-recording layers 	<ul style="list-style-type: none"> ◆ Targeted drug delivery/gene therapy ◆ Multifunctional nano-coatings



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Technological Impact Present and Potential (Cont.)

Technology	Present	Potential
High Surface Area Materials	<ul style="list-style-type: none"> ◆ Molecular sieves ◆ Drug delivery ◆ Tailored catalysts ◆ Absorption/adsorption materials 	<ul style="list-style-type: none"> ◆ Molecule-specific sensors ◆ Large hydrocarbon or bacterial filters ◆ Energy storage ◆ Grätzel solar cells



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Technological Impact Present and Potential (Cont.)

Technology	Present	Potential
Nanodevices	<ul style="list-style-type: none"> ◆ GMR recording heads 	<ul style="list-style-type: none"> ◆ Terabit memory and microprocessing ◆ Single molecule DNA sizing and sequencing ◆ Biomedical sensors ◆ Low noise, low threshold lasers ◆ Nanotubes for high brightness displays



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Technological Impact Present and Potential (Cont.)

Technology	Present	Potential
Consolidated Materials	<ul style="list-style-type: none"> ◆ Low-loss soft magnetic materials ◆ High hardness, tough WC/Co cutting tools ◆ Nanocomposite cements 	<ul style="list-style-type: none"> ◆ Superplastic forming of ceramics ◆ Ultra-high strength tough structural materials ◆ Magnetic refrigerants ◆ Nano-loaded polymer composites ◆ Ductile cements



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Conclusion

Nanomaterials and nanotechnology will have an important and growing impact on biomedical applications in the coming years...



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Nanotechnology in Materials

Ilhan A. Aksay
Department of Chemical Engineering and
Princeton Materials Institute
Princeton University
Princeton, NJ 08540



Princeton Materials Institute
Princeton University

NANOTECHNOLOGY IN MATERIALS

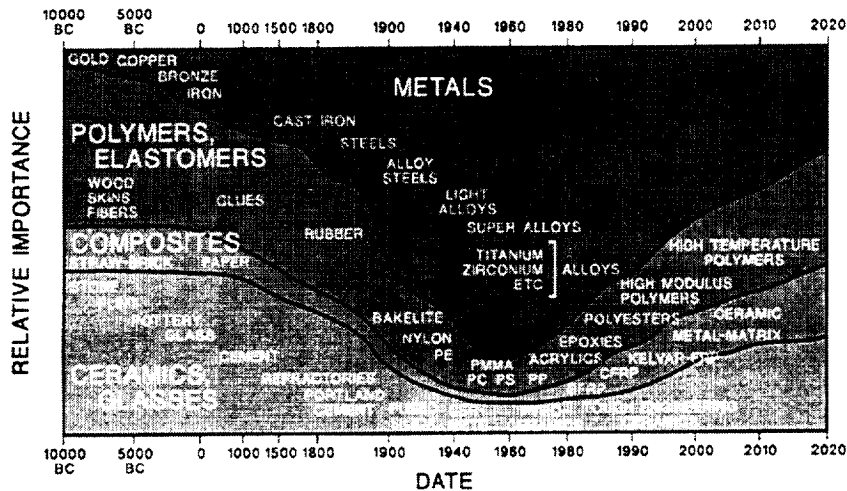
ILHAN A. AKSAY

Department of Chemical Engineering and
Princeton Materials Institute
Princeton University, Princeton, New Jersey



Princeton University

Evolution of Engineering Materials





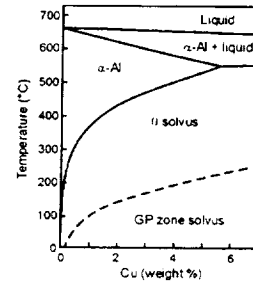
Princeton University

What is Nanotechnology?

Precipitation Hardening in the First Aerospace Aluminum Alloy: The Wright Flyer Crankcase

Frank W. Gayle and Martha Goodway

SCIENCE • VOL. 266 • 11 NOVEMBER 1994



"An aluminum copper alloy (with a copper composition of 8 percent by weight) was used in the engine that powered the historic first flight of the Wright brothers in 1903. Examination of this alloy shows that it is precipitation-hardened by Guinier-Preston zones in a bimodal distribution, with larger zones (10-22 nanometers) originating in the casting practice and finer ones (3 nanometers) resulting from ambient aging over the last 90 years."



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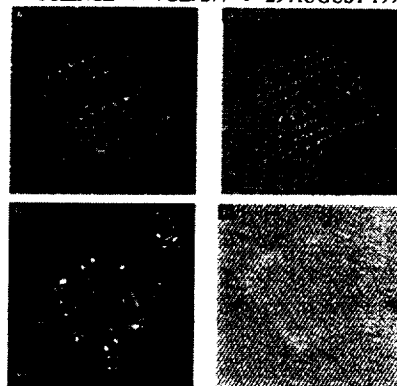
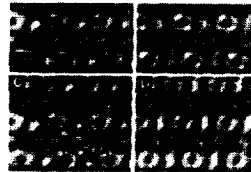
ARTICLES

Structure Determination of Mg_5Si_6 Particles in Al by Dynamic Electron Diffraction Studies

H. W. Zandbergen, S. J. Andersen, J. Jansen

SCIENCE • VOL. 277 • 29 AUGUST 1997

Precipitation hardening, in which small particles inhibit the movement of dislocations to strengthen a metal, has long been used to improve mechanical strength, especially of aluminum alloys. The small size of precipitates and the many possible variants of the orientation have made their structural determination difficult. Small precipitates in commercial aluminum-magnesium-silicon alloys play a crucial role in increasing the mechanical strength of these alloys. The composition and structure of the β' phase in an aluminum-magnesium-silicon alloy, which occur as precipitates typically 4 nanometers by 4 nanometers by 50 nanometers and are associated with a particularly strong increase in mechanical strength, were determined. Element analysis indicates that the composition is Mg_5Si_6 . A rough structure model was obtained from fast Fourier reconstruction from high-resolution electron microscopy images. The structure was refined with electron microdiffraction data (overall R value of 3.1 percent) with the use of a recently developed least-squares refinement procedure in which dynamic diffraction is fully taken into account.



"Precipitation hardening, in which small particles inhibit the movement of dislocations to strengthen a metal, has long been used to improve mechanical strength, especially of aluminum alloys."

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Hierarchy in Bone

Level 1: Major components (100 nm)

Level 2: Mineralized collagen fibril (200 nm)

Level 3: Fibril array

Level 4: Fibril array patterns

Level 5: Cylindrical motifs: osteons (10 μm)

Level 6: Spongy vs compact bone

Level 7: Whole bone

S. Weiner and H. D. Wagner, *Ann. Rev. Mater. Sci.* 28, 271-98 (1998).

Princeton University

Three Key Lessons:

- Discrete levels and/or scales with organization starting at 1-100 nm.
- Levels of structural organization are held together by specific interactions.
- Hierarchical composite systems designed to meet a wide range of functional requirements.



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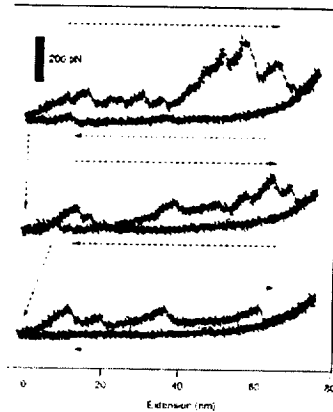
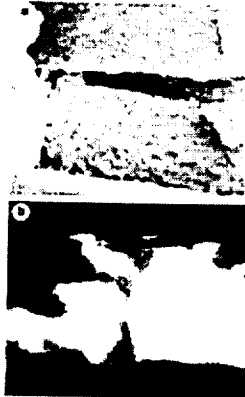
letters to nature

Molecular mechanistic origin of the toughness of natural adhesives, fibres and composites

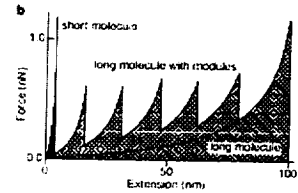
Bette L. Smith¹, Timon E. Schlierf¹, Mario Viani¹, James B. Thompson², Neil A. Frederick³, Johannes Kind⁴, Angela Belcher⁵, Alan D. Sacks⁶, Daniel E. Morse⁷ & Paul K. Hansma¹

¹Department of Physics, ²Department of Chemistry and Materials, and ³Department of Molecular, Cellular, and Developmental Biology, University of California at Santa Barbara, California 93106, U.S.A. ⁴Department of Materials Science, Max-Planck-Gesellschaft, Physikalische Chemie, 37077 Göttingen, Germany. ⁵Department of Chemistry, The University of Texas at Austin, Austin, Texas 78712, U.S.A. ⁶These authors contributed equally to this work.

NATURE VOL 429 20 JULY 2006 WWW.NATURE.COM



"Thus the break strength of each adhesive molecule would be the force required to break a strong bond: of the order of one nano-newton (estimate by dividing one electron volt by an extension of one ångström). For a material with many strongly bound molecules in parallel, the macroscopic tensile strength is expected to be of the order of several giga-pascals."



Princeton University

Goals and Organization

Self Assembly

(a) Amphiphilic and Protein Membranes
Groves, Hecht, Saville, Aksay 1-10 nm

(b) Liquid Crystal Templating
Cubic phase 1-10 nm
Sponge phase
Dabbs, Saville, Prud'homme, Aksay

(c) Block Copolymer Templating
10 - 100 nm
Register, Aksay, Chaikin

(d) 2D and 3D Colloidal Structures
Saville, Aksay

PROCESSING TECHNIQUES

Laminating and Micropatterning by Field-Assisted Flow

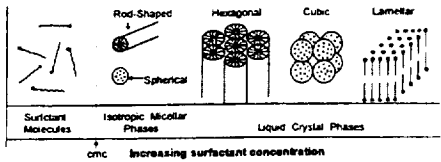
(a) Micropatterning (b) Cone/Jet (c) Electrodeposition

Hierarchically Structured Nano- and Microlaminates
Suo, Evans, Soboyejo, Saville, Groves, Aksay

OPTIMAL PROPERTIES

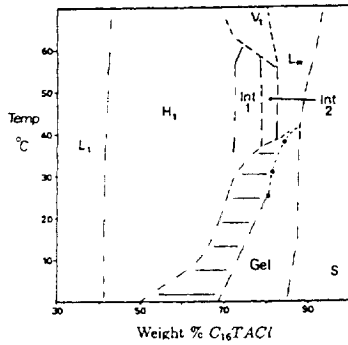


CTAC (Cetyltrimethyl Ammonium Chloride)



Phase sequence of surfactant-water binary system

D. Myers, *Surfactant Science and Technology*, VCH: New York (1992)



Partial phase diagram for the CTAC-water system

- L₁: micellar solution;
- H₁: hexagonal phase;
- L_α: Lamellar phase;
- Gel: Monolayer interdigitated gel phase;
- V₁: bicontinuous cubic phase;
- S: Solid phase; Int-1 and Int-2, intermediate phases.

Gel phase is separated from the H₁ phase by a two-phase region

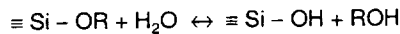
U. Henriksson *et al.*, *J. Phys. Chem.* **96** 3894-902 (1992)



TEOS (Tetraethoxysilane)

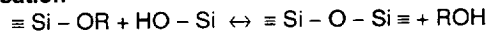
Hydrolysis and Condensation

1) Hydrolysis



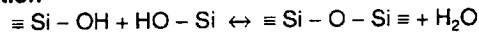
The R represents an alkyl group. In this reaction, the alkoxide groups (OR) are replaced by hydroxyl (OH) groups.

2) Alcohol Condensation



Siloxane bonds (Si - O - Si) and Alcohol (ROH) are produced.

3) Water Condensation



Siloxane bonds and water (H₂O) are produced.

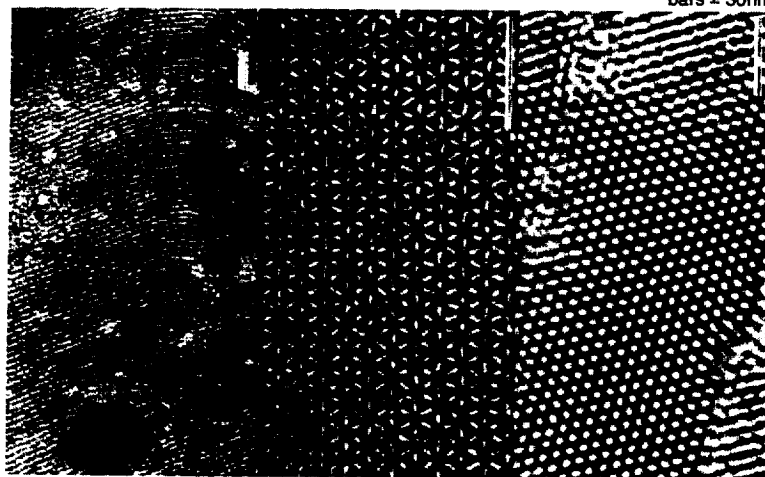
At low pH and high water concentration: The hydrolysis finishes in a very short period of time; therefore, the hydrolysis and condensation reactions are well separated.

C. Jeffrey Brinker *et al.*, *Sol-gel Science* (Academic Press, San Diego, 1986)



Princeton University

Lamellar, Cubic and Hexagonal Mesoporous Structures

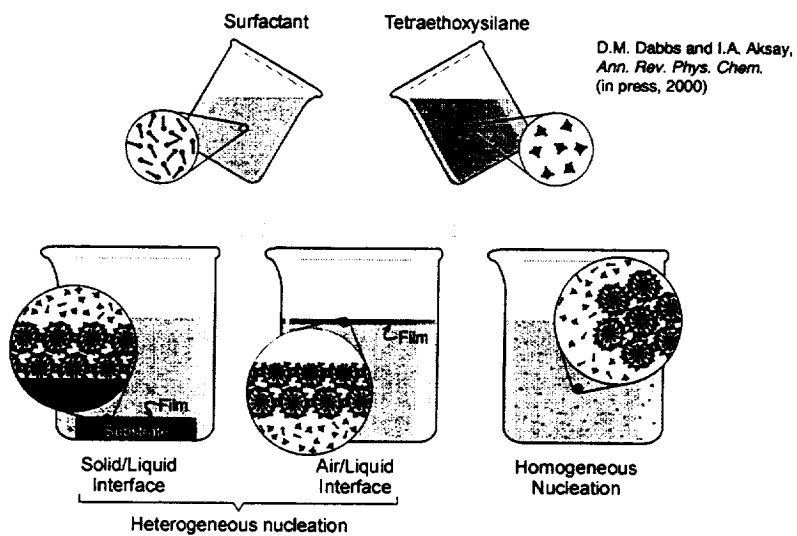



M. D. McGehee, S. M. Gruner, N. Yao, C. M. Chun, A. Navrotsky, and I. A. Aksay, *Proc. 52nd Ann. Mtg. MSA* 448-9 (1994)



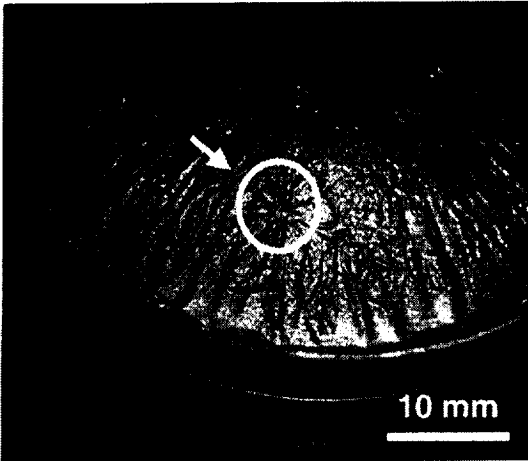
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Templating Self-Assembled Surfactants




 Princeton University

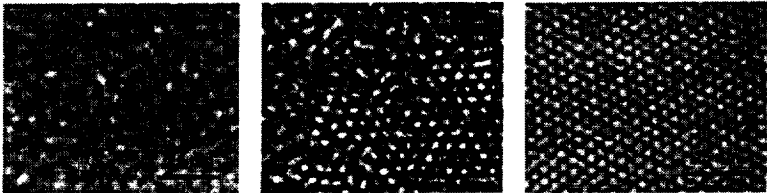
Self Healing Inorganic/Organic Films



N. Yao, A. Y. Ku, N. Nakagawa, T. Lee, D. A. Saville, and I. A. Aksay, *Chem. Mater.* 12 [6] 1536-548 (2000)

 Princeton University

Film Growth: Mesoscopic Crystallization

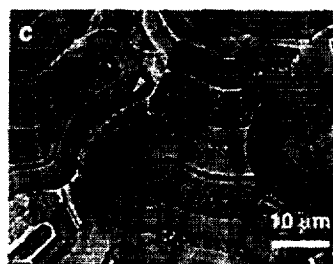
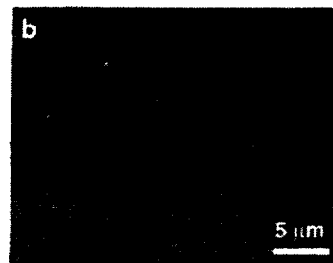
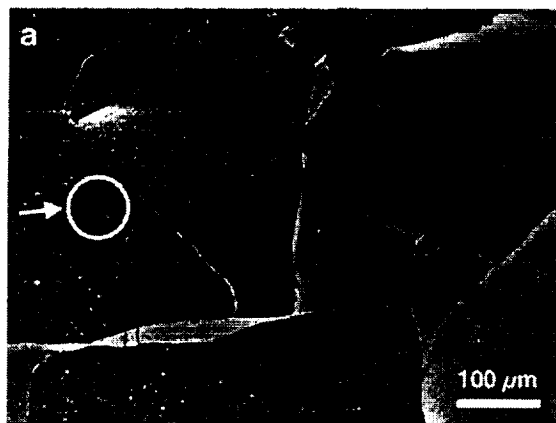


30 minutes 5 hours 2 days

N. Yao, A. Y. Ku, N. Nakagawa, T. Lee, D. A. Saville, and I. A. Aksay, *Chem. Mater.* 12 [6] 1536-548 (2000)



Princeton University




N. Yao, A. Y. Ku, N. Nakagawa, T. Lee, D. A. Saville, and I. A. Aksay, *Chem. Mater.* 12 [6] 1536-548 (2000)



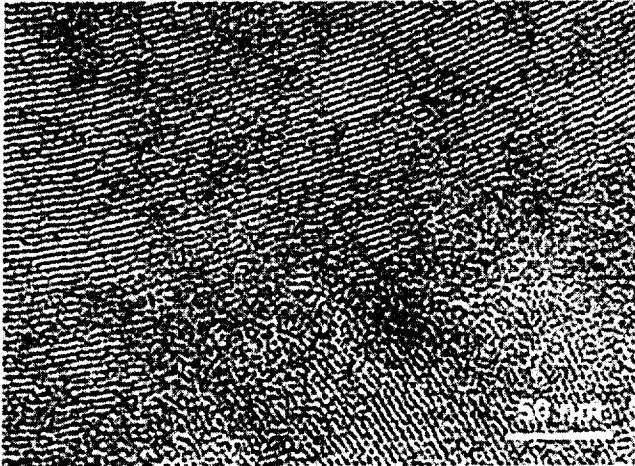
Princeton University

Mesostructured Silica Film on Mica




 Princeton University

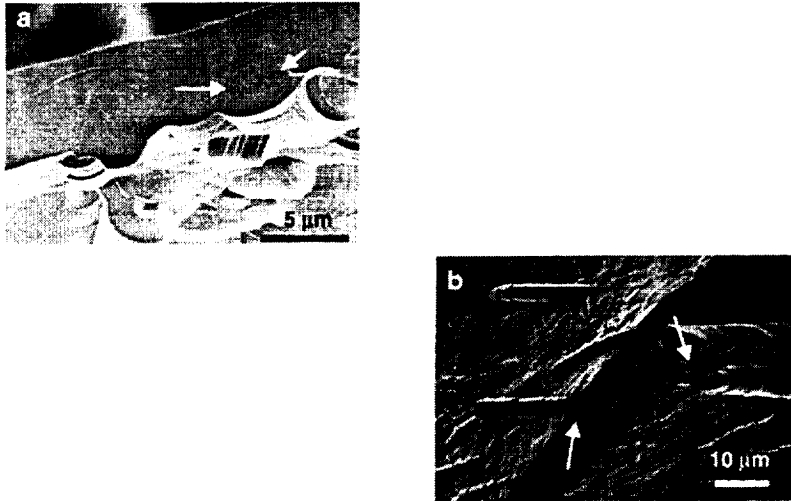
Cross-Sectional TEM: Film at the Air-Water Interface



N. Yao, A. Y. Ku, N. Nakagawa, T. Lee, D. A. Saville, and I. A. Aksay, *Chem. Mater.* 12 [6] 1536-548 (2000)

 Princeton University

Film Grown at the Air/Water Interface



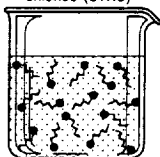
N. Yao, A. Y. Ku, N. Nakagawa, T. Lee, D. A. Saville, and I. A. Aksay, *Chem. Mater.* 12 [6] 1536-548 (2000)



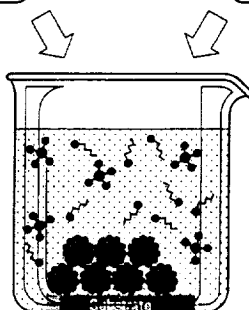
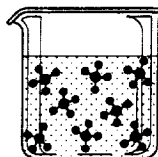
Princeton University

Synthesis of Mesostructured Silica Films

Cetyltrimethyl ammonium chloride (CTAC)

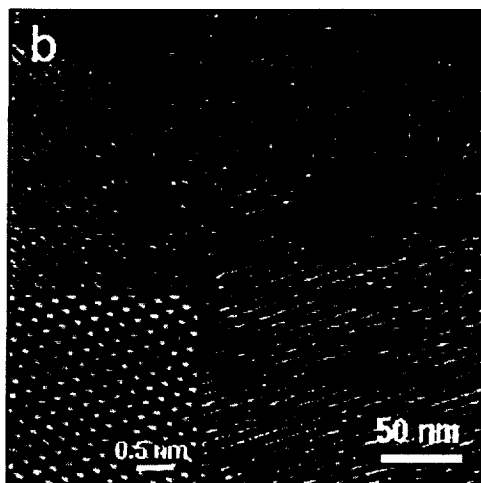


Tetraethoxysilane



Princeton University

Mesostructured Silica on Graphite-AFM



Princeton University

Mesostructured Inorganics Through Liquid Crystal Templating

- **Surfactant-based procedure yields mesostructured inorganic materials**
 C. T. Kresge *et al.*, *Nature* 359 (1992); and, J. S. Beck *et al.*, *J. Am. Chem. Soc.* 114 [27] (1992).

I. A. Aksay, M. Trau, S. Manne, I. Honma, N. Yao, L. Zhou, P. Fenter, P. M. Eisenberger, S. M. Gruner *Science* 273 892-98 (1996).

Mica Graphite Silica

Princeton University

In-plane Orientational Alignment: On Mica

A 2-D azimuthal scan of the (101) Bragg peak for the film grown on mica for 24 hours. Note that peaks are observed at $\phi = \pm 30^\circ$, corresponding to the tubules along N1 and N2 ($\phi = \pm 60^\circ$), but no peak is observed at $\phi = \pm 90^\circ$, which would correspond to tubules laying along the b-axis direction.

Schematic of the lattice structure of the mica surface. The tubules of the film are aligned along the two next-nearest-neighbor directions N1 and N2 of the pseudo-hexagonal structure.

• Silicon ○ Oxygen



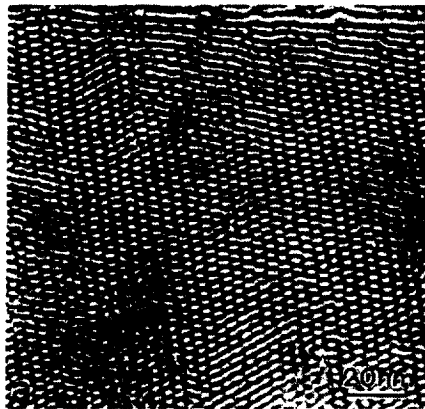
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Mesostructured Thin Film on Mica



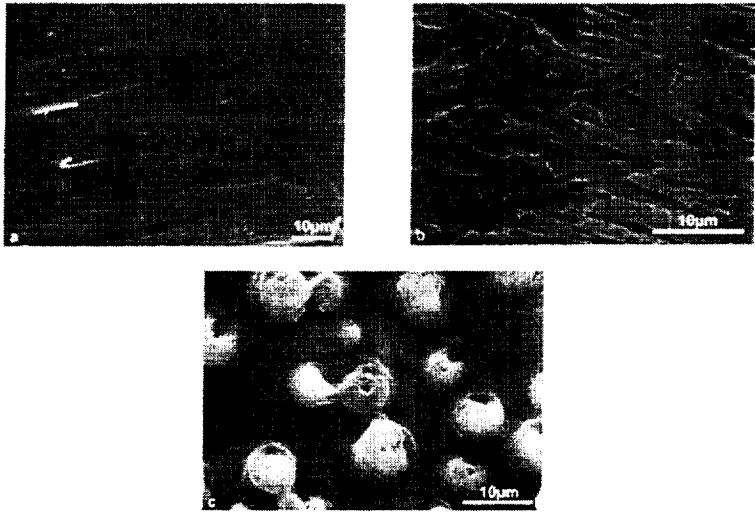
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Mesostructured Silica Film on Mica




 Princeton University

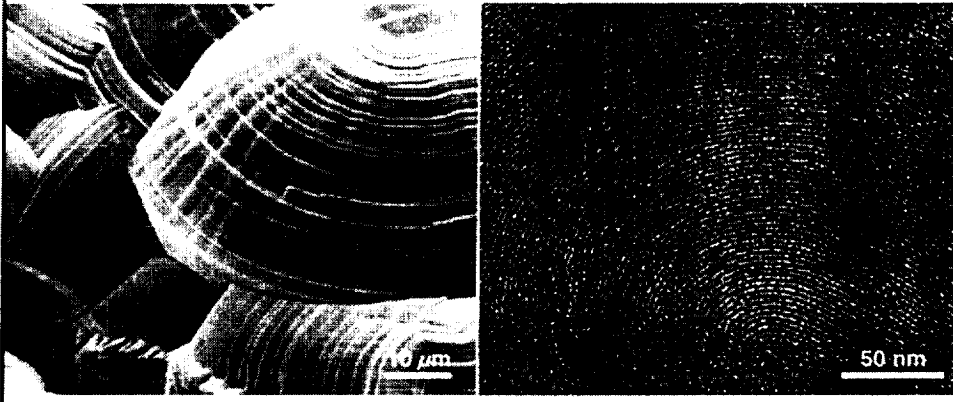
Mesostructured Thin Films



(a) (b) (c)

 Princeton University

Hierarchically Structured Mesoscopic Silica Film

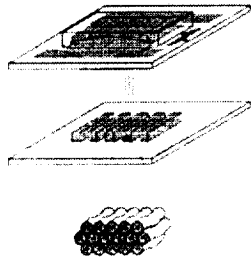


10 μm 50 nm

On silica substrate



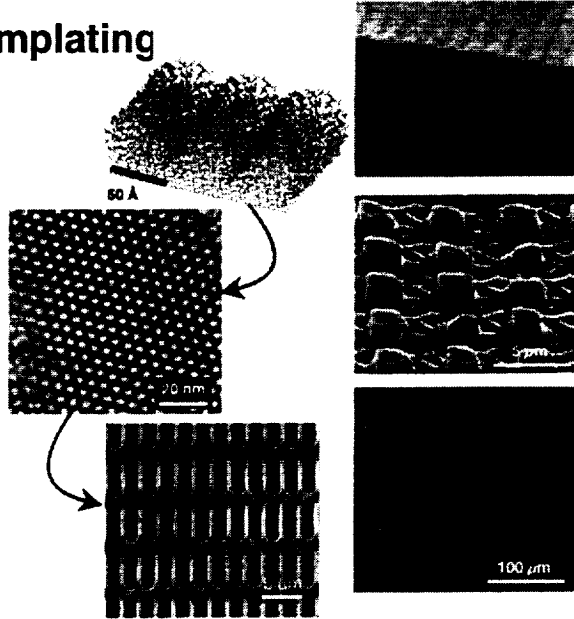
Liquid Crystal Templating



I. A. Aksay, M. Trau, S. Manne, I. Honma, N. Yao, L. Zhou, P. Fenter, P. M. Eisenberger, S. M. Gruner, *Science* 273 892-98 (1996);

M. Trau, N. Yao, E. Kim, Y. Xia, G. M. Whitesides, I. A. Aksay, *Nature* 390 [6661] 674-76 (1997)

A. Y. Ku, D. A. Saville, I. A. Aksay, unpublished research (2000)

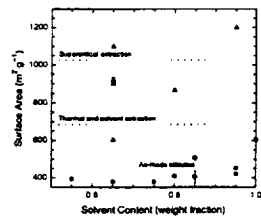
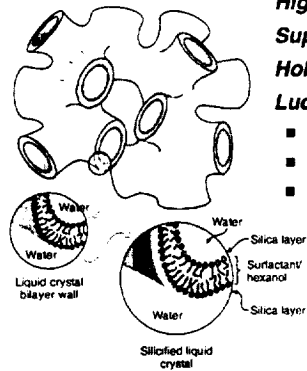


L₃-Templated Silicates

High surface area with contiguous, uniform pore structure
Supercritically extracted to remove template (N. Mulders)
Holographic storage medium (H. Katz,

Lucent Technologies):

- High permeability for precursors
- *In-situ* reaction and curing
- Two-photon write-and-read

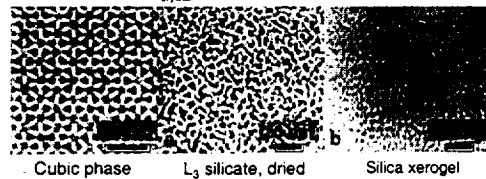


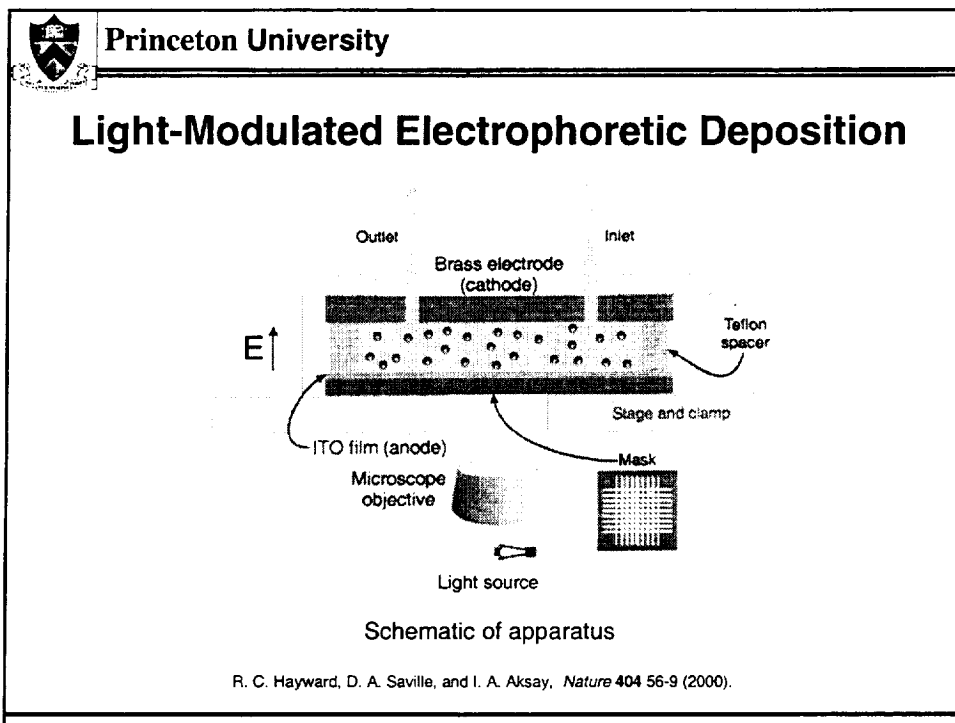
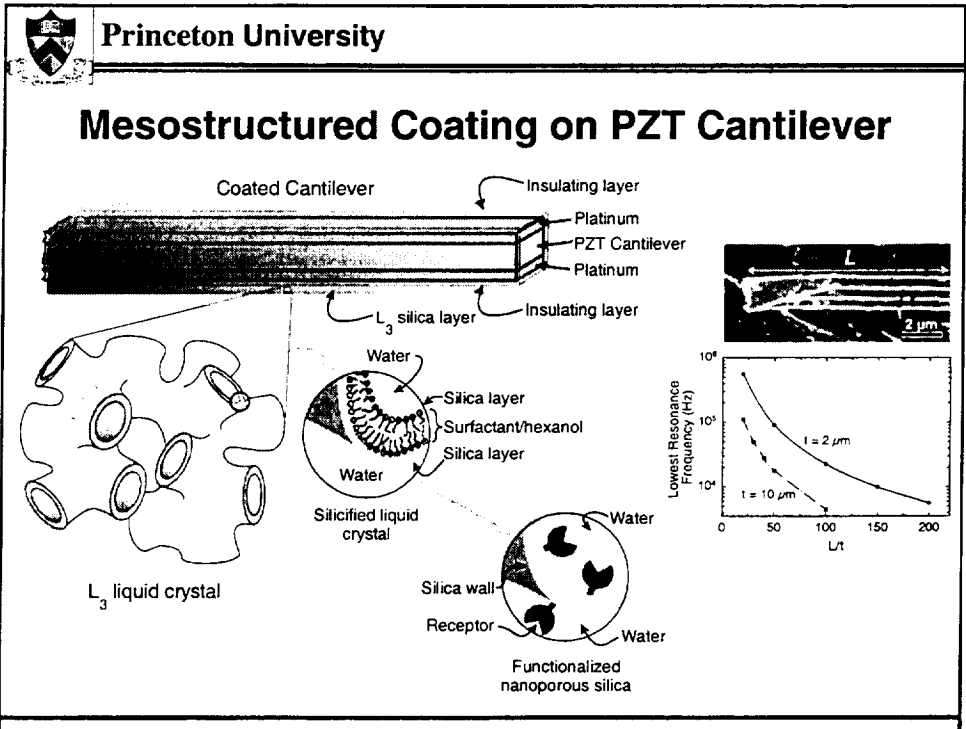
Cubic Phase:
M. D. McGehee, S. M. Gruner, N. Yao, C. M. Chun, A. Navrotsky, and I. A. Aksay, *Proc. 52nd Ann. Mtg. MSA* (1994) 448-9.

L₃ Silicates:
K. M. McGrath, D. M. Dabbs, N. Yao, I. A. Aksay, and S. M. Gruner, *Science* 277 552-6 (1997).

K. M. McGrath, D. M. Dabbs, K. J. Edler, N. Yao, I. A. Aksay, and S. M. Gruner, *Langmuir* 16 398-406 (2000).

D. M. Dabbs, S. M. Gruner, N. Mulders, and I. A. Aksay, unpublished research (2000).

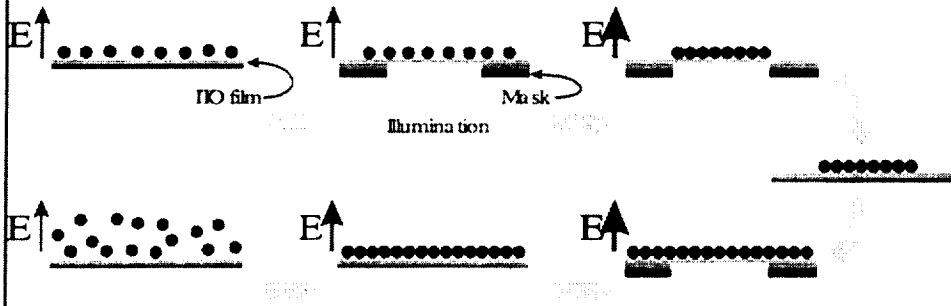






Pattern Formation

Patterned assembly followed by fixing to substrate



General assembly followed by patterned fixing to substrate


R. C. Hayward, D. A. Saville, and I. A. Aksay, *Nature* 404 56-9 (2000).



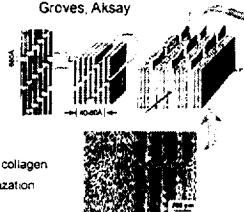
Patterned Colloidal Particles



R. C. Hayward, D. A. Saville, and I. A. Aksay, *Nature* 404 56-9 (2000).

 **Princeton University**


(a) Living Cells
Schwarzbauer, Carbeck,
Groves, Aksay



- Templated collagen
- Biomineralization

HYBRID-SYNTHONS

(b) Templates through Laser Rastering
Prud'homme, Aksay

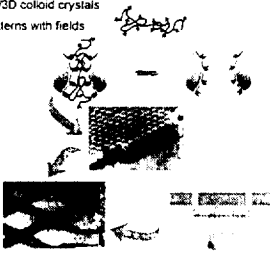


- Stereolithography
- 2-Photon beam scanning
- 2D/3D scaffolds

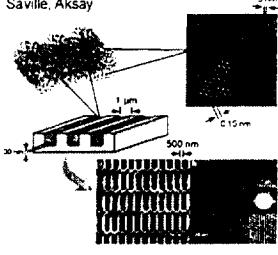
NOVEL NANOLITHOGRAPHIES

(c) Patterned Colloidal Crystals
Carbeck, Saville, Aksay

- 2D/3D colloid crystals
- Patterns with fields



(d) Nanolithography through Self-Assembly in Templates
Saville, Aksay



- Soft lithography
- E-beam lithography
- Templates/fields

58/76


12P

Carbon Nanotubes for Space Applications

Meyya Meyyappan
NASA Ames Research Center
Moffett Field, CA 94035


Carbon Nanotubes for Space Applications

Meyya Meyyappan
NASA Ames Research Center
Moffett Field, CA 94035
meyya@orbit.arc.nasa.gov

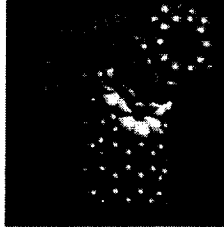


Ames Research Center

Carbon Nanotubes for Space Applications




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<http://www.ipt.arc.nasa.gov>



Invited Talk
UVA-NASA Workshop on Nano-Biotechnology
NASA LaRC, June 14-15, 2000

Acknowledgment

	<h1>Acknowledgment</h1>	
<hr/>		
Alan Cassell	M. Anantram	
Lance Delzeit	Charlie Bauschlicher	
Jie Han	Fedor Dzegilinko	
Jim Kaysen	Richard Jaffe	
Bishun Khare	Madhu Menon	
Cattien Nguyen	Natalio Mingo	
Ramsey Stevens	Deepak Srivastava	
Jonathan Trent	Toshi Yamada	
Sunita Verma	Liu Yang	


Ames Nanotechnology Research Focus

NASA Ames' nanotechnology program started about five years ago, and the carbon nanotube research is the largest in any federal government lab and one of the largest in the world. The broad focus includes experimental work with complementary theoretical and simulation work. The group has won two Feynmann prizes awarded by the Foresight Institute. A list of journal publications can be found at www.ipt.arc.nasa.gov.


 <p style="text-align: center;">Ames Nanotechnology Research Focus</p> 	
<p><i>Nanotubes</i></p> <ul style="list-style-type: none">• Controlled, patterned growth of CNT• Large scale production of CNT• CNT-based biosensor for cancer diagnostics• Functionalization of nanotubes• AFM study of Mars dust• AFM study of Mars meteorite• CNT-based sensors for astrobiology• Hydrogen storage in nanotubes• Protein nanotubes: growth and applications• Reactor/Process Modeling of CNT growth• Computational investigation of electronic, mechanical and other properties of CNT• Transport in CNT, nanoelectronics• BN nanotubes, structure and properties• Design of CNT-based mechanical components	<ul style="list-style-type: none">• Chemical storage of data• Atomic chain electronics• Bacteriorhodopsin based holographic data storage <p><i>Computational Electronics, Computational Optoelectronics</i></p> <ul style="list-style-type: none">• Development of multidimensional quantum simulators to design Ultra-small semiconductor devices• Development of semi-classical methods with quantum correction terms• Investigation of device technologies suitable for petaflop computers• Modeling of optoelectronics devices, VCSEL, THz modulation• Optical interconnect modeling

Why Nanotechnology at NASA?

As a result of the National Nanotechnology Initiative currently being implemented by all federal agencies, NASA is earnestly evaluating the potential of nanotechnology for the agency's missions. The pay-off to NASA, particularly for investment in nanotube based nanotechnology, appears to be significant.




why Nanotechnology at NASA?




- Advanced miniaturization, a key thrust area to enable new science and exploration missions
 - Ultrasmall sensors, power sources, communication, navigation, and propulsion systems with very low mass, volume and power consumption are needed
- Revolutions in electronics and computing will allow reconfigurable, autonomous, "thinking" spacecraft
- Nanotechnology presents a whole new spectrum of opportunities to build device components and systems for entirely new space architectures
 - Networks of ultrasmall probes on planetary surfaces
 - Micro-rovers that drive, hop, fly, and burrow
 - Collection of microspacecraft making a variety of measurements
- In vivo and noninvasive astronaut health diagnosis and prognosis, in vivo therapy

Carbon Nanotube

Carbon nanotube (CNT), a tubular form of carbon, is an extraordinary material in terms of its mechanical and electronic properties. The remarkable figures-of-merit of CNT have caused much excitement among researchers about the future of this technology. The anticipated investment is expected to accelerate the speed of innovation in the field.



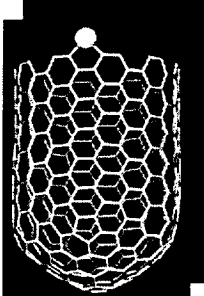
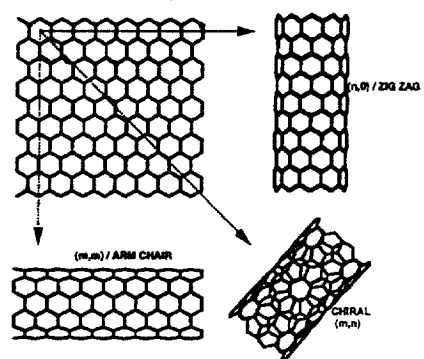
Carbon Nanotube



CNT is a tubular form of carbon with a diameter as small as 1 nm.
Length: few nm to microns.

CNT is configurationally equivalent to a two-dimensional graphene sheet rolled into a tube.

• STRIP OF A GRAPHENE SHEET ROLLED INTO A TUBE




CNT exhibits extraordinary mechanical properties: Young's modulus over 1 Tera Pascal, as stiff as diamond, and tensile strength ~ 200 GPa.


CNT can be metallic or semiconducting, depending on chirality.

CNT Properties

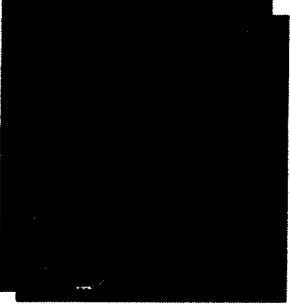

Comparison with materials such as aluminum, titanium, and steel, shows that CNT has much superior strength-to-weight ratio. CNT's thermal conductivity is second only to CVD-grown diamond. Thermal conductivity appears to be a function of temperature, chirality, etc. Also, the remarkable combination of properties enables CNT to be a multifunctional material in structural applications.



CNT Properties




- The strongest and most flexible molecular material because of C-C covalent bonding and seamless hexagonal network architecture
- Young's modulus of over 1 TPa vs 70 GPa for aluminum, 700 GPa for C-fiber
 - Strength to weight ratio 500 times > for Al; similar improvements over steel and titanium; one order of magnitude improvement over graphite/epoxy
- Maximum strain 10-30% much higher than any material
- Thermal conductivity ~ 3000 W/mK in the axial direction with small values in the radial direction




CNT Properties (Cont'd.)

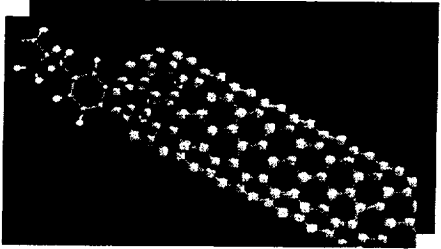
CNT's electrical properties are unique. Depending in chirality, the nanotube can be metallic or semiconducting. Creative functionalization can also lead to insulating nanotubes. All of this allows us to dream of building an entire architecture predominantly based on this one material. The excellent field emission properties have led Japanese and Korean companies to make serious investments on exploiting for display technology.



CNT Properties (cont.)



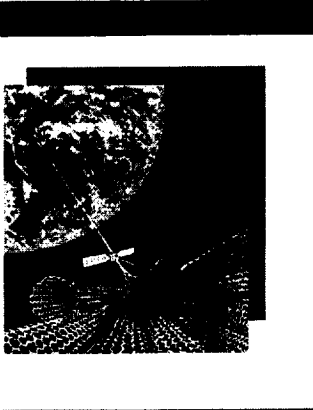


- Electrical conductivity six orders of magnitude higher than copper
- Can be metallic or semiconducting depending on chirality
 - 'tunable' bandgap
 - electronic properties can be tailored through application of external magnetic field, application of mechanical deformation...
- Very high current carrying capacity
- Excellent field emitter; high aspect ratio and small tip ratio of curvature are ideal for field emission
- Can be functionalized




CNT Applications: Structural, Mechanical

The applications mentioned herein are based on what we know about the properties. No serious demonstrations of any kind have been made yet.


	<h3>CNT Applications: Structural, Mechanical</h3>	
<ul style="list-style-type: none">• High strength composites• Cables, tethers, beams• Multifunctional materials• Functionalize and use as polymer back bone<ul style="list-style-type: none">- Plastics with enhanced properties like "blow molded steel"• Heat exchanges, radiators, thermal barriers, cryotanks• Radiation shielding• Filter membranes, supports• Body armor, space suits		
<h3>Challenges</h3> <ul style="list-style-type: none">- Control of properties, characterization- Dispersion of CNT homogeneously in host materials- Large scale production- Application development		

CNT Applications: Electronics

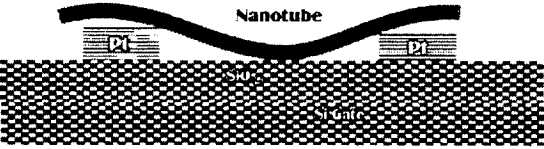
Nanotube based molecular computing is a couple of decades away. A key to the development is to focus on novel circuits and architectures at an early stage (now), and not to try to create field effect transistors to fit into the existing CMOS-like scheme.



CNT Applications: Electronics



- CNT quantum wire interconnects
- Diodes and transistors for computing
- Capacitors
- Data storage
- Field emitters for instrumentation
- Flat panel displays
- THz oscillators





Challenges

- Control of diameter, chirality
- Doping, contacts
- Novel architectures (not CMOS based!)
- Development of inexpensive manufacturing processes


CNT Applications: Sensors, NEMS, Bio

Applications in the fields of sensors and nanodevices are amazingly numerous. In a few years, when research becomes successful in control of nanotube diameter and chirality, characterization, and development of nano-fabrication and nano-manipulation techniques, some of these dream applications will become reality.


 CNT Applications: Sensors, NEMS, Bio 	
<ul style="list-style-type: none">• CNT based microscopy: AFM, STM...• Nanotube sensors: force, pressure, chemical...• Biosensors for astrobiology• Molecular gears, motors, actuators• Batteries, Fuel Cells: H₂, Li storage• Nanoscale reactors, ion channels• Biomedical<ul style="list-style-type: none">- in vivo real time crew health monitoring- Lab on a chip- Drug delivery- DNA sequencing- Artificial muscles, bone replacement, bionic eye, ear...	<h3>Challenges</h3> <ul style="list-style-type: none">• Controlled growth• Functionalization with probe molecules, robustness• Integration, signal processing• Fabrication techniques

CNT Synthesis

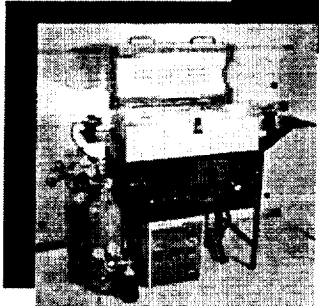
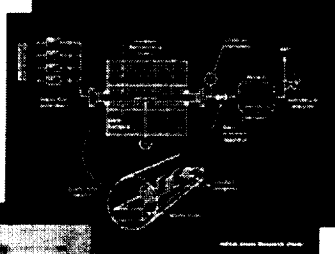
Laser ablation provides ~ 70% purity single wall nanotubes. It is not a suitable process for mass production. Universities and companies across the country are investigating new approaches to producing nanotubes in large quantities. CVD on the other hand enables controlled growth on patterned substrates. NASA Ames runs three CVD reactors to grow nanotubes on substrates. Parameters controlling the outcome are numerous: feed gas composition, temperature, choice of catalyst material, catalyst preparation technique, resulting catalyst particle size, substrate preparation.... Ames' work includes a combinatorial chemistry analysis to speed up this investigation.



CNT Synthesis

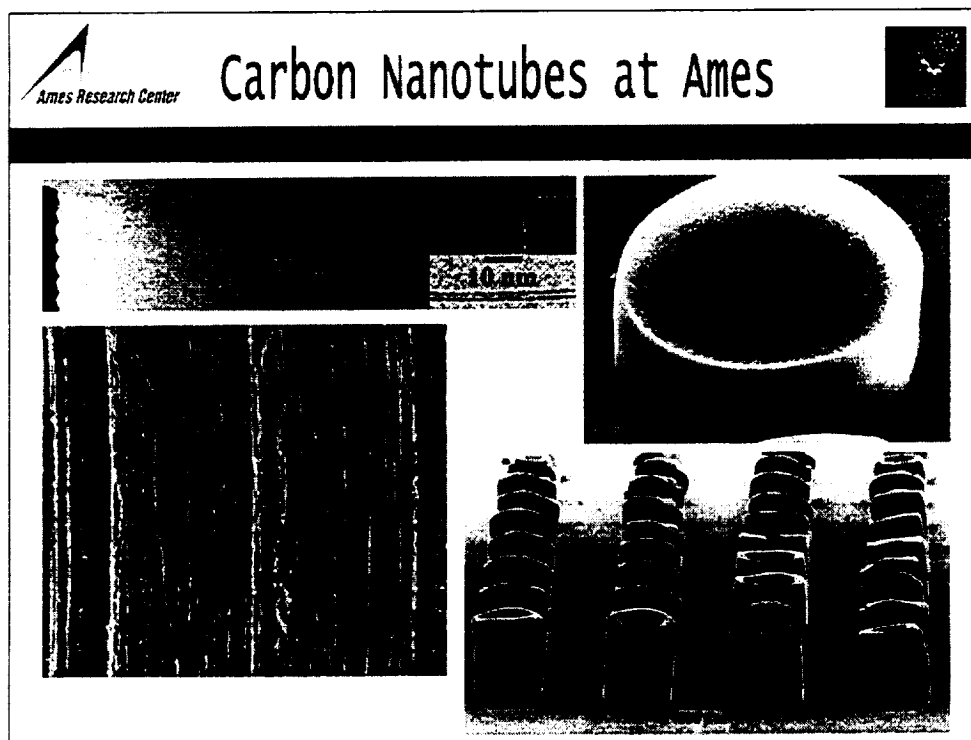


- CNT has been grown by laser ablation (pioneering at Rice) and carbon arc process (NEC, Japan) - early 90s.
 - SWNT, high purity, purification methods
- CVD is ideal for patterned growth (electronics, sensor applications)
 - Well known technique from microelectronics
 - Hydrocarbon feedstock
 - Growth needs catalyst (transition metal)
 - Multi-wall tubes at 500-800° deg. C.
 - Numerous parameters influence CNT growth




Carbon Nanotubes at Ames

The top left picture shows a single wall nanotube between two contacts. The top right shows a multi-wall nanotube pillar. A close examination of this pillar is shown in the bottom left picture. When the catalyst is arranged in a ring-like pattern on the substrate, then structures resembling a nano-trash can emerge as shown on the bottom right. All of this CVD work was done by Alan Cassell of the Ames team.




CNT in Microscopy

Using CNT as a tip in AFM is well known. However, most groups attach the CNT to the cantilever manually using epoxy or glue. This is tedious. Stevens and Nguyen of Ames are able to attach nanotubes directly to the cantilever by CVD. At Ames, an AFM with a nanotube tip is used to study simulated Mars dust as well as ALH 84001. The image on the right extreme is from H. Dai of Stanford University and Jie Han of NASA Ames which shows a 10nm line lithographic pattern on silicon. The bottom image is nano-lithography as well as nano-calligraphy where the White House nano-website address was written out as 10nm size letters using nanotube tip in an AFM at Ames.

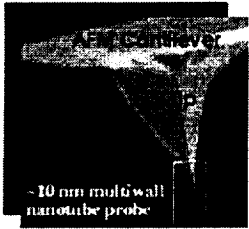


CNT in Microscopy

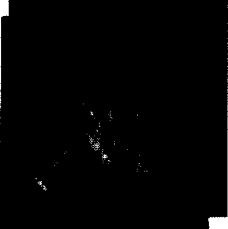


Atomic Force Microscopy is a powerful technique for imaging, nano-manipulation, as platform for sensor work, nanolithography...


Conventional silicon or tungsten tips wear out quickly. CNT tip is robust, offers amazing resolution.




~10 nm multiwall nanotube probe



Simulated Mars dust



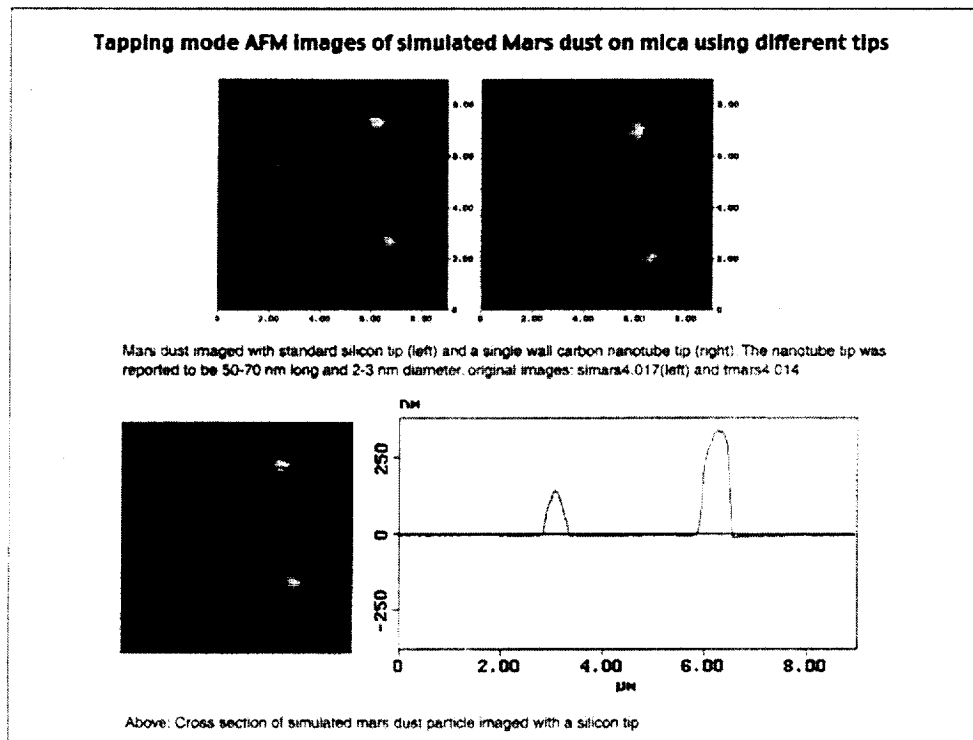
H. Dai



NASA Ames Research Center
Ramsey Stevens, Lance Delzeit, Cattien Nguyen

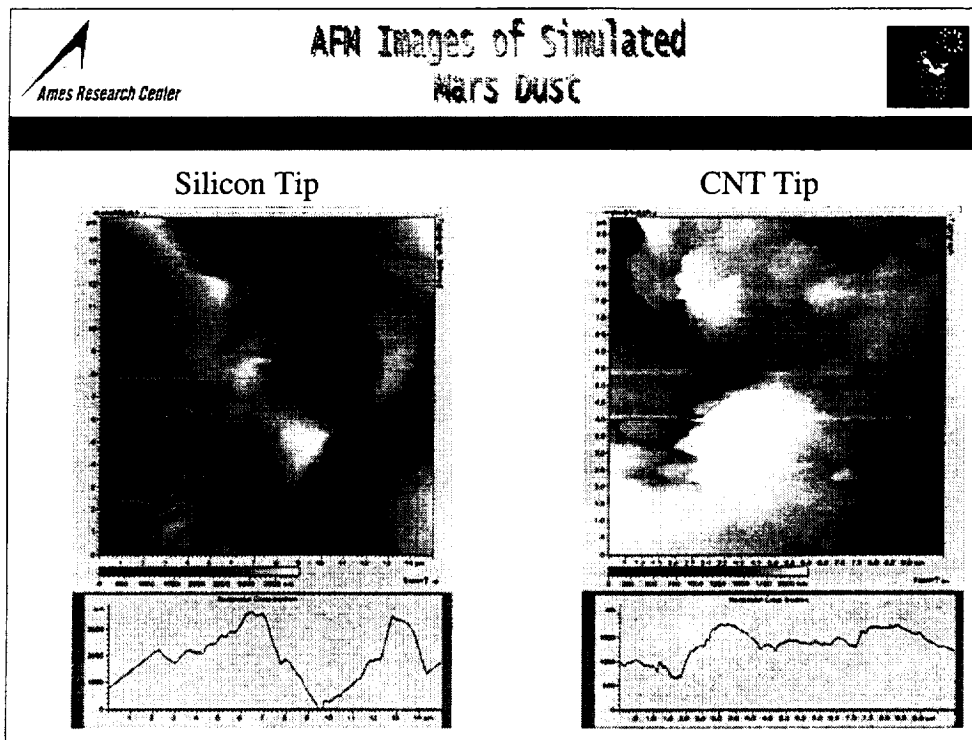
Tapping Mode AFM Images of Simulated Mars Dust on Mica Using Different Tips

Srin Manne of the University of Arizona did a comparison of nanotube tips and silicon tips in an AFM. When the particle size is small, the silicon tip cannot capture the shape correctly; all particles appear to be triangular on one side. In contrast, the nanotube tip captures the shape very well. The tip is also very robust and long lasting.




AFM Images of Simulated Mars Dust

This comparison, done by Ramsey Stevens of Ames, shows the image of 20 μm simulated Mars dust. The image using silicon tip, though topologically smooth, is a false image and is an artifact due to the pyramidal tip of the cantilever making contact with a tall feature before the apex of the tip reaches the surface. In contrast, the image using the nanotube tip shows a complex topography. The cross section at the bottom shows that the tip is tracking the surface even into deep valleys and over sharp peaks. It does, however, exhibit a 'record skipping' type artifact because the tip is reaching so deep past tall features that sometimes the side of the pyramid bumps into a tall feature as the tip scans past. This artifact has been overcome by altering tip size.




CNT Based Biosensors

The National Cancer Institute (NCI) is funding NASA Ames to develop a nanotube based cancer sensor. The focus is on developing a sensor for Leukemia. David Loftus, Ames medical officer, is a hematologist working on this project along with the Ames nanotube team. The experience gained in aligned nanotube growth and functionalization for this project would be directly beneficial to the sensor efforts in astrobiology.


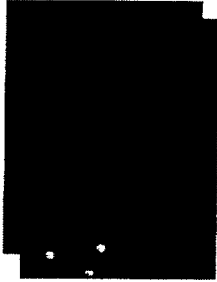
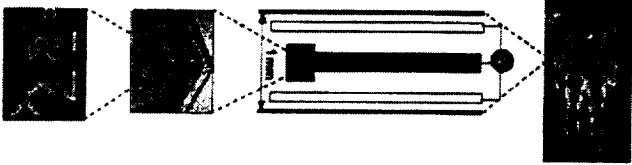


CNT Based Biosensors




- Our interest is to develop sensors for astrobiology to study origins of life. CNT, though inert, can be functionalized at the tip with a probe molecule. Current study uses AFM as an experimental platform.
- The technology is also being used in collaboration with NCI to develop sensors for cancer diagnostics:
 - Identified probe molecule that will serve as signature of leukemia cells, to be attached to CNT.
 - Current flow due to hybridization will be through CNT electrode to an IC chip.
 - Prototype biosensors catheter development.

- **High specificity**
- **Direct, fast response**
- **High sensitivity**
- **Single molecule and cell signal capture and detection**




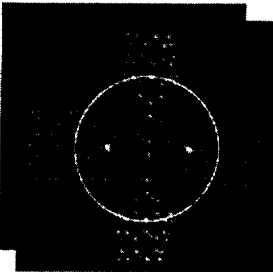
Computational Nanotechnology

Computational modeling and simulation have been valuable in the nanotube field. Numerous papers in the literature have been devoted to evaluation of properties and transport in nanotubes. The Ames team has made significant contributions to the field of computational nanotechnology. The CNT networks shown here, as modeled by Srivastava, appear to have the potential for revolutionary electronics. The nanogear designed by Han and Srivastava has captured the imagination of nano-enthusiasts across the world and represents one of the most widely used images in nanotechnology.



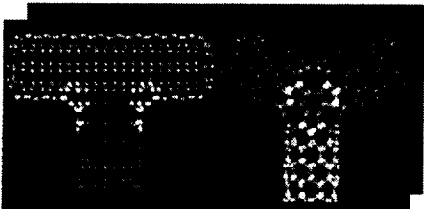
Computational Nanotechnology



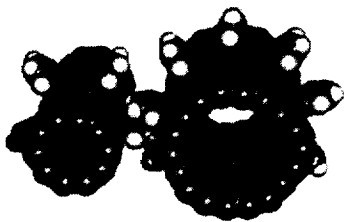


CNT Molecular Network

- Large scale computer simulations based on ab initio methods enable understanding nanotube characteristics and serve as design tool
- Evaluation of mechanical properties
- Evaluation of electronic properties
- Electron transport in CNT devices
- Functionalization of the nanotubes
- Design of electrical and mechanical devices
- Evaluation of storage potential (H_2 , Li)

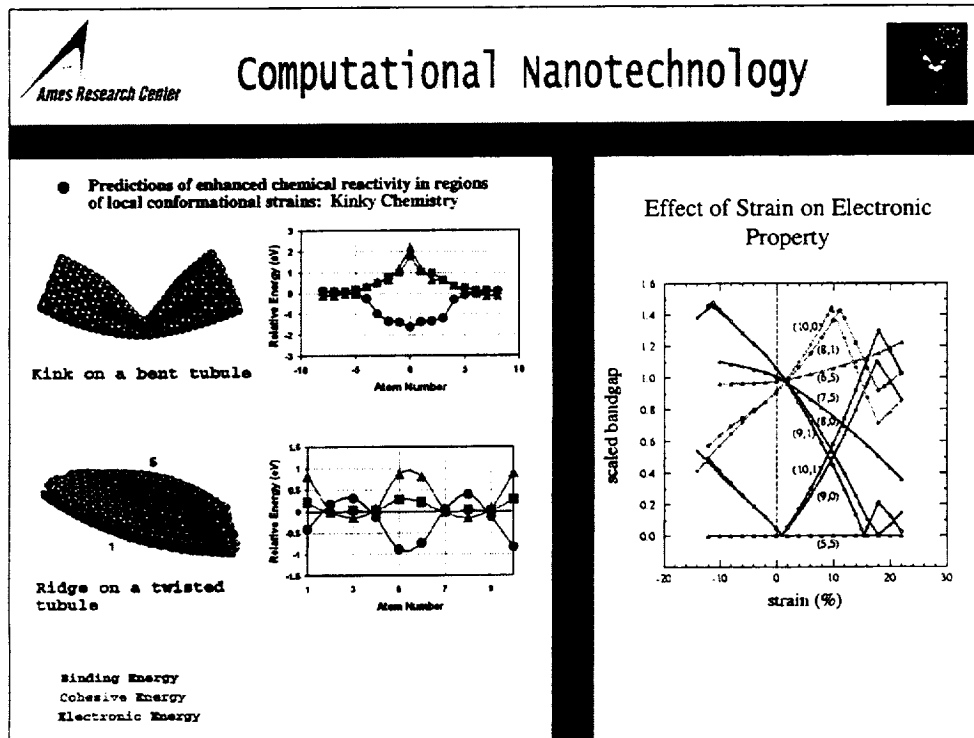


CNT "T" and "Y" Junctions




Computational Nanotechnology

CNT itself is chemically inert. Srivastava's simulations show enhanced chemical reactivity at locations of conformational strain. This prediction has been experimentally verified by Rodney Ruoff's group at Washington University. The electronic properties of CNT are tightly coupled to the mechanical properties. Liu Yang of Ames has computed the bandgap as a function of elongational and torsional strain. In addition, several papers by Anantram focus on transport in nanotubes and metal-nanotube contact characteristics. See www.ipt.arc.nasa.gov for a bibliography.




Protein Nanotubes

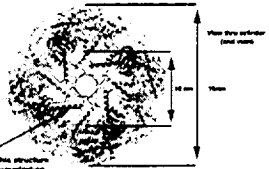

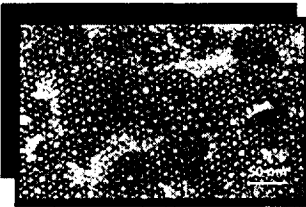
The study of extremophiles is an area of interest to Ames Astrobiology scientists. Jonathan Trent at Ames has been able to assemble HSP 60 into nanotubes. These protein tubes are about 12-15nm in diameter and a few microns long. The image on the left shows a self-assembly pattern of the protein nanotubes.



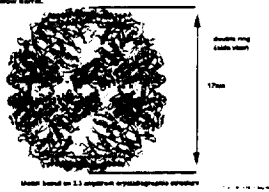
Protein Nanotubes



- Heat shock protein (HSP 60) in organisms living at high temperatures (“extremophiles”) is of interest in astrobiology.
- HSP 60 can be purified from cells as a double-ring structure consisting of 16-18 subunits. The double rings can be induced to self-assemble into nanotubes.



Removal of this structure prohibits polymerization, creating a hollow barrel.



12nm


17nm

12nm


17nm

Summary

The potential of nanotube technology for NASA missions is significant and is properly recognized by NASA management. Ames has done much pioneering research in the last five years on carbon nanotube growth, characterization, atomic force microscopy, sensor development and computational nanotechnology. NASA Johnson Space Center has focused on laser ablation production of nanotubes and composites development. These in-house efforts, along with strategic collaboration with academia and industry, are geared towards meeting the agency's mission requirements.



Summary



- Nanoscale science and technology will have significant impact on the future of NASA missions by enabling cheaper, more capable and reliable, and more frequent missions.
- Given the tremendous potential, there is a need for investment from all enterprises.
- Given the breadth of nanotechnology subfields, there is significant overlap with DoD, DOE missions and opportunity to share fundamental research sponsored by NSF.
- Nano-revolution has just begun; there is a long way to go before significant system level payoff. It is time to focus on:
 - Fundamental research
 - Material development, characterization
 - Novel instrumentation
 - Cost effective manufacturing routes
 - Identification of most promising applications
 - System level concepts

59/76

18p

Computational Nanotechnology of Materials, Devices and Machines: Carbon Nanotubes

Deepak Srivastava
NASA Ames Research Center
Moffett Field, CA 94035



Computational Nanotechnology of Materials, Devices and Machines: Carbon Nanotubes



Deepak Srivastava
Computational Nanotechnology at CSC/NAS
NASA Ames Research Center
Moffett Field, CA 95014

Collaborators:

- M. Menon – University of Kentucky
- K. Cho – Stanford University
- D. Brenner – North Carolina State University
- R. Ruoff – University of Washington, St. Louis



NASA Mission Needs



- Onboard computing systems for future autonomous intelligent vehicles
 - powerful, compact, low power consumption, radiation hard
- High performance computing (Tera- and Peta-flops)
 - processing satellite data
 - integrated space vehicle engineering
 - climate modeling
- Revolutionary computing technologies
- Smart, compact sensors, ultrasmall probes
- Advanced miniaturization of all systems
- Microspacecraft
- 'Thinking' spacecraft
- Micro-, nano-rovers for planetary exploration





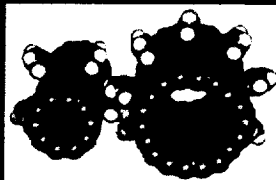
CARBON NANOTUBES

Carbon nanotube (CNT) is a new form of carbon, configurationally equivalent to two dimensional graphene sheet rolled into a tube. It is grown now by several techniques in the laboratory and is just a few nanometers in diameter and several microns long.



CNT can be metallic or semiconducting and offers amazing possibilities to create future nanoelectronics devices, circuits, and computers.

CNT exhibits extraordinary mechanical properties. The Young's modulus is over 1 Tera Pascal. It is stiff as diamond. The estimated tensile strength is 200 Giga Pascal. These properties are ideal for reinforced composites, nanoelectromechanical systems (NEMS).



<http://www.ipt.arc.nasa.gov> at Ames Research Center



Simulation Techniques

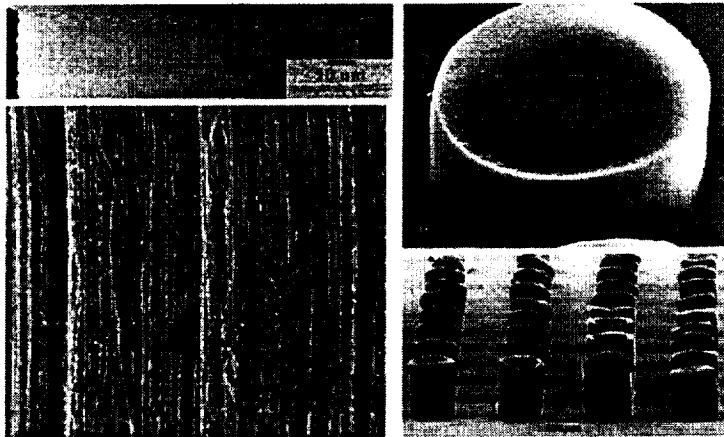


- **Large-scale Classical Molecular Dynamics Simulations on a Shared Memory Architecture Computer**
 - Tersoff-Brenner reactive many-body potential for hydrocarbons with long range LJ(6-12) Van der Waals interactions
 - Parallel implementation on a shared memory Origin2000
- **Quantum Molecular Dynamics Simulations**
 - Tight-binding MD in a non-orthogonal atomic basis.
 - Previous parametrization: silicon and carbon (M. Menon and K. R Subbaswami, Phys. Rev. B 1993-94).
 - Extended to heteroatomic systems including C, B, N, H



Experimental Nanotechnology at Ames Research Center

CVD Carbon Nanotube SEM Images



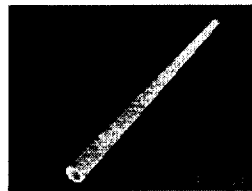
<http://www.ipt.arc.nasa.gov> at Ames Research Center



Nanomechanics of Nanomaterials: Characterization



- Nanotubes are extremely strong, highly elastic nanofibers.
 - ~ High value of Young's modulus (1.2 -1.3 T Pa for SWNTs)
 - ~ Elastic limit up to 10-15% strain
- Dynamic response under axial compression, bending and torsion.



- *Redistribution of strain*
- *Sharp buckling leading to bond rupture*
- *SWNT is stiffer than MWNT*



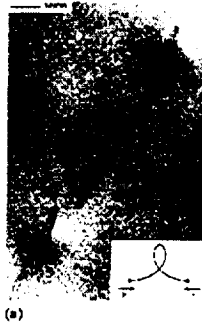
Application: Nanotubes in Composites



- Experiment: Buckling and collapse of nanotubes embedded in polymer composites.

- Experiment: Buckling and Collapse of Embedded Carbon Nanotubes
O. Lourie et al. Phys. Rev. Lett. Vol. 81, 1638 (1998).

Buckle, bend and loops of thick tubes.



(a)



(b)

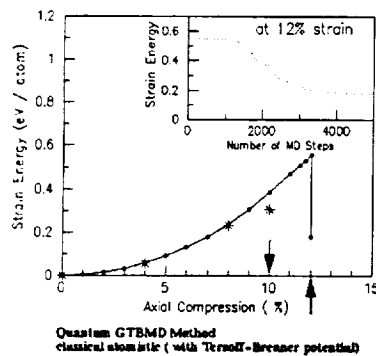
Local collapse or fracture of thin tubes.



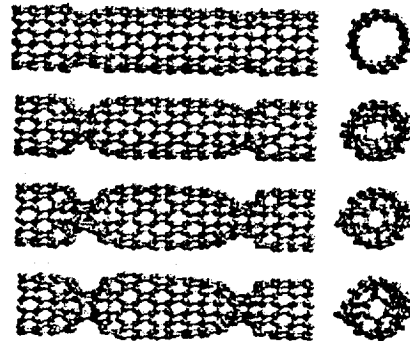
Stiffness and Plasticity of Compressed C Nanotubes



- Energetics of collapse-plasticity of (8,8) CNT at 12% compression strain.



- Spontaneous collapse-plasticity of (8,8) CNT through graphitic (sp²) to diamond like (sp³) type transition.



(a) side view

(b) top view

- Linear response regime ($Y = 1.3$ TPa) followed by pinching/buckling (classical MD) or collapse/plasticity (quantum MD).

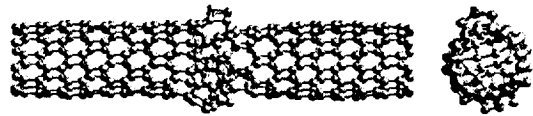
Shows the same collapse as observed in experiment.



Plastic Collapse by Design



● With a single B point defect



- Tube plastically collapses at the location of the defect.
- New types of hetero-junctions can be created.
- Quantum dot effect in one-dimensional system.
- Application: Molecular electronics.

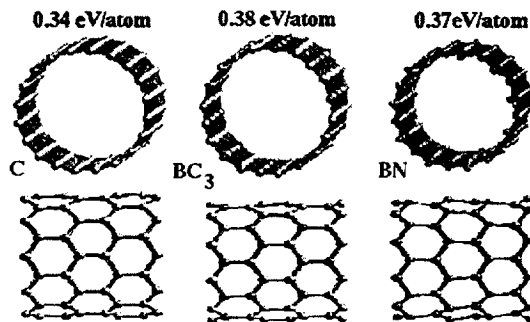


Heteroatomic C_xByN_z Nanotubes



- Band gap engineering over a larger range is possible

- | | |
|---------------------|------------|
| • BN | ~ 5 eV |
| • BC ₂ N | ~ 2 eV |
| • C | ~ 0 - 1 eV |
| • BC ₃ | ~ 0.5 eV |



reconstruction due to polar BN bond

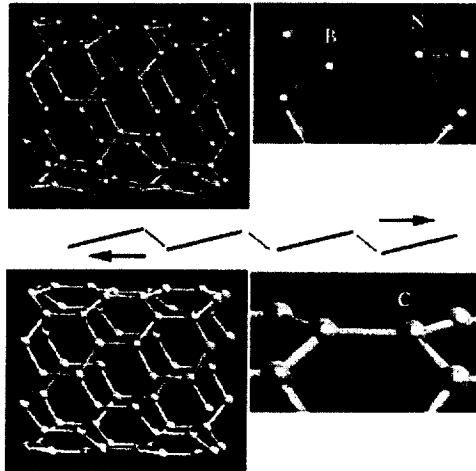


BN Nanotubes - Structural Characteristics



- BN bond buckling effect to minimize the energy

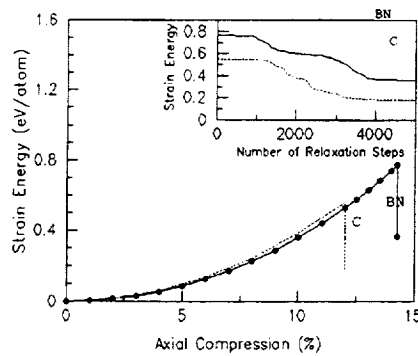
- BN bond buckling effect



BN Nanotubes: Nanomechanics and Plasticity



- Comparison of Young's modulus and elastic limit with carbon nanotubes



- $Y(\text{BN}) = 1.2 \text{ TPa}$ ~ BN is 92% as strong as CNT!
 $Y(\text{C}) = 1.3 \text{ TPa}$
- BN nanotube plastically collapses at even higher strain than C nanotube.

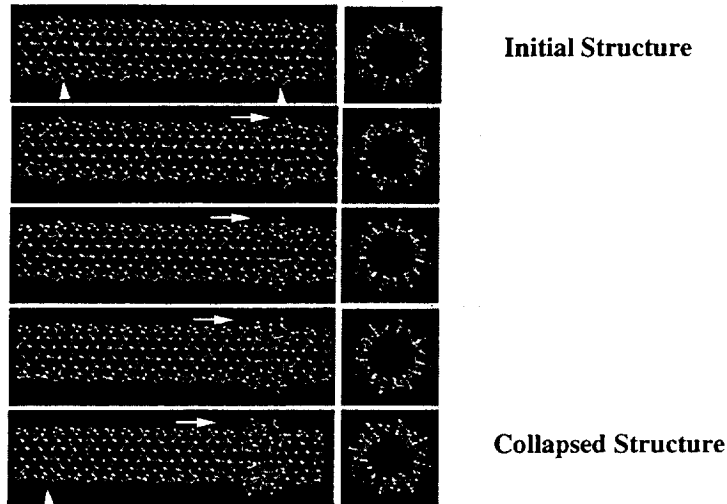
D. Srivastava, M. Menon and K. Cho, submitted (2000)



Anisotropic Plasticity of Compressed BN Nanotube



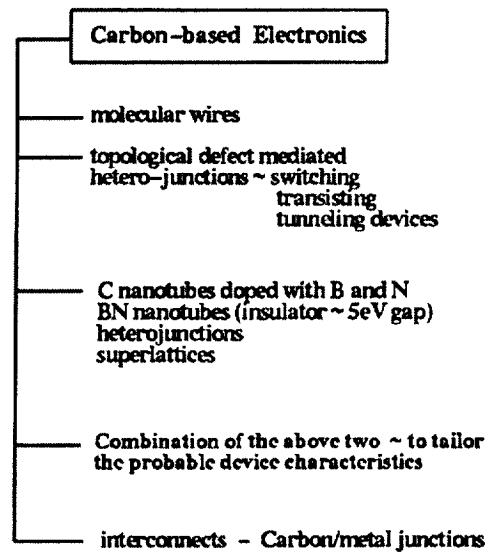
- Plastic collapse at 14.75% strain – damage is limited to only one side of the material.



D. Srivastava, M. Menon and K. Cho, submitted (2000)

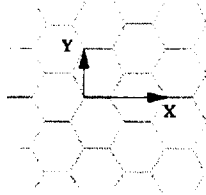


Nanotube Electronics: Scheme

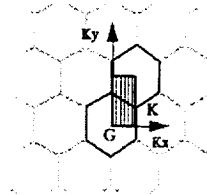




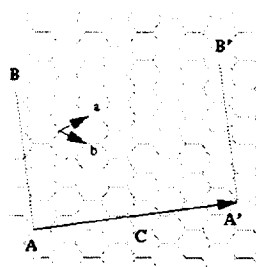
Nanotube Electronics (Characterization)



Hexagonal Lattice of a Graphene Sheet - (2xunit cell)



First Brillouin zone for an arm-chair tube.



$Ch = n a + m b$ (chiral vector)

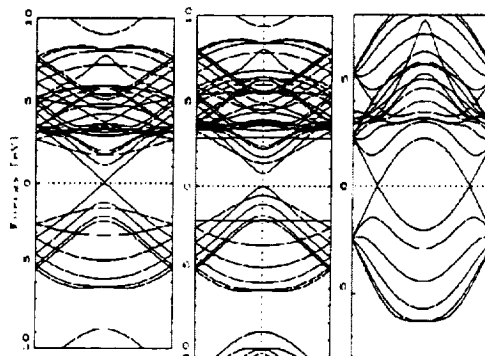
Boundry condition decide if nanotube is metallic or semiconducting



Band Structure of Different Nanotubes



Electron bands in (9,0) tube Electron bands in (10,0) tube Electron bands in (5,5) tube



Wave vector Wave vector Wave vector
 (9,0) tube (10,0) tube (5,5) tube

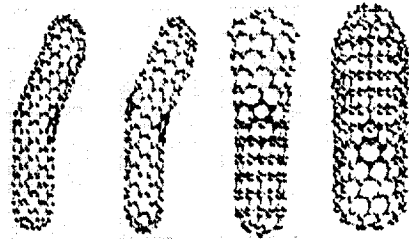
Arm chair tubes (n,n) - metal like
 Otherwise $m-n = 3l$ (l- integer) metal like



Nanotube Heterojunctions: 2-point



2- point Nanotube Heterojunctions
Molecular Electronic Switches



(10,0) - (6,6) (9,0) - (5,5) (8,0) - (7,1) (12,0) - (11,0)

Bent Junctions

Straight Junctions

Chico et al. Phys. Rev. Lett., 96
Charlier et al. Phys. Rev. B, 96
Lambine et al. Chem. Phys. Lett., 96
Saito et al. Phys. Rev. B, 96

Semiconductor-Metal
Semimetal-Metal

We studied the effect of capping the tubes and relaxing the junctions with a quantum GTBMD method.



Nanotube Heterojunctions: 3-point



VOLUME 79 NUMBER 22 PHYSICAL REVIEW LETTERS 11 DECEMBER 1997

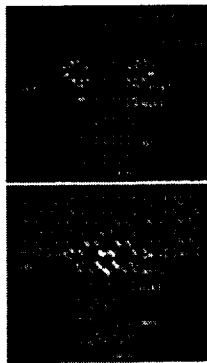


FIG. 1. Scanning tunneling microscopy image of a (10,0)-(9,0) T-junction. The frequency, color, and scale bar are shown. The color scale is the current. The structure contains two heterojunctions and two junctions. The tube width is 10 nm. The diameter of each tube is 10 nm. The heterojunctions are shown by white dots. The structure contains two heterojunctions and two junctions.

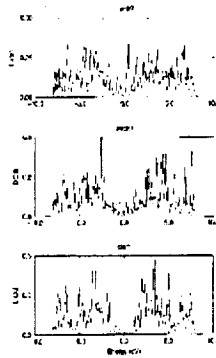


FIG. 2. LDOS of the (10,0)-(9,0) T-junction at bias voltages of 0.1 V, 0.2 V, and 0.3 V. The bias contribution in the plot is due to the presence of two tubes. The bias contribution is shown in the inset.

LDOS of (10,0)-(9,0) "T-junction"

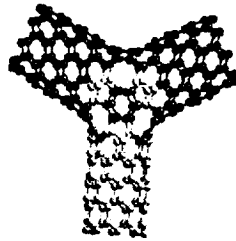
3-terminal "T-tunnel" Junctions of Nanotubes



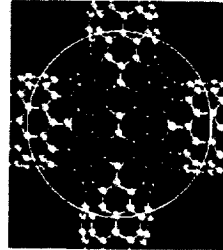
Molecular Networks with Nanotubes



Pathways to Two Dimensional Molecular "Networks"



Metal-Semiconductor-Metal "Y" Tunnel Junction



A four-terminal nanotube heterojunction

"It turns out that all of our proposed junctions satisfy - Generalized Euler's Rule about the global topology of connected networks"



Nanotube Electronics with Doping



- Band gap engineering over a larger range should be possible:

BN	~5.5 eV
BC ₂ N	~2.8 eV
C	~0 - 1 eV
BC ₃	~0.5 eV

- a variety of junctions, quantum dots and superlattices should be possible

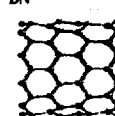
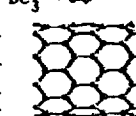
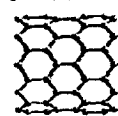
- should be more robust

- Example: Composite (10,0) nanotube

0.34 eV/atom

0.38 eV/atom

0.37 eV/atom



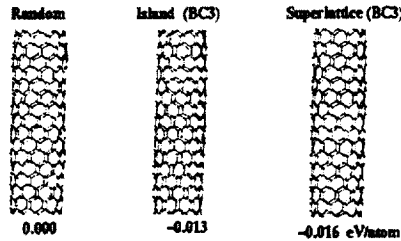
reconstruction due to polar BN bond



Nanotube Electronics with Doping

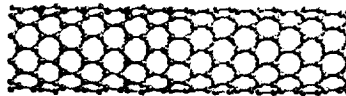


• B doping of Carbon Nanotube



phase separation of doped and undoped regions is thermodynamically stable !

• BN/C Junctions

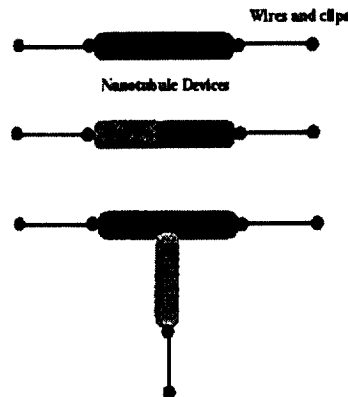


Interface Energy = 2*BN/C - BN - C
Interface Energy = 0.33eV/CB bond

Stable interfaces should be possible !



Nanotube/Molecules Hybrid Electronics

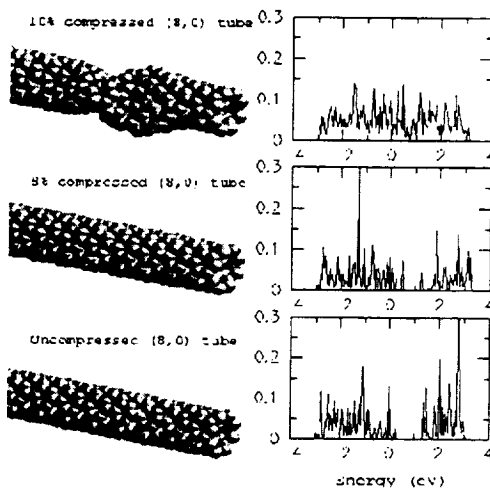


Negative "World-image" is also possible

- Amenable to self-assembly through shape and color interactions
- Provision for molecular interconnects to the outside metallic contacts



Nano Electromechanical Effects (NEMS)



Mechanical deformation alters the electronic deformation of nanotubes. Effect is chirality dependent.



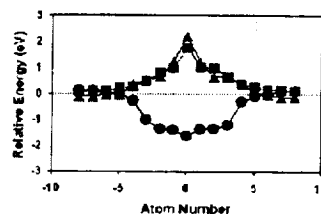
Mechano-Chemical Effects: Kinky Chemistry



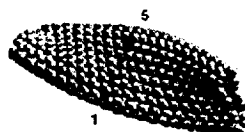
- Predictions of enhanced chemical reactivity in regions of local conformational strains: Kinky Chemistry



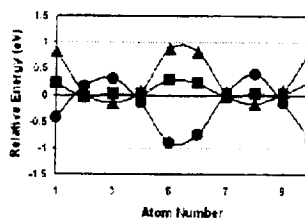
Kink on a bent tubule



Cohesive Energy
Binding Energy



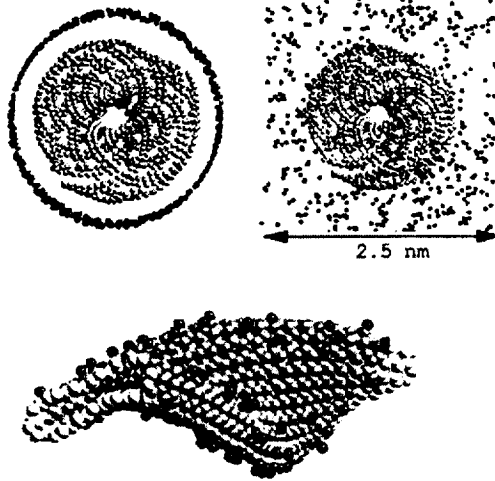
Ridge on a twisted tubule



Reactivity is enhanced at the location of mechanical kinks



Kink Driven Functionalization of Nanotubes



Torsionally twisted SWNT equilibrated in an H bath

More Hydrogen is adsorbed at the sharp edges of a kink !

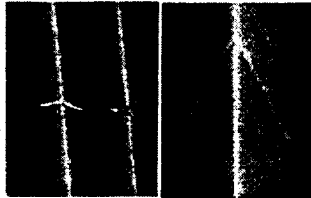


Mechano-Chemical Effects: Kinky Chemistry

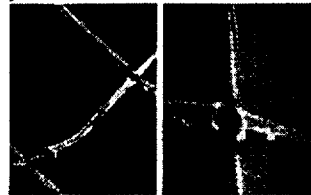


SEM images of MWNTs dispersed on a V-ridged Formvar substrate

(a) Before Reaction



(b) Same sample after exposure to nitric acid vapor at room temperature



Nanotube etching occurs preferentially at the location of a kink.

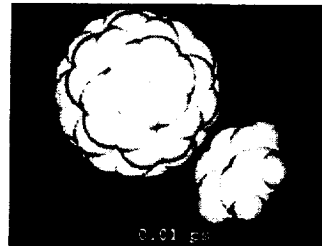
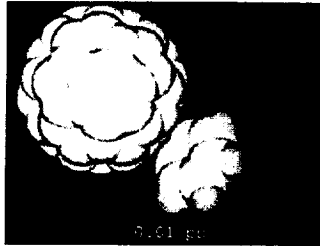
D. Srivastava, J. D. Schall, D. W. Brenner, K. D. Ausman, M. Feng and R. Ruoff, J. Phys. Chem. Vol. 103, 4330 (1999).



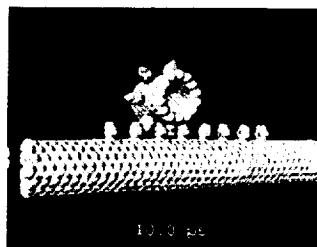
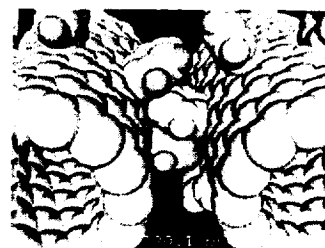
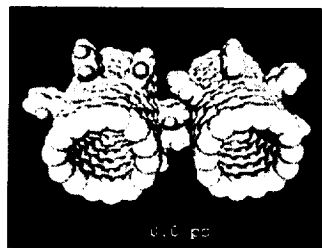
Molecular Machines and Laser Motor



J. Han, A Globus and R. Jaffe



Molecular Machines and Laser Motor



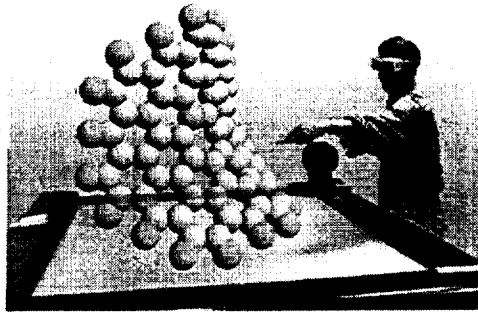


Computational Nanotechnology: Future: PSE



Nanomanipulation in Virtual World

Simulations



Experiments

Next Generation of Technology and Products

2/15/2016

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Carbon Nanotubes: Properties and Functionalization

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Properties and Functionalization**

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Training Workshop on Nano-Biotechnology
NASA Langley Research Center, June 14-15, 2000

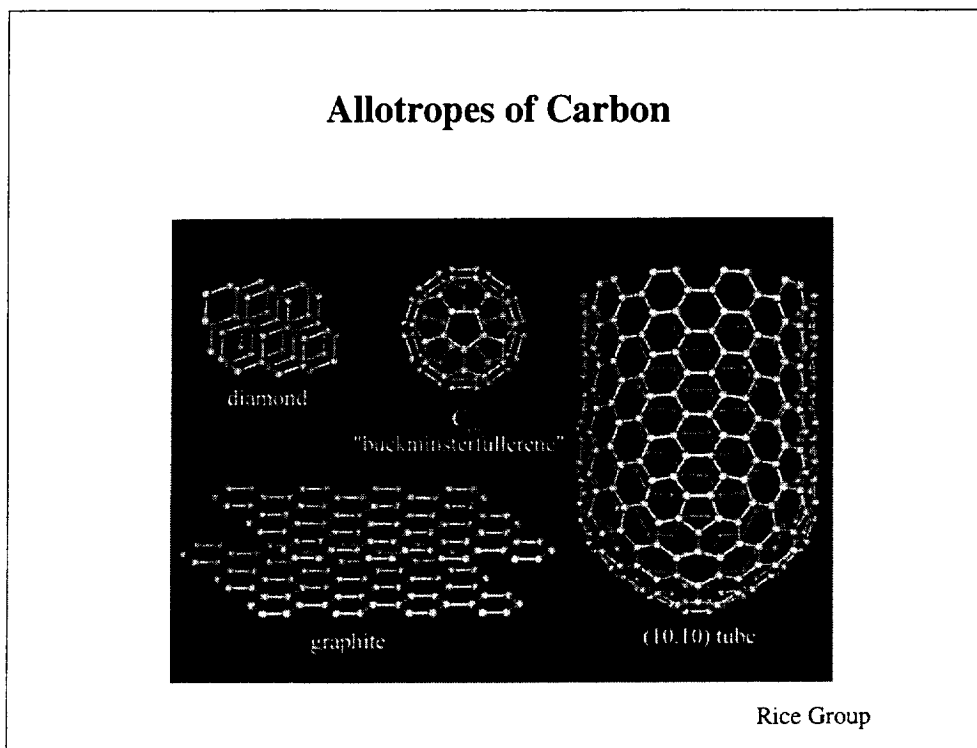


Introduction

- **Nanoscale Hybrid Materials**
- **Chemistry in Confined Environments**
- **Single Molecule/Single Atom Detection**

Allotropes of Carbon

The different allotropes of carbon by class. Clockwise from upper left. Diamond, C_{60} , representing the many fullerene closed cage structures formed from mixtures of five and six member carbon rings, (10,10) nanotube, representing the many nanotube structures, achiral and chiral formed by wrapping a single, or multiple nested graphene sheets into a tube, graphite. This figure is from the Rice University web page of Rick Smalley.



Production of Nanotubes

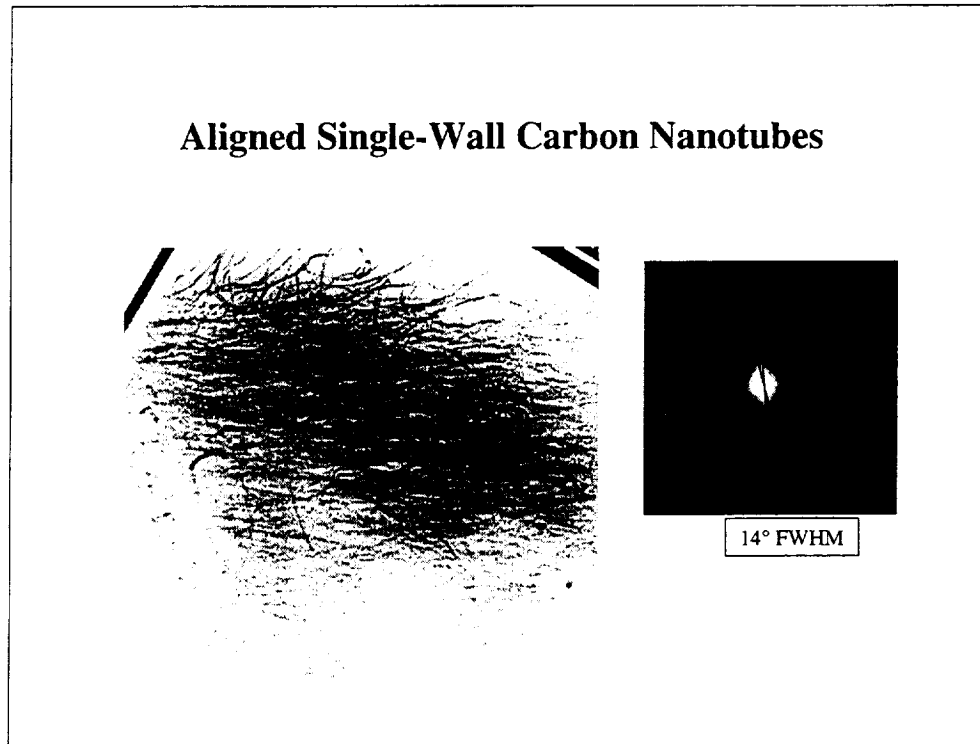
A complete summary (as of the time of the workshop) of the methods used to produce nanotubes with the year of publication and responsible organization listed. The list is confined to those methods for which rigorous evidence of the existence of closed tubes of graphene sheets extending over long distances has been presented, usually via transmission of electron microscope (TEM) images.

Production of Nanotubes

- **Discovery**
 - Multi-wall Carbon Nanotubes (MWNTs) - NEC, 1991
 - Single-wall Carbon Nanotubes (SWNTs) - NEC, IBM, 1993
- **Production Methods**
 - Electric Arc (CA) - NEC, IBM, 1993, Montpellier, 1997
 - Pulsed Laser Vaporization (PLV) - Rice, 1996
 - Solar Furnace - Montpellier, 1998
 - Chemical Vapor Deposition - Stanford, 1998
 - High Pressure CO Disproportionation (HIPCO) - Rice, 2000
 - Combustion - TDA Research, 2000

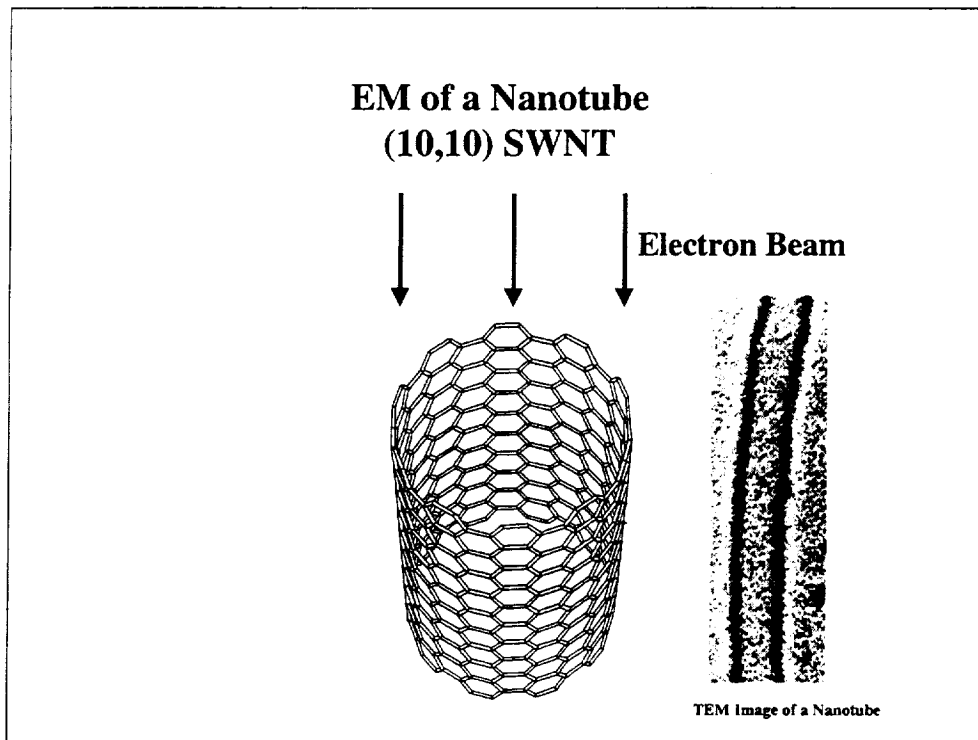
Aligned Single-Wall Carbon Nanotubes

Carbon nanotubes have been aligned by three methods: under high magnetic fields; by melt spinning within a polymer matrix; and under the influence of an electric field. The micrograph is of tubes@rice material (PLV method) aligned with a 25T magnetic field (Rice group). Measurement of the FWHM alignment was done using electron diffraction (Penn).



EM of a Nanotube (10, 10) SWNT

A high magnification image of a single-wall carbon nanotube (SWCNT) compared to a schematic. In the phase imaging condition, all scattered and unscattered electrons that pass through the lens pole pieces are used to produce the image. Due to its low atomic number, carbon scatters electrons weakly. Under phase imaging conditions, nanotubes can, therefore, be considered as weak phase objects. Images of weak phase objects will be two-dimensional projections along the electron beam direction of the three dimensional specimen convoluted with the point transfer function of the electron microscope. With the resolution of the microscope significantly better than the finest scale detail in an image, the image can be considered to be a direct magnification of the carbon shells. The intra-shell structure of the modified graphene sheet is below the resolution limit of the microscope and appears as a uniform contrast level (gray). Since the maximum scattering potential of the nanotube exists where the structure is tangent to the electron beam, the images will appear as a pair of parallel lines.



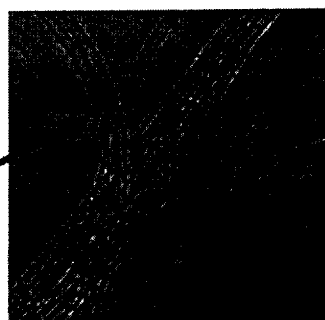
Cutting Nanotubes to Length

The ideal structure of a carbon nanotube is a perfect closed sheet of hexagonal rings of carbon atoms. Exposure to an oxidizing environment has been shown to damage the nanotube, even producing sizeable holes in the sidewall and opening the ends. It is not known why this process is localized, but the result is useful for certain applications.

Cutting Nanotubes to Length

Key capability for electronic, biochemical
and mechanical applications

Processes leading to this
condition need to be
understood and controlled



Thermal and Chemical Stability of Carbon Nanotubes

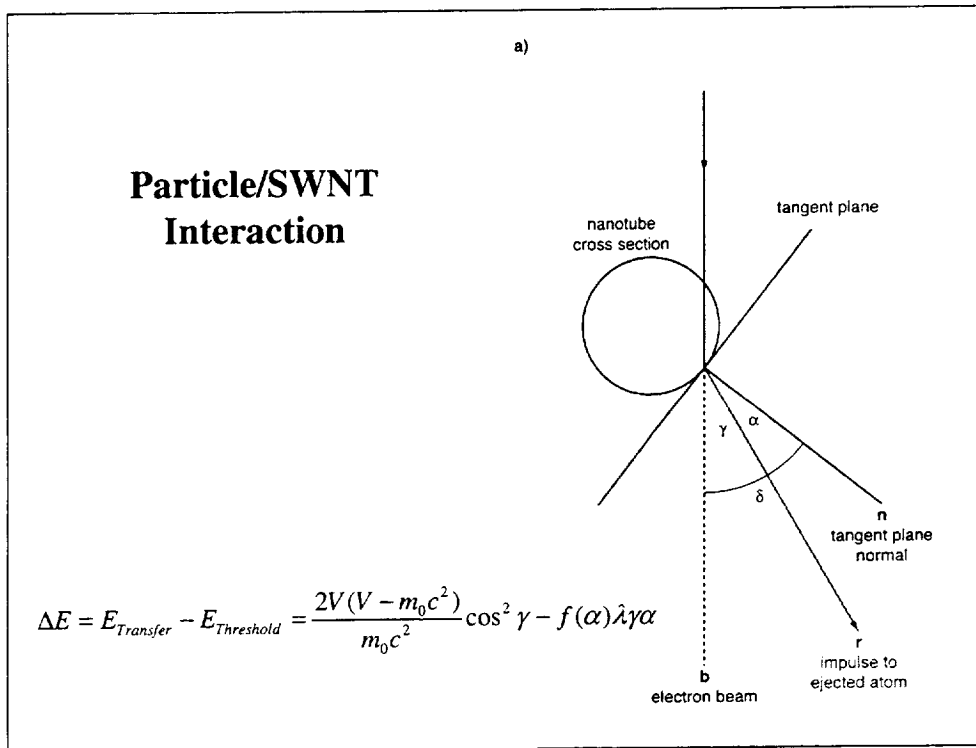
This is an incomplete summary of the response of nanotubes to some environments – included for guidance only.

Thermal and Chemical Stability of Carbon Nanotubes

- In vacuum
 - Stable range - from < 90 K to > 1500 K
 - Some reports above 1500 K, but unconfirmed
- In argon
 - Tested range RT to 1200 °C - stable
 - Coalesce at high temperatures
- In air
 - Decompose at ~ 400 °C
- Chemically stable, however
 - Attacked in oxidizing environments
 - Attacked by strong ultrasonic disturbance

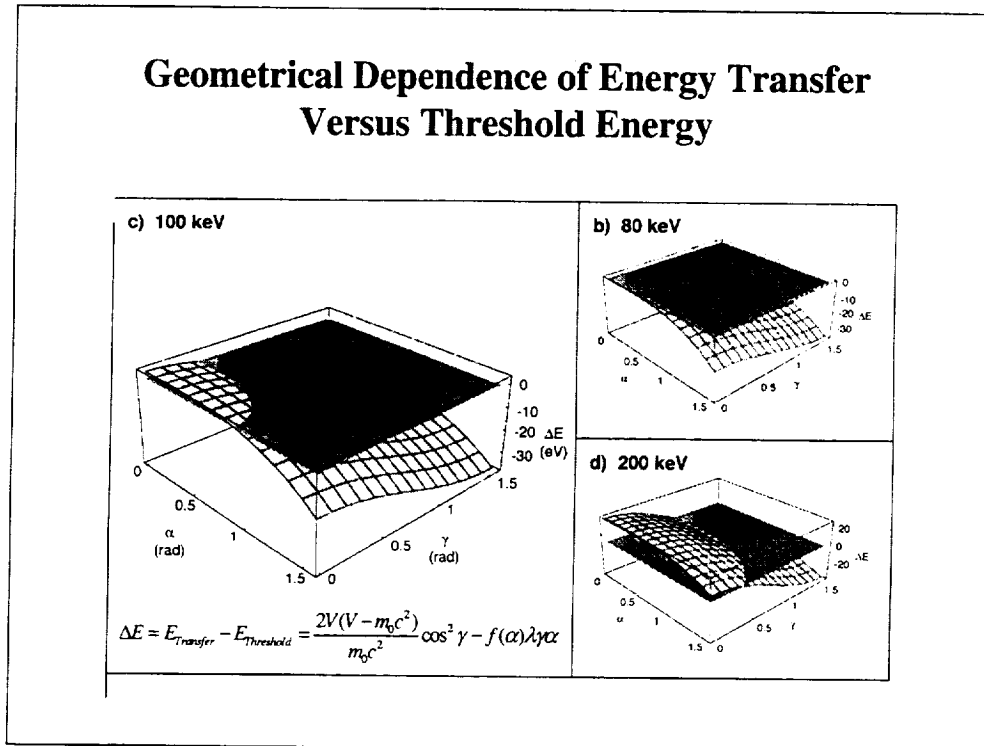
Particle/SWNT Interaction

In order to electron irradiation damage in nanotubes, we can calculate the minimum incident electron energy (e.g., accelerating voltage) required for ballistic ejection of a carbon atom to occur. To facilitate this calculation, we define the primary knock-on atom (PKA) as the carbon atom targeted for displacement. Since a nanotube may adopt any spatial orientation with respect to the electron beam, a complete description of the relevant interaction geometry is required. The PKA is contained by a tangent plane to the nanotube, where \mathbf{n} is the normal vector to that plane. The vector \mathbf{r} points along the direction of impulse to the PKA (i.e., the direction of ejection). The vector \mathbf{b} points along the direction of the incident electron beam. Finally, the angle α is between \mathbf{n} and \mathbf{r} , the angle γ is between \mathbf{r} and \mathbf{b} , and the angle δ is between \mathbf{n} and \mathbf{b} such that $\delta = \alpha + \gamma$. It will be shown that it is only necessary to consider the case where \mathbf{n} , \mathbf{r} , and \mathbf{b} are coplanar. Two factors must be considered in determining whether or not the PKA will be ejected: (1) the energy transferred from the electron beam to the PKA; and (2) the energy barrier that the PKA must overcome to escape from the nanotube. These are embodied in the two terms in the equation, the first governing the energy transfer to the PKA, the second a function fit to discrete tight binding calculations of the anisotropic binding energy of the PKA to the nanotube.



Geometrical Dependence of Energy Transfer Versus Threshold Energy

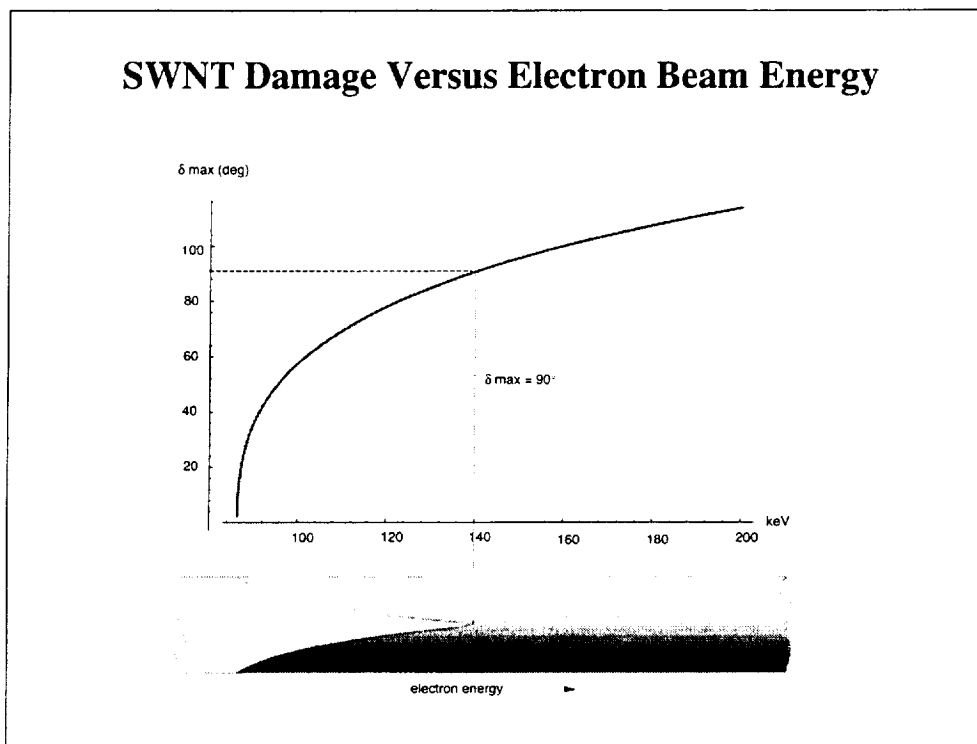
At a given incident electron energy (V), at those (α, γ) geometries where E_{transfer} exceeds E_{escape} the PKA will be ejected. These conditions are indicated in the figures which show $\Delta E = E_{\text{transfer}} - E_{\text{escape}}$ plotted for three different electron energies. For 80 keV electrons, ΔE is negative for all (α, γ) such that ejection of the PKA is impossible. At 100 keV, ΔE is positive for a small (α, γ) range such that ejection of the PKA is possible only within a narrow angular spread of both \mathbf{n} and \mathbf{b} . Similarly, at 200 keV the energy transfer is sufficiently high that ejection is possible at more severe angles. Note that the cross section for ejection will increase as ΔE becomes more positive, indicating that ejections are most probable for the geometry $(\alpha, \gamma) = (0, 0)$. Finally, the threshold energy for knock-on damage occurs where the ΔE surface has its maximum at 0 eV. This is calculated to occur at an electron energy of 86.4 keV.



SWNT Damage Versus Electron Beam Energy

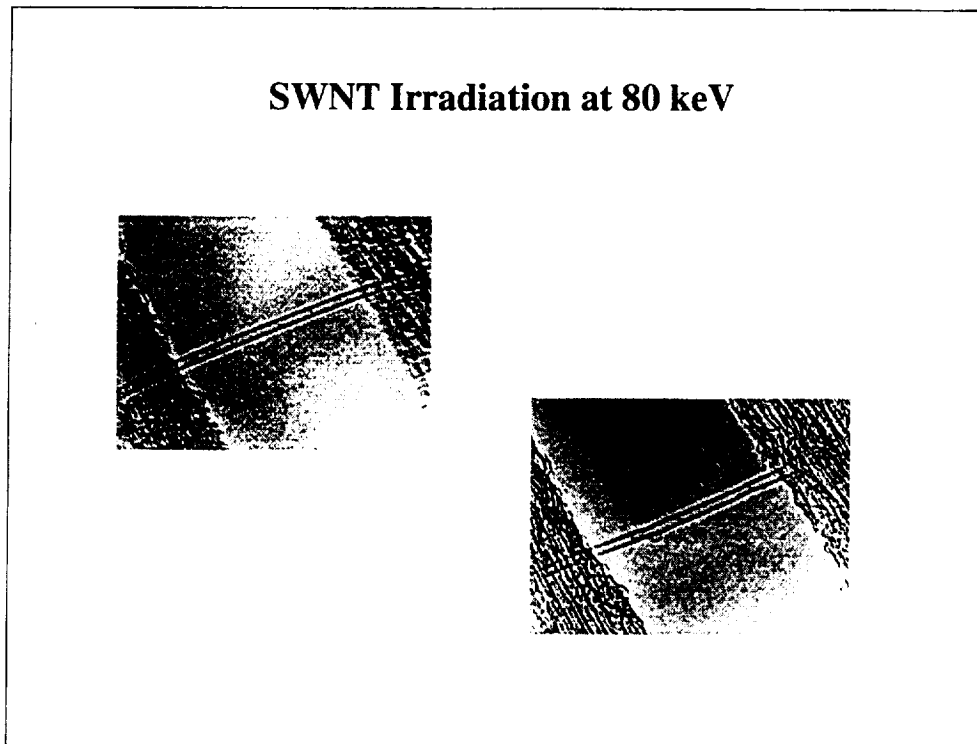
For a known electron beam direction and energy, it is possible to determine which atoms on an SWNT (as defined by their tangent planes) are susceptible to knock-on damage. Consider that the angle δ can be calculated for each (α, γ) having positive ΔE . The largest δ for any such (α, γ) occurs when α and γ are coplanar. Finally, the ΔE surface intersects the $\Delta E = 0$ plane along a curve that has the property of giving the largest allowed γ for a given α , and vice versa. Maximizing the sum $\alpha + \gamma$ along this curve gives the largest possible δ that can occur for *any* (α, γ) at that beam energy. Any carbon atoms whose tangent plane normals are further from \mathbf{b} than this angle, which we call δ_{\max} , cannot undergo ballistic ejection.

A numerical calculation of δ_{\max} as a function of electron energy is plotted. The corresponding illustration is drawn on the same abscissa as the plot above it and graphically shows which surfaces of a nanotube can be damaged as a function of electron energy for a beam directed down the figure. As before, at 80 keV no carbon atoms can be ejected. At 100 keV, atoms can be ejected for $\delta < 57.5^\circ$, destroying the top and bottom surfaces and leaving only the side walls intact. Above 138.8 keV, all carbon atoms can be ejected.



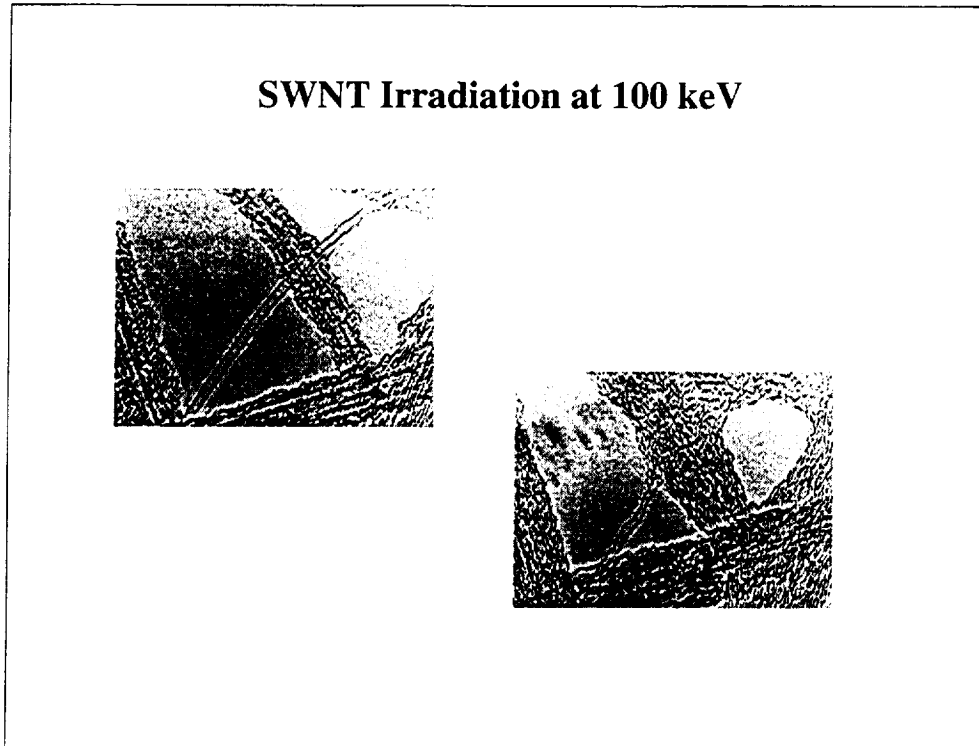
SWNT Irradiation at 80 keV

At 80 keV, the SWCNT is not damaged by the electron beam even after extensive irradiation.



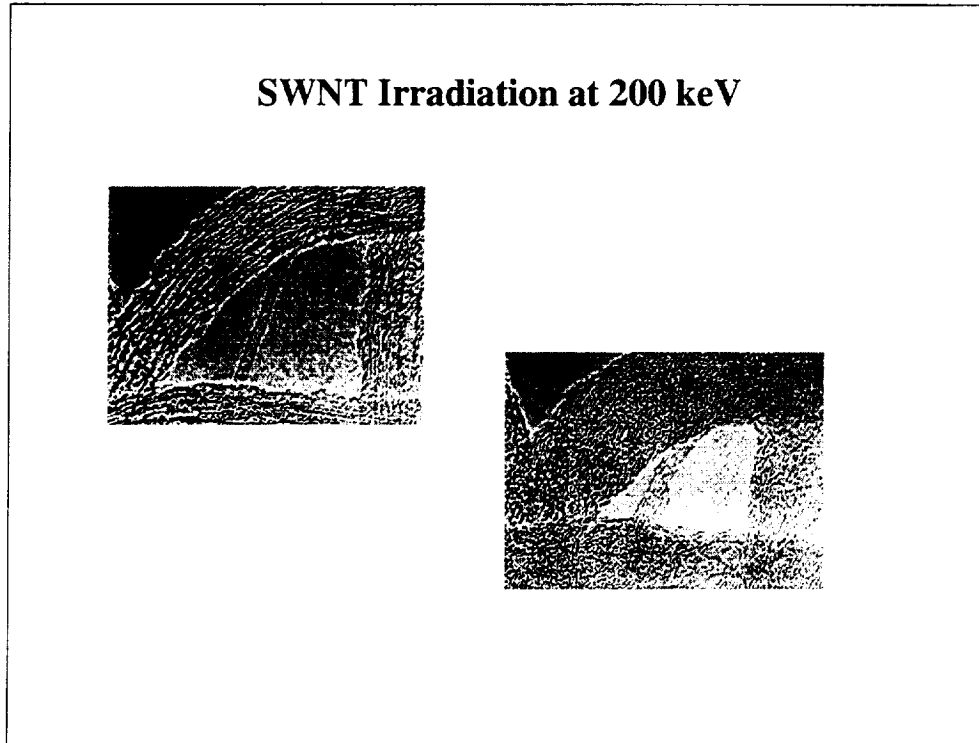
SWNT Irradiation at 100 keV

At 100 keV, the top and bottom of the nanotube is damaged with the side walls remaining intact as can be seen from the strong continuous contrast. The loss of top and bottom surfaces is detectable by the lack of parallel registry between the two side walls.



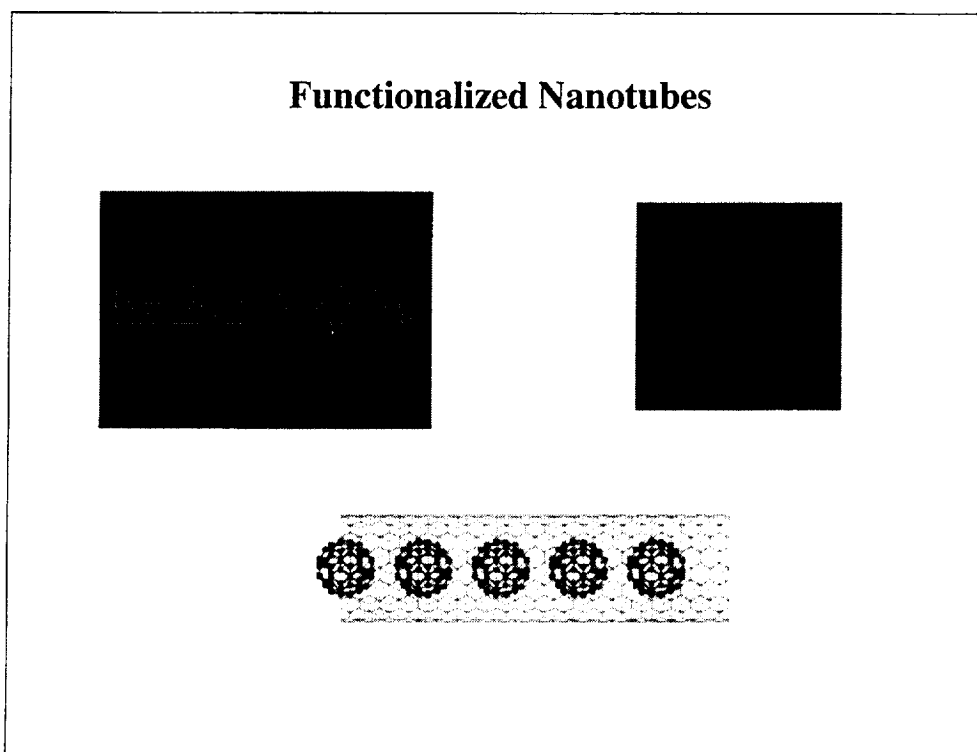
SWNT Irradiation at 200 keV

At 200 keV, the nanotube is amorphized with all surfaces destroyed.



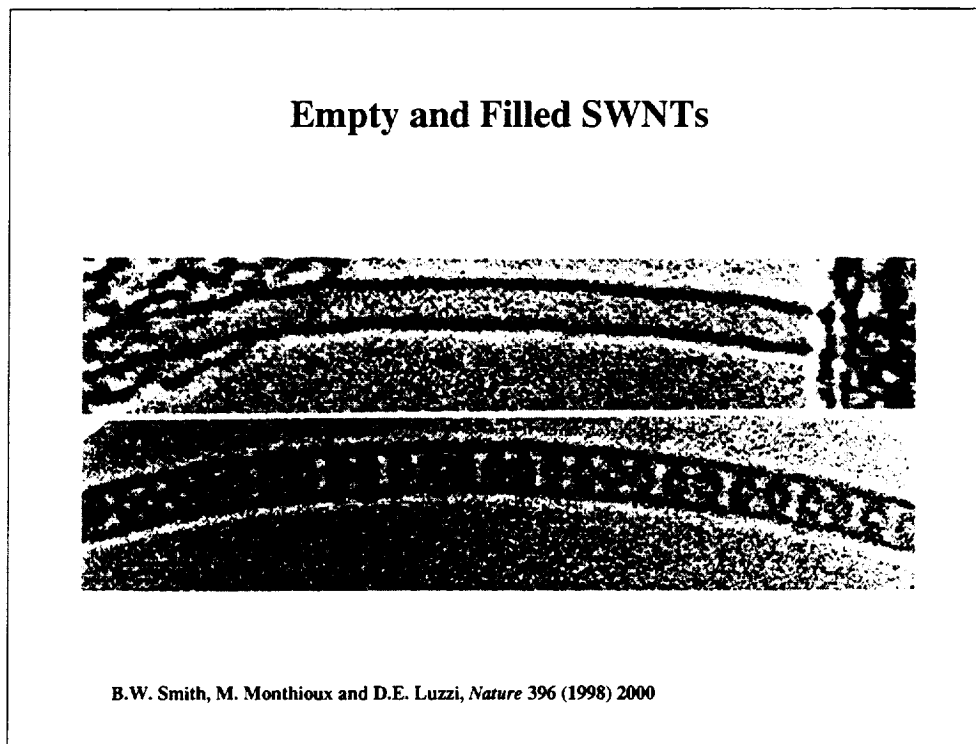
Functionalized Nanotubes

There are three possible paths to SWCNT functionalization: clockwise from upper left – attachment of side groups to the nanotube walls and ends; intercalation of the interstices in the SWCNT lattice; and intracalation of molecules within the lumen of the SWCNT. Schematics from the Smalley group (Rice), the Fischer group (UPenn), the Luzzi group (UPenn).



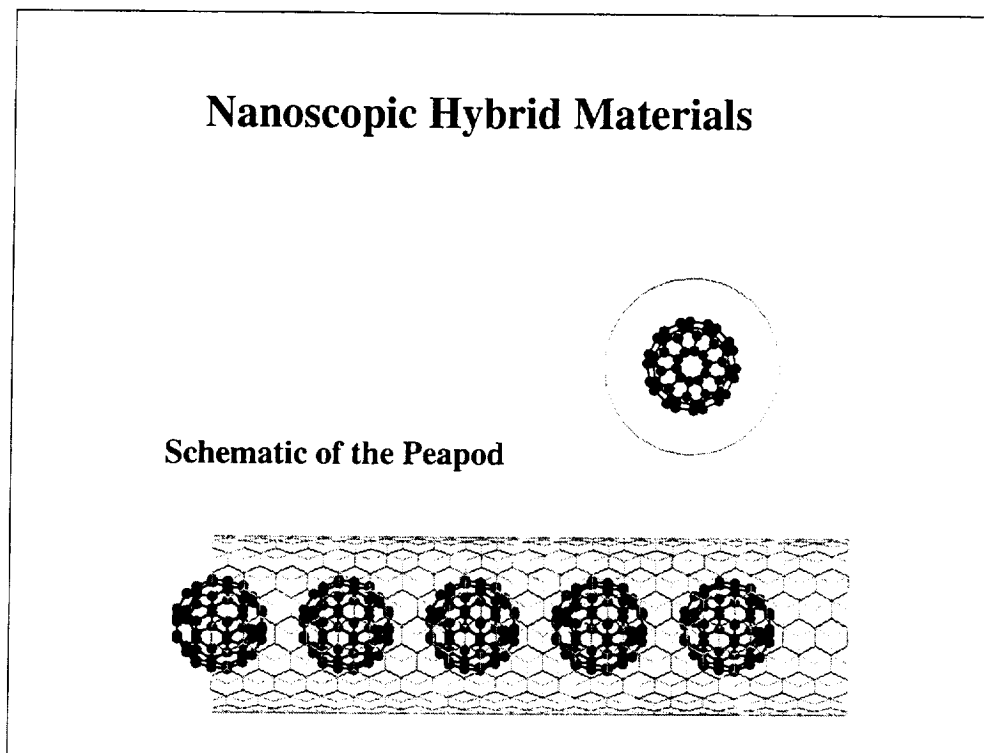
Empty and Filled SWNTs

High magnification TEM micrographs of an empty SWCNT and a SWCNT filled with a linear chain of C_{60} molecules. The scale bar is 2 nm.



Nanoscopic Hybrid Materials

Schematic of the structure of a linear chain of C_{60} molecules within an SWCNT.



Detection of C₆₀ Liberated From Peapods

Early UV-VIS experimental results used to prove that the interior molecules of the peapod were indeed C₆₀. This experiment also provided the first indication that molecules could be extracted from the inside of an SWCNT.

Detection of C₆₀ Liberated From Peapods

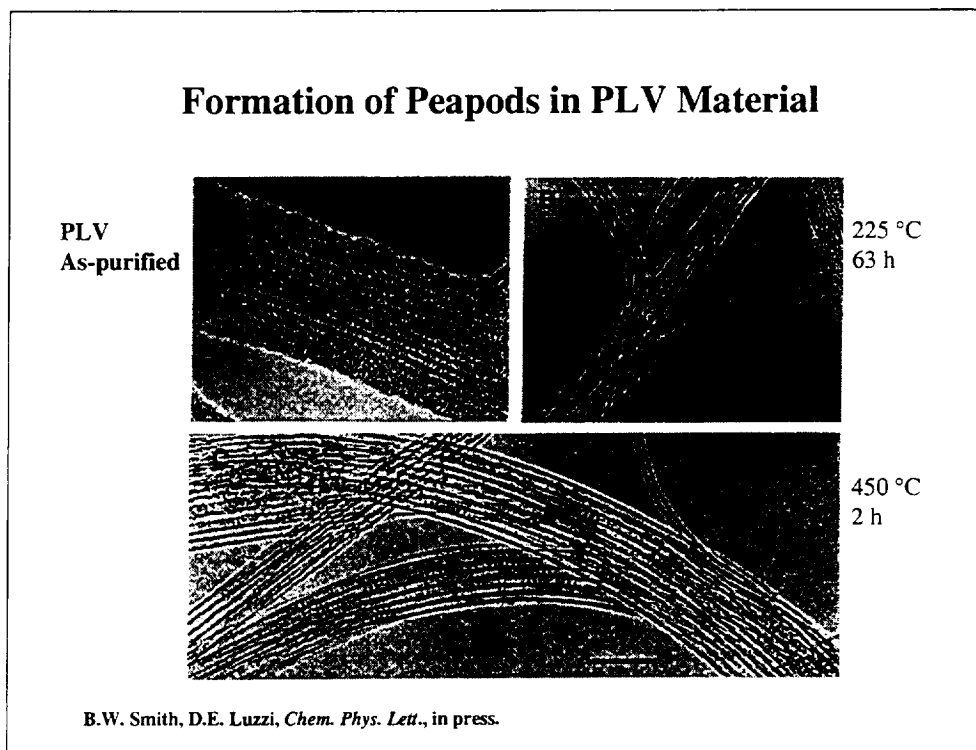
- PLV/Purified/Annealed Material Containing Peapods
- UV-VIS Spectroscopy (Control)
- Strong Acid Etch H₂SO₄ (90%):HNO₃ (70%) (3:1)
– 90 °C, 10 min
- UV-VIS Spectroscopy

Sample	Mass (mg)	C ₆₀ Mass (mg)	C ₆₀ Mass Fraction	Etched Tube Length Fraction
Etch-1	0.857	0.0074	0.0087 ± 0.0001	0.023
Etch-2	1.1	0.0175	0.016 ± 0.003	0.040
Etch-3	1.45	0.0297	0.0205 ± 0.0003	0.054
Control	1	undetected	<0.00008	<0.0004

B. Burtiaux, A. Claye, B.W. Smith, M. Monthieux, D.E. Luzzi, J.E. Fischer, *Chem. Phys. Lett.*, 310 (1999) 21.

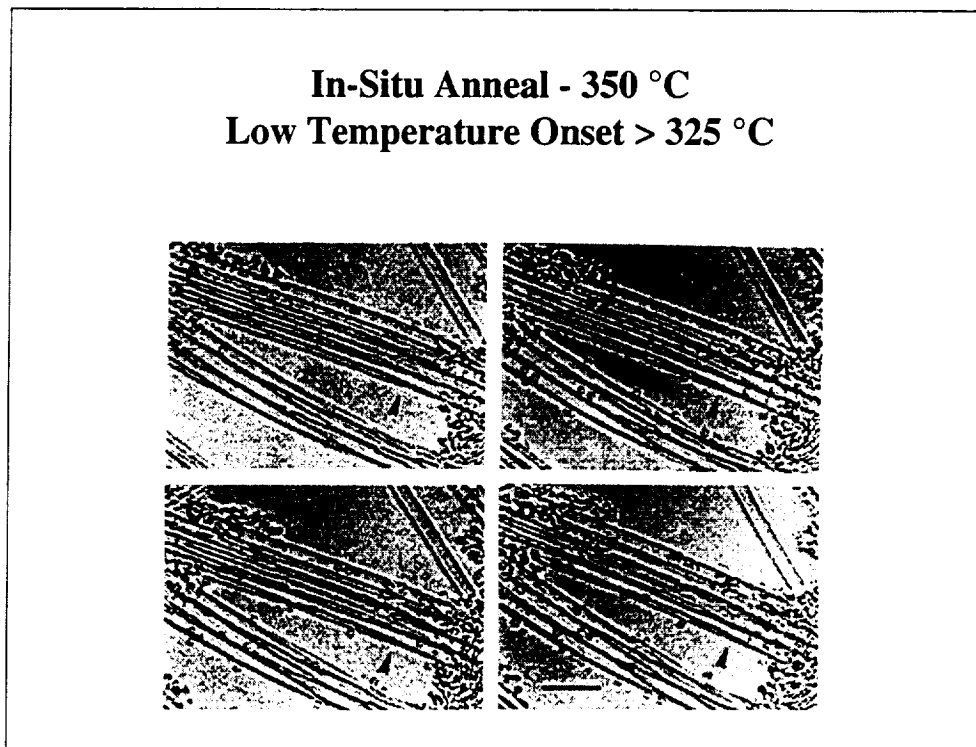
Formulation of Peapods in PLV Material

Upper left – as-received PLV material that has been acid purified and is coated with surfactant. Upper right – the same material (not same location) after removal of the surfactant; the acid-damaged nanotubes can be seen (as shown earlier).



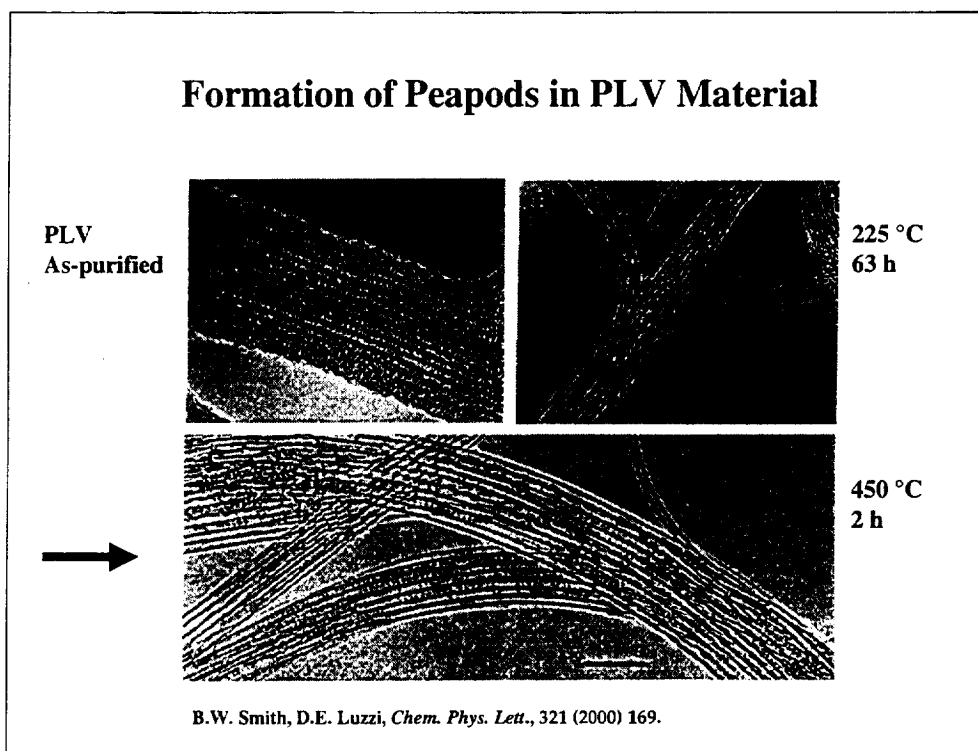
In-Situ Anneal - 350 °C
Low Temperature Onset > 325 °C

At temperatures above 325 °C in high vacuum, residual C₆₀ within the sample becomes mobile and comes into contact with nanotube exterior walls.



Formation of Peapods in PLV Material

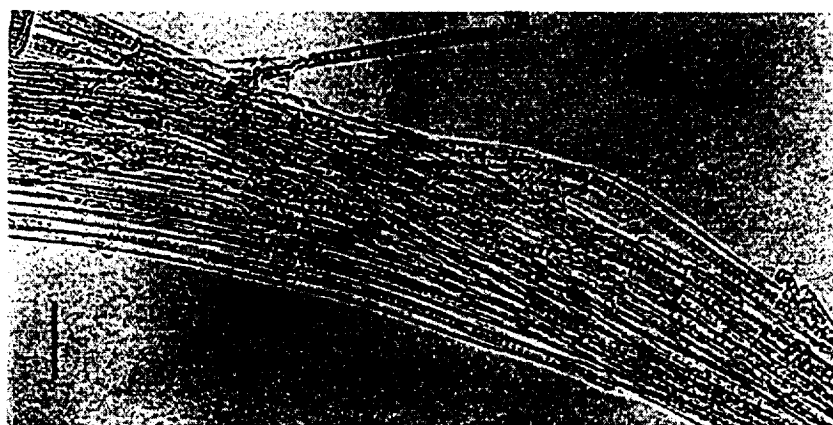
Bottom figure – C₆₀ then enters the nanotubes forming 1-D chains.



CA Material (Peapod Specimen) - 400 °C, 1 h

Filling is possible at high efficiency and in nanotubes produced by different methods. This SWCNT material was produced using the CA method. C₆₀ was added to the material from a solution.

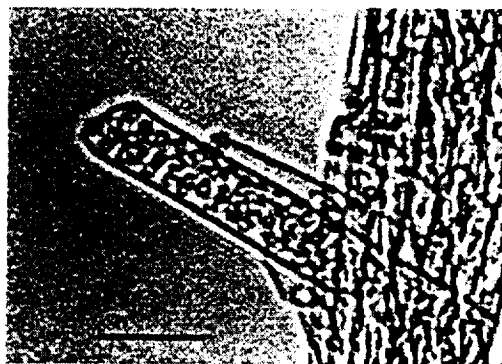
CA Material (Peapod Specimen) - 400 °C, 1 h



**Disordered C₆₀ Filling a 2.7 nm Nanotube
CA Material - 400 °C, 1 hour**

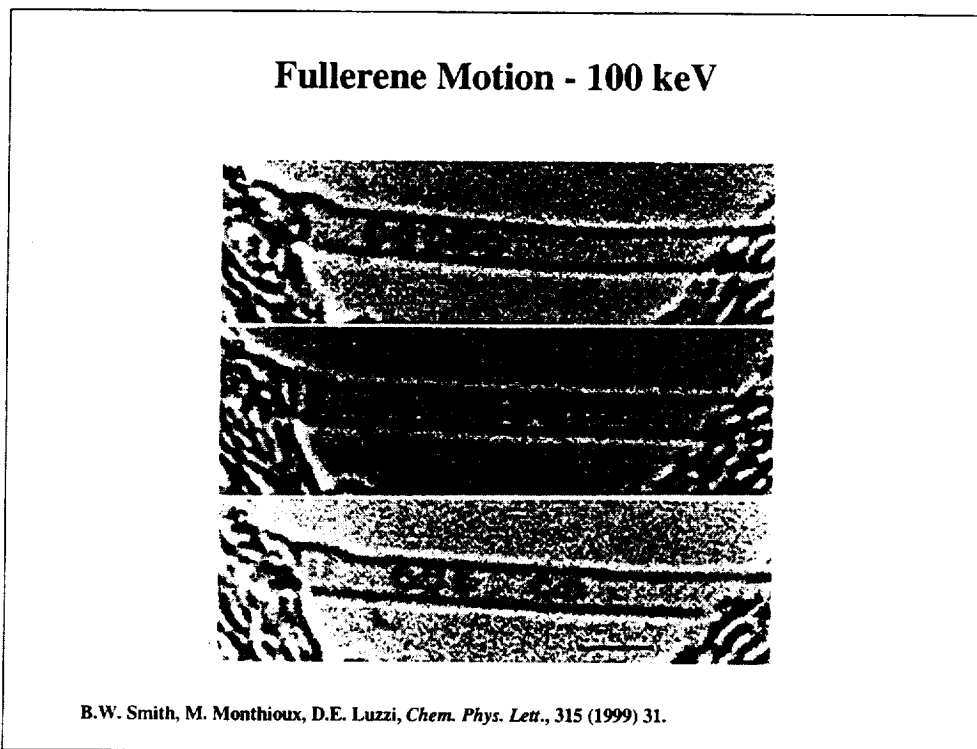
Image of a disordered cluster of C₆₀ filling a large diameter SWCNT. Scale bar is 5 nm. This provides important evidence that nanotubes can be filled with molecules, even when the size of the molecules does not match the diameter of the nanotube lumen.

**Disordered C₆₀ Filling a 2.7 nm Nanotube
CA Material - 400 °C, 1 hour**



Fullerene Motion - 100 keV

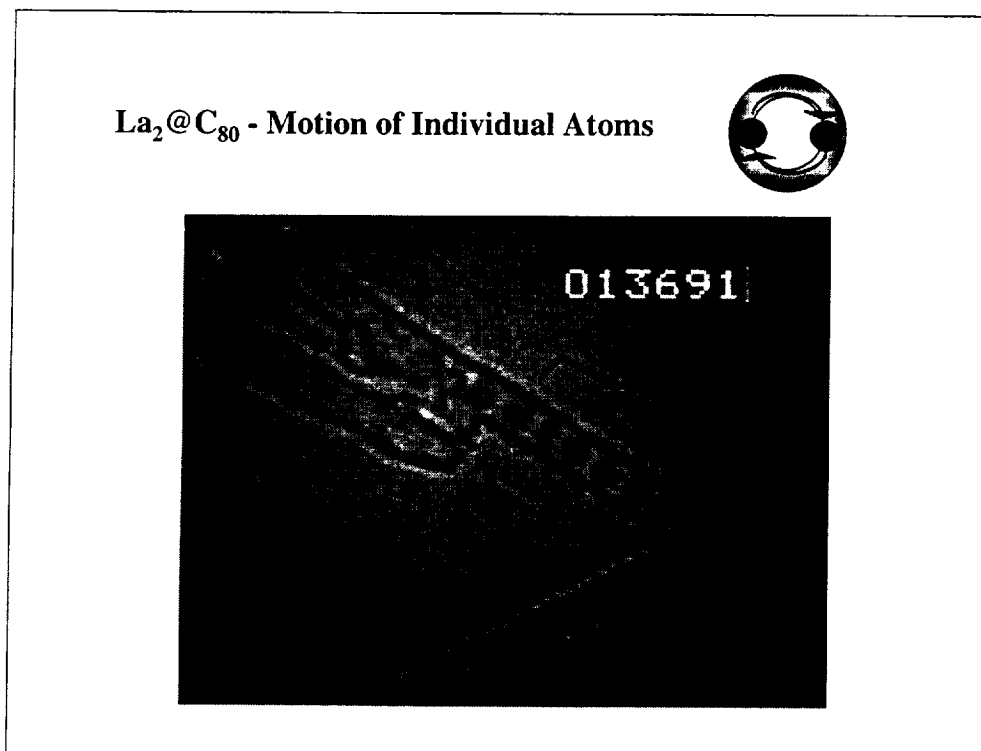
C_{60} 's can be induced to move within the SWCNT through interactions with the electron beam. This is a time sequence of the same cluster of five molecules with approximately 20s between images. Controlled mass transport along the lumen of nanotubes opens the possibility for a number of enabling nanotechnology applications.



La₂@C₈₀ - Motion of Individual Atoms

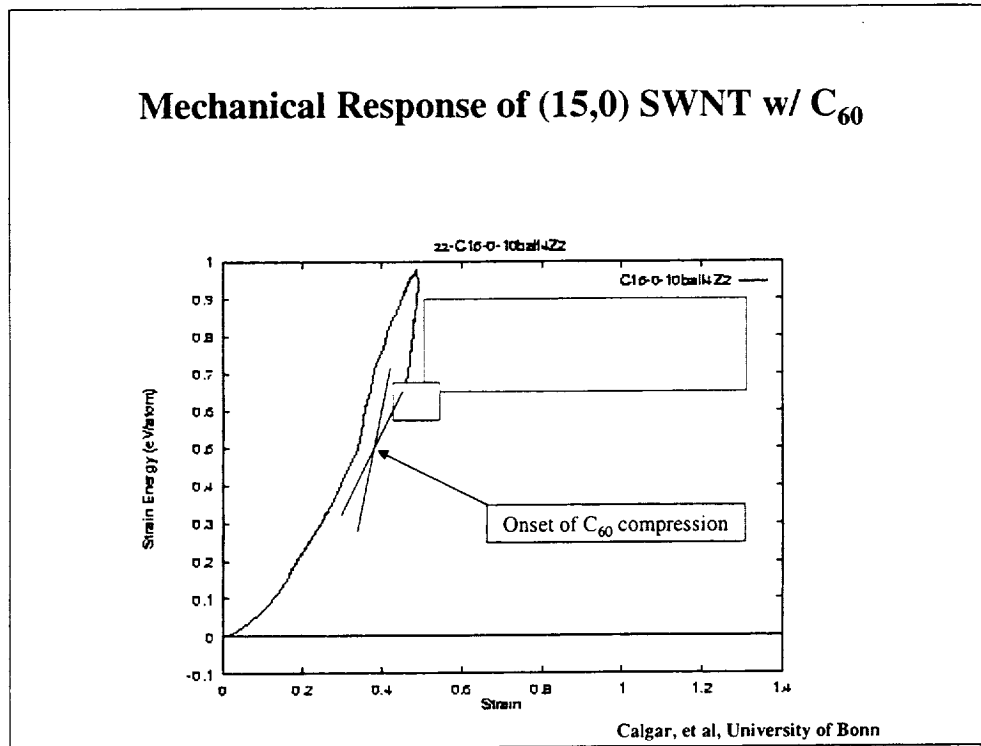
A TEM image of a 1-D chain of endohedral metallofullerene La₂@C₈₀ molecules within a 1.4 nm diameter SWCNT. This is a single frame of an in-situ video, so shot noise is present. However, the two La atoms can be seen as dark spots within the circles which are the C₈₀ cage.

Go to slide show view, move your mouse cursor over the image until a picture of a pointing finger appears and click. The video will show the tumbling motion of the two La atoms within the C₈₀ cages. These images were recorded at temperatures near room temperature.



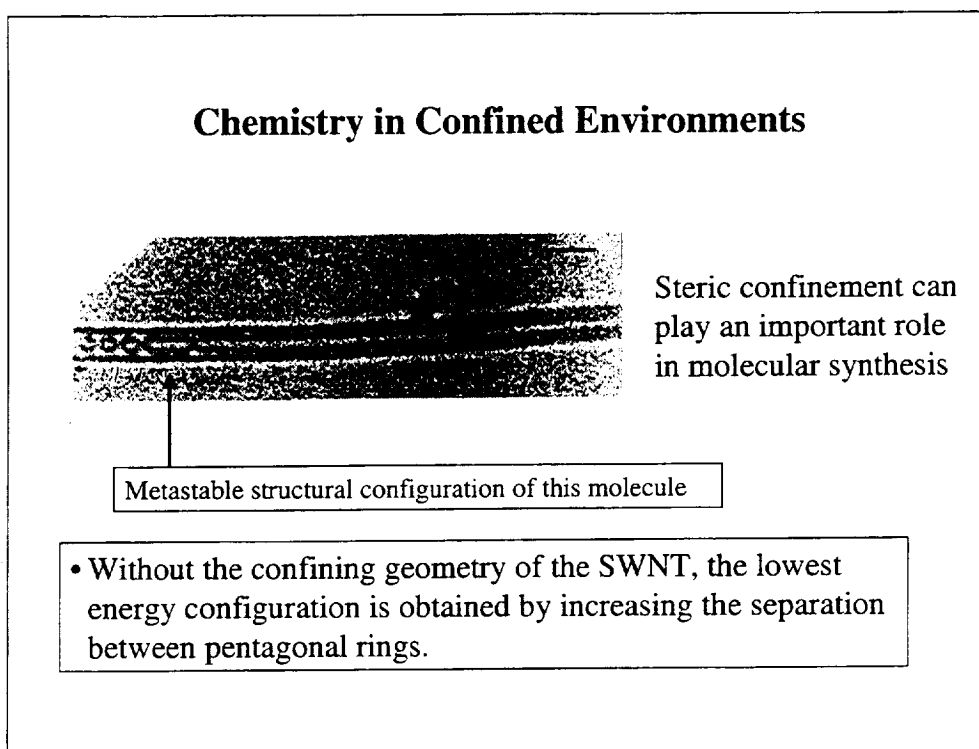
Mechanical Response of (15,0) SWNT w/ C_{60}

When a nanotube is deformed in tension, the extension of the nanotube induces a Poisson contraction that reduces its diameter. If the interior of the nanotube is filled with molecules such as C_{60} , the molecules will resist this compression and therefore increase the stiffness of the nanotube. This is seen in this atomistic simulation that shows a slope change in the strain energy versus tensile strain curve at the point at which the interior C_{60} 's begin to undergo compressive deformation. Thus, it is expected that the hybrid nanotubes containing C_{60} will be stiffer than the nanotube alone, which is already the stiffest material known.



Chemistry in Confined Environments

When the hybrid nanotube containing C_{60} is heated to high temperatures, the C_{60} molecules coalesce into interior cylindrical capsules and tubes. These capsules are mobile within the nanotube indicating that no reaction occurs between the nanotube and the interior molecules. Thus, the nanotube provides two functions: it catalyzes the reaction by confining the reactants in close proximity and, controls the structure of the reaction product through steric confinement. A clear example is the indicated capsule of C_{180} . The equilibrium structure of this molecule is more spherical. Within the nanotube, it is restricted to form this cylindrical form, which is a metastable configuration.



Nanometer-sized Furnace Tubes

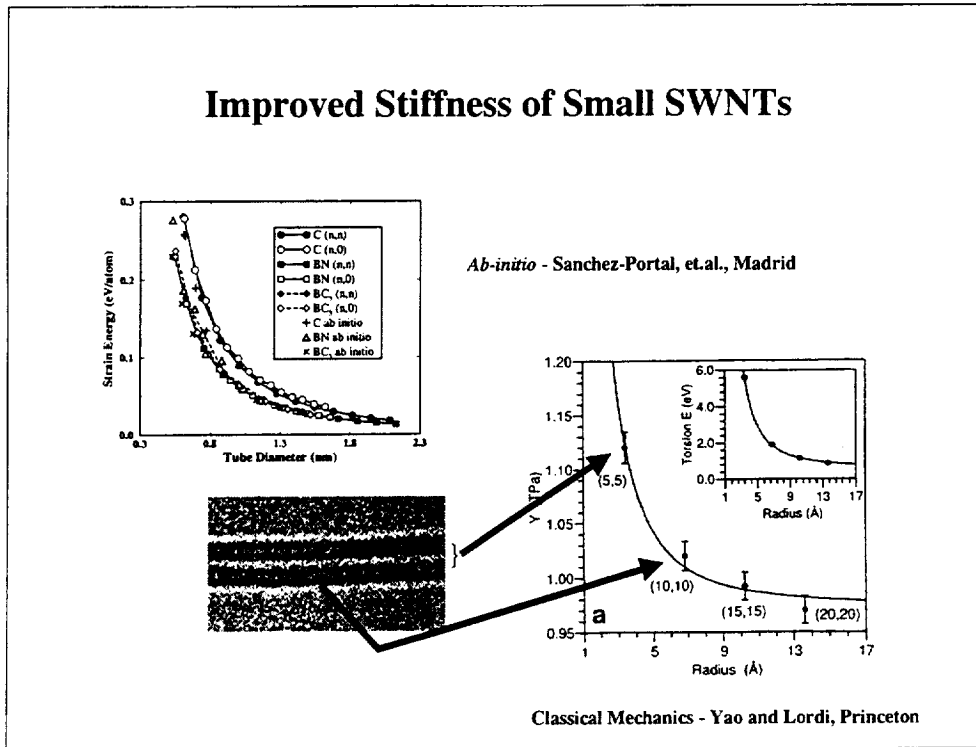
In order to carry out useful chemistry in nanometer-sized reaction vessels, one must be able to carry out three tasks listed below in yellow. In the present work, each of these concepts has been developed. It remains to be tested whether nanotube-based synthesis can be used on a bulk scale.

Nanometer-sized Furnace Tubes

- **Charge the Reaction Chamber**
 - Synthesis of hybrids
- **Carry out the Reaction**
 - Formation of metastable C_{180}
- **Recover the Product**
 - Extraction of C_{60} from nanotubes

Improved Stiffness of Small SWNT's

Both ab-initio and statics calculations have shown that the stiffness of nanotubes in bending will increase with decreasing diameter. Thus, the production of small tubes within the larger nanotubes from the C_{60} -nanotube hybrid should yield a stiffer nanotube, but without significant changes to other nanotube properties, such as the chemical reactivity.



Using SWNTs for the Study of Single Molecules

The work has also demonstrated the efficacy of nanotubes as substrates for the study of individual molecules. It has been extraordinarily difficult to study single molecules due to the problems posed by background signals from substrates. Nanotubes provide a stable, radiation damage resistant (at low voltages), extremely high observation area substrate.

Using SWNTs for the Study of Single Molecules



7 Angstroms!

Any molecule that will enter a SWNT or bind/physisorb to the exterior of a nanotube can be studied by imaging, diffraction or spectroscopy

We are imaging stable single molecules at close to atomic resolution without effort!

Acknowledgments

Smith and Monthioux at Penn (MM permanent address: CEMES, Toulouse, France)

Nanotube materials (pre-filling) graciously provided by Rice, Montpellier and CNRS Strasbourg.

Funding from NSF and ONR.



Brian W. Smith
Marc Monthioux



Rice - Rick Smalley, Dan Colbert, et al.
Montpellier - Patrick Bernier, et al.
CNRS Strasbourg - Pierre Petit

National Science Foundation
Office of Naval Research

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Nanotube Mechanics

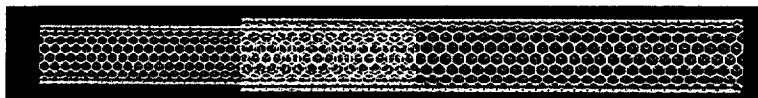
Rodney S. Ruoff
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Nanotube Mechanics

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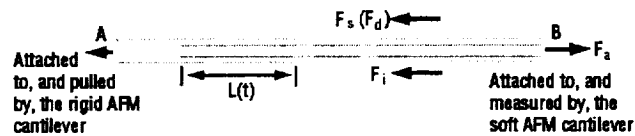
Shear Strength and Nanotribology



- Ⓐ MWCNT is a perfect object for the study of friction in nanoscale.
- Ⓐ MWCNT consists of nested cylinders of single wall carbon nanotubes that can be conceptual as cylinders rolled from graphene sheet. The layer-layer separation is about 0.34 nm and the layer-layer interaction is due to van der Waals forces.
- Ⓐ Nested tubes in MWCNT can have same or different helicity.



Sliding Between Nested Shells

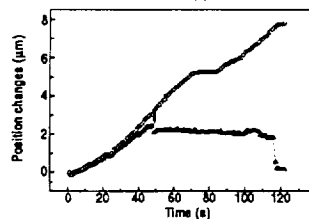
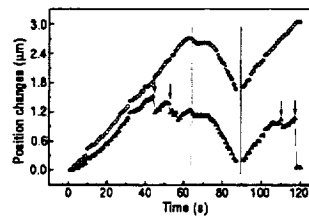


- ⊞ Shear force $F_s = \tau A$, A is the contact area = $\pi dL(t)$.
- ⊞ Interface force F_i : 1. Capillary force; 2. Edge effect force. It only depends on the perimeter length of the nanotube cylinder.
- ⊞ So $F_a = \pi d \tau L(t) + F_i$. From the F_a versus $L(t)$ dependence, τ can be obtained.



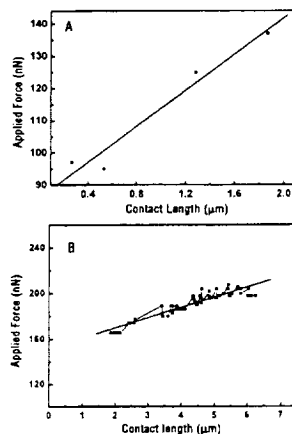
Stick-Slip and Smooth Pullout

- ⊞ The position change at each end of the MWCNT is recorded.
- ⊞ Stick slip sliding: static friction > dynamic friction.
Smooth sliding: static friction = dynamic friction (normally both are small).



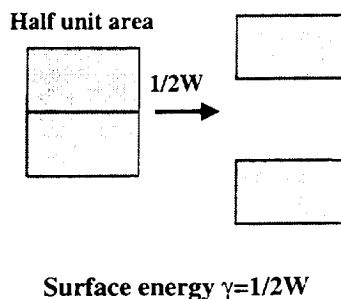
Shear Strength and Interface Interactions

- 🔔 In stick-slip sliding: static shear strength ~ 0.3 MPa.
- 🔔 In smooth pullout: static shear strength ~ 0.08 MPa.
- 🔔 Possible explanation: sliding between commensurate or incommensurate surfaces. The overall surface/surface interactions depend on the arrangement of atoms on surfaces. Another evidence for the existence of super-lubricity.



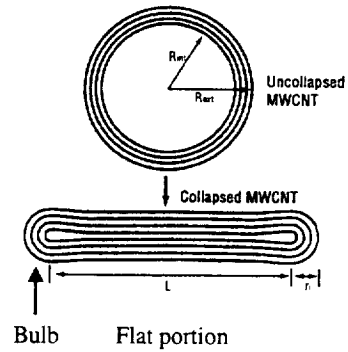
Surface Energy of MWCNT

- 🔔 $F_i = 2\pi\gamma d$ can be obtained from the intersection of the linear fit with the F axis.
- 🔔 The upper limit values of γ obtained from two cases are 0.45Jm^{-2} and 0.67Jm^{-2} . The γ value has contributions from both surface energy and edge effect.
- 🔔 For comparison, $\gamma_g = 0.11\text{Jm}^{-2}$



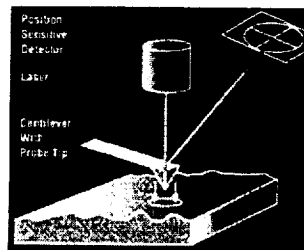
Radial Deformability of Carbon Nanotube

- Nanoscale objects are excellent candidates for revealing nanoscale interactions.
- The collapse of carbon nanotube relates to: strain energy
van der Waals interactions.



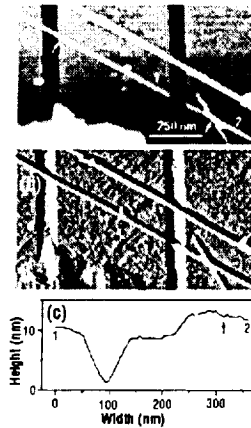
Atomic Force Microscopy

- Invented in 1986 with the help of good vibration isolation, piezo-materials and electronics.
- Sensitive to the atomic interactions (pN to μ N) between the force sensing probe tip and the studied surface.
- Lateral resolution up to 0.1nm and vertical resolution up to 0.01nm.



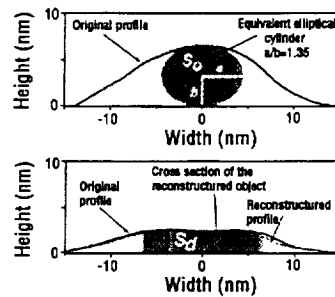
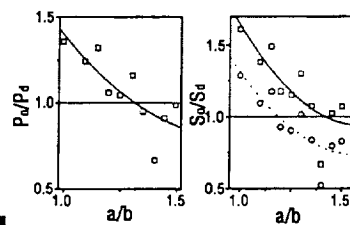
Collapsed Carbon Nanotube

- The collapsed nanotube is significantly more flexible than the uncollapsed nanotube; it drops ~ 8nm into the trench.
- Collapse initiates at the bend and terminates before crossing the trench.
- The height of the collapsed nanotube is ~ 2.3nm; the uncollapsed nanotube is ~ 6.5nm.



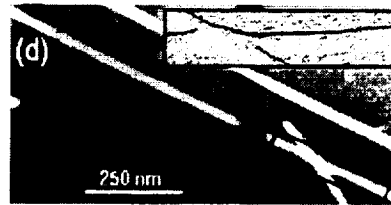
Structural Analysis

- Erosion and dilation is used to get the true shape of the MWCNT.
- Perimeter fitting and area fitting indicate that the nanotube is a MWCNT having three cylinders.



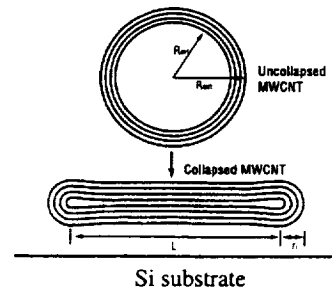
Metastability of Carbon Nanotube

- Metastability is the nature of some cylindrical carbon nanotubes having certain types of structures: certain diameters, certain number of walls.



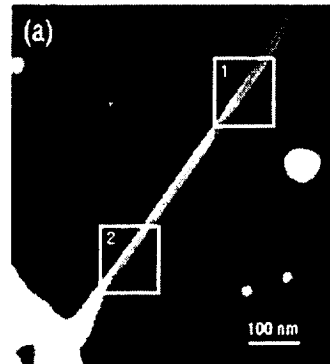
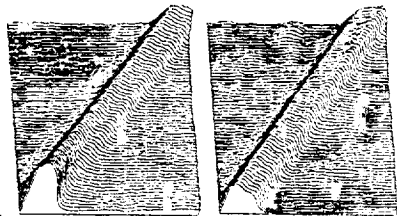
What Can It Tell Us

- The energetic:
 - Strain energy increase $\Delta E_s = E_b - E_{nt}$
 - Surface energy decrease $\Delta E_v = E_{nv} + E_{snv}$
 - where $E_b = \pi k / r$, $E_{nt} = \pi k / R$, $E_{nv} = -2\gamma L$, $E_{snv} = -W_{sn}L$
- If $\Delta E_s + \Delta E_v < 0$, collapse is favored.
- $\Delta E_s = 36 \text{ eV/nm}$, $\Delta E_v = -12 \text{ eV/nm} - W_{sn}L$
- We need $W_{sn} > 2.8 \text{ eV/nm}^2$ (or 440 mJ/m^2)
- $W_{sn} = 2(\gamma_{si} \gamma_c)^{1/2} = 785 \text{ mJ/m}^2$



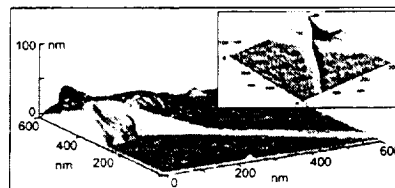
Twisted and Collapsed Nanotube

- ⌚ Rarely observed.
- ⌚ More information can be obtained from the twisted nanotube. Good for theoretical simulation.



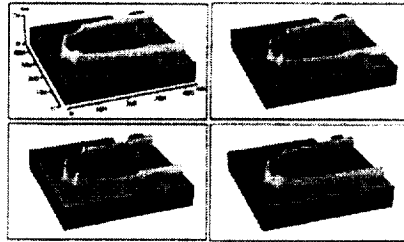
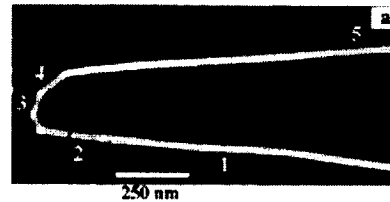
Anisotropic Mechanical Properties

- ⌚ Anisotropic mechanical property is also present in collapsed nanotube depending on its orientation.
- ⌚ Two factors: the different moment of inertia ($\propto wd^3$) and the different elastic constant.



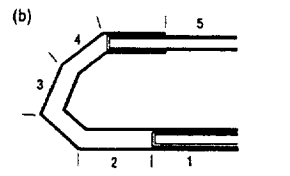
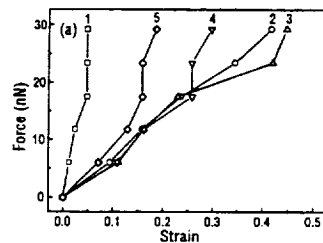
Dynamic Study of the Deformability

- Dynamic compressing of individual MWCNT is performed and recorded.
- It reveals different rigidities along the MWCNT.



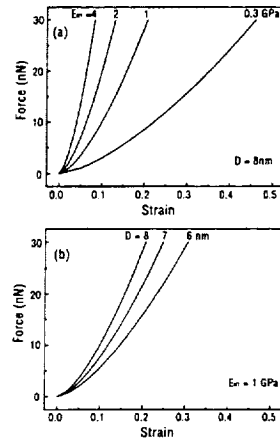
Structural Information

- The applied force by AFM tip is calibrated in a separate experiment and in a simulation.
- The obtained force-strain curve indicates that MWCNT is relatively soft in its radial direction and sensitive to the structure.



Mechanical Property in the Radial Direction

- ⌚ A simplified model is used to estimate how MWCNT can be compared to other solid materials.
- ⌚ MWCNT is considered as a elastic cylindrical rod and AFM tip as a sphere. Hertz model is applied to solve the contact problem.
- ⌚ MWCNT is comparable to an elastic rod having Young's modulus around several GPa; for example, rubber, polymer.



Conclusions

- ⌚ New tools and methods are developed for studying carbon nanotubes.
- ⌚ First measured the tensile strength: $\sim 30 \text{ GPa}$.
- ⌚ Young's modulus $\sim 1000 \text{ GPa}$.
- ⌚ First measured the shear strength: around 0.3 MPa or 0.08 MPa depending on the degree of commensurance between neighboring shells.
- ⌚ In the radial direction, carbon nanotube is deformable having an effective Young's modulus value of about several GPa.
- ⌚ The stability of a carbon nanotube depends on its structure.
- ⌚ Nanoscale interactions can have significant effects on the behavior of carbon nanotubes (e.g., capillary force, substrate effect, edge effect).



Further References:

- M.-F. Yu et al. *Nanotechnology* 10, 244 (1999)
- M.-F. Yu et al. *Science* 287, 637 (2000)
- M.-F. Yu, B. S. Files, S. Arepalli, R. S. Ruoff *Phys. Rev. Lett.*, June (2000)
- M.-F. Yu, B. I. Yakobson, R. S. Ruoff *Nature*, Submitted.
- M.-F. Yu, T. Kowalewski, R. S. Ruoff *Phys. Rev. Lett.*, Submitted.
- M.-F. Yu, T. Kowalewski, R. S. Ruoff *Phys. Rev. Lett.*, Submitted.



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30P

A Virtual Presence Interface for a Scanning Probe Microscope

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A Virtual Presence Interface for a Scanning Probe Microscope

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NanoManipulator™ System

A Virtual-Environment Interface to a ThermoMicroscopes™ SPM

Aron Helser
NanoManipulator Project Leader
3rdTech, Inc.



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Agenda



Agenda

- About 3rdTech
- NanoManipulator System Overview
 - Components
 - Features/Functions
- What Science has the NanoManipulator Enabled?
 - Adenovirus
 - Carbon Nanotubes
 - DNA
 - Fibrin

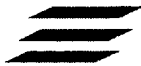
 **3rdTech™**

About 3rdTech

3rdTech is a foundry for new companies. Located in Chapel Hill, NC, directly across the street from the University of North Carolina, 3rdTech is working to turn the most advanced technologies into leading edge products.

The Computer Science Dept. at UNC-CH has one of the world's best computer graphics and virtual environments research efforts. The department also enjoys a world-class reputation in medical image analysis, networking, and hardware systems design, and has significant strengths in other areas. And there are many other technology development groups within the University with similar reputations and potential.

3rdTech is driven by the opportunities to build new businesses around these world-class technologies and this exceptional talent pool. We are leveraging these resources by creating a channel and a culture to enable the rapid development of new products and new businesses.



About 3rdTech

- New Kind of High-Tech Incubator
 - Working with researchers at UNC-CH
 - Creating a channel to bring advanced technology from the university to the marketplace
 - Productize technology; develop sales/distribution channels
 - Enable spin-off of independent companies

 **3rdTech™**

Ideal Microscopy: Virtual Environment Interface to SPM

In Scanning Probe Microscopy, we are working with objects a million times smaller than everyday objects. How can we make it intuitive and easy to manipulate them? With the NanoManipulator system, an environment with the computer is created where it seems like the viruses and molecules are sitting on the table in front of you, and you can see, feel and move them.



Ideal Microscopy: Intuitive Merging of User and Sample

A virtual environment interface to SPM

The Goal:

- Remove boundaries between user and sample
- Can we make experiments on the molecular scale as easy as rolling a pencil or pushing a golf ball?



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NanoManipulator System

The Computer Science Dept. has been working to build tools to help the Physics Dept. do SPM microscopy for about seven years. 3rdTech has worked with the researchers in both departments to develop a commercial version of these tools – the NanoManipulator System. The components of the NanoManipulator make manipulations and experiments easier, more intuitive and more efficient.

Three-dimensional display of the sample during the experiment enables new interpretation of the shape of the sample.

Force feedback gives you information about the sample location and surface features during a manipulation.

Automatic recording of the entire experiment session enables new discoveries and analysis on recorded data.



What is the NanoManipulator System?

- Real-time Control for ThermoMicroscopes SPMs
 - Integrated software and hardware
- Virtual-Environment Interface
 - See, feel, manipulate your sample
- 3D Graphics
 - Improved visualization during the experiment
- Force Feedback to Guide Manipulations
 - Real-time position information
- Virtual Tips
 - Oscillating/contact switch
- Automatic Lab Notebook
 - Store/replay/re-analyze data

 **3rdTech™**

NanoManipulator System Components: SPM

We provide an interface to these ThermoMicroscopes SPMs. The Explorer is pictured. The NanoManipulator communicates to the SPM control software through a standard network connection.



NanoManipulator System Components

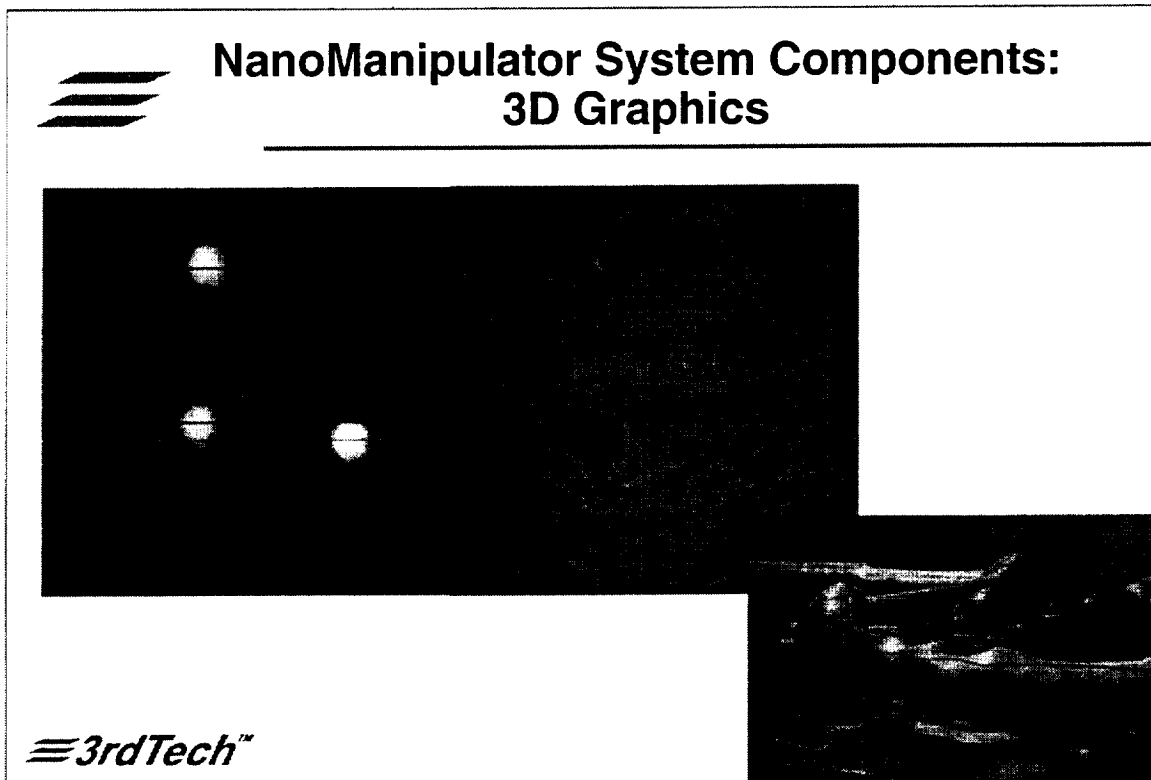
- A ThermoMicroscopes™ SPM
 - Explorer™
 - Discoverer™
 - Lumina™
 - Observer™



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NanoManipulator System Components: 3D Graphics

A key component of the NanoManipulator is real-time display of the sample surface with 3D graphics. Here is a side-by-side comparison of two views of adenovirus. One of the adenoviruses is leaking DNA on the surface, and you can see how the highlights from the light on the right is picking out the DNA on the surface. It is also showing some subtle shape changes on the tops of the adenoviruses which are lost on the left. The user has interactive control of the view and lighting, which means one can zoom and rotate in any direction, getting views like this during the experiment.



NanoManipulator System Components: Force Feedback

The Phantom Desktop from SensAble Technologies is the other key component. It is a 6D input tool, which makes it easy to interact with the 3D environment of the NanoManipulator. It also is a 3D force-feedback tool enabling one to “feel” the sample surface. This provides additional data about the surface topography of the sample.

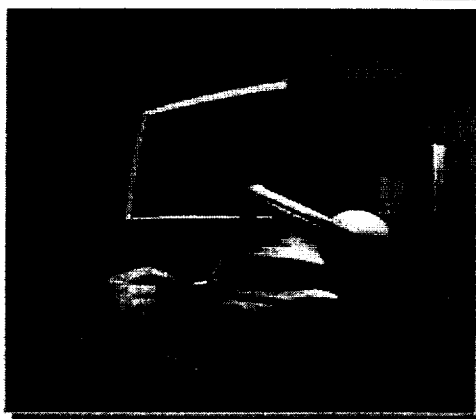
It is also particularly valuable during a sample modification because it lets you feel the shape of your sample as you guide the SPM tip while it is modifying your sample. Hysteresis and drift have no effect on the tactile feedback – you can find exactly the right spot to modify, and feel what is happening during a modification. This is unlike the visual feedback which is not current and accurate during a modification.

This results in the ability to do modifications which would otherwise not be possible – or would be extremely difficult.



NanoManipulator System Components

- Haptic/force feedback output
 - A SensAble Technologies PHANTOM™ Desktop
 - Continuous, real-time location identification
 - Find the right spot to modify; feel it during manipulation



“It was really a remarkable feeling for a chemist to be running his hand over atoms on a surface,” R. Stanley Williams, UCLA Chemistry

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NanoManipulator System: Virtual Tips


The NanoManipulator software has been developed over the years to enable a number of different techniques for sample modification.

The simplest is to move the Phantom over the surface, and have the SPM tip follow, pushing down into the sample as it goes.

A second simulates a "Virtual Tip" shape. For example, to clear out an area of photo-resist, to etch and separate electrical contacts, as pictured here, SPM tip can simulate a broom or scraper by moving side-to-side as you move forward.

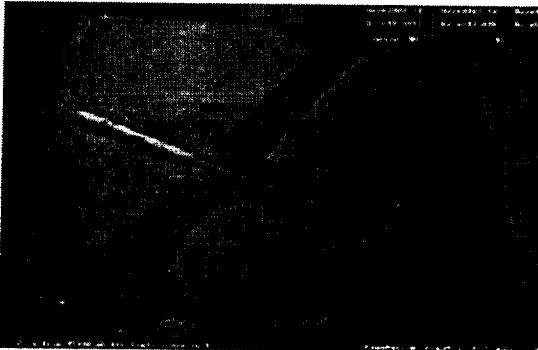
In addition, one can specify movements across the surface to move freely, to be constrained to a line, or to automatically have the SPM tip follow a pre-planned path.

Finally, the NanoManipulator provides an automatic switch-over from oscillating imaging mode to contact mode, so one can scan and feel the sample with the light touch of oscillating mode, but modify and measure lateral forces using contact mode.

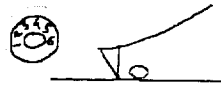


NanoManipulator: Virtual Tips

- Whisk broom
- Freehand, constrained or automatic
- Oscillating/contact

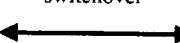


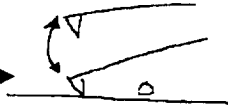
Touching, Modifying: need to switch quickly between imaging mode and manipulation mode



Contact-quantitative manipulation

transparent
switchover





Oscillating-imaging

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NanoManipulator System: Store/Replay

A vital feature of the NanoManipulator is the “automatic lab notebook,” which records a complete record of all the data obtained during an experiment. This file can be replayed and reviewed at any later time, at the speed of the original experiment or it can be “fast forwarded” to locate specific data more rapidly. This enables new analysis of data that might not have been understood while the experiment was taking place. One clear example of its value was the discovery, days after an experiment was performed, that a nanotube was rolling and not sliding. This had not been noted at the time of the experiment.



NanoManipulator: Store/Replay

“If it’s not in the lab notebook, it didn’t happen.”

- Store data for the entire experiment
- Enables replay from different points of view
- Playback at different speeds
- Perform new analysis on old data
- Results:
 - tube slid on top of another
 - tube rolling, not tip artifact

All the best science seems to happen at 3 AM

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Science Enabled by the NanoManipulator

Let's look at four areas of science that members and collaborators of the NanoManipulator Project at UNC Chapel Hill have investigated.



Science

- What science has been enabled by the NanoManipulator System?
 - Adenovirus
 - Carbon Nano Tubes
 - DNA
 - Fibrin

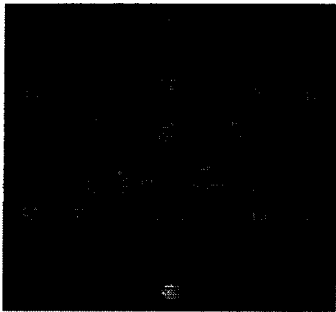
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Application 1: Adenovirus

Adenovirus causes the common cold, and can be used as a vector in gene therapy. Scientists would like to understand how the adenovirus infects a cell in detail. Using the NanoManipulator, scientists have found out more about how they work.



Application 1: Adenovirus



Icosahedral Virus
85 nm diameter

Why are they interesting?

- Responsible for common human illness
- Model virus for understanding basic virology
- Vector for gene therapy

Questions:

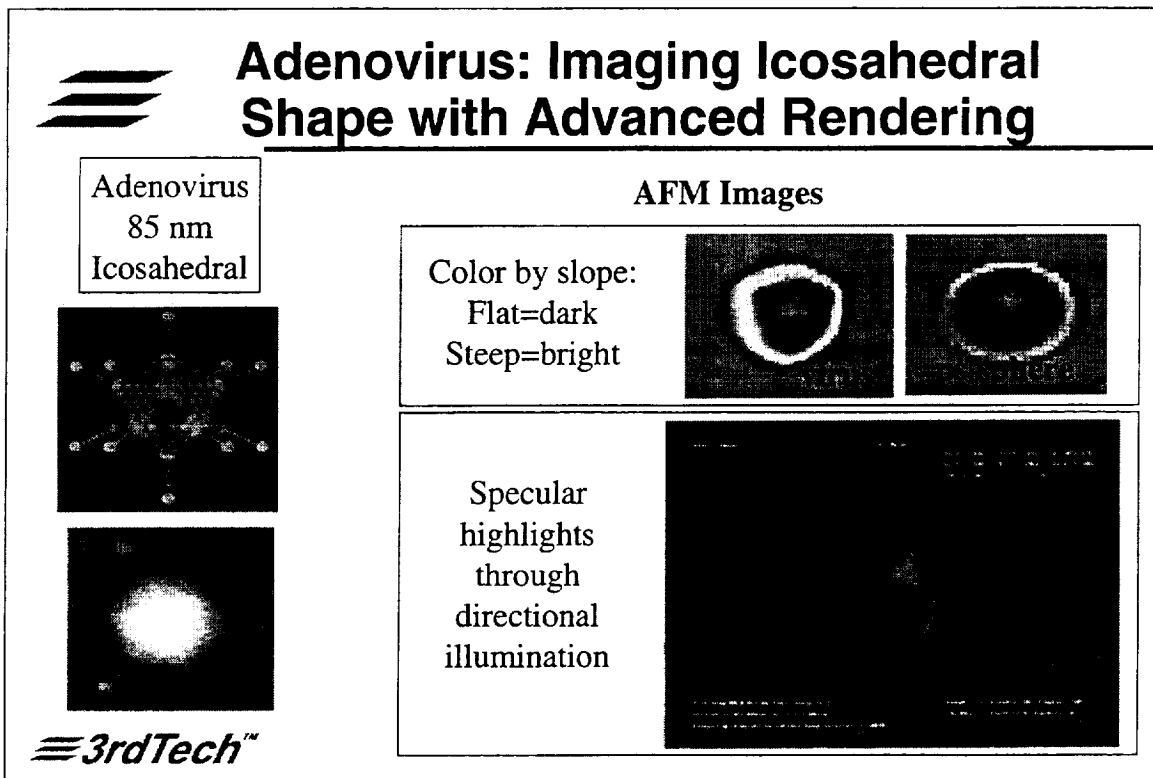
- Can we correlate shape (form) with function?
- How does virus bind to cell?
- How do virus capsid mechanical properties relate to infectivity?

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Application 1: Adenovirus Icosahedral Shape

First, one can confirm the icosahedral structure of the virus from a three-dimensional rendering using a directional light which shows the triangular facets. Above that is a color map based on the slope of the surface. This clearly shows that the adenovirus has facets and that the polystyrene bead does not. Multiple rendering techniques like this enable one to show more than one kind of data on the surface at the same time.

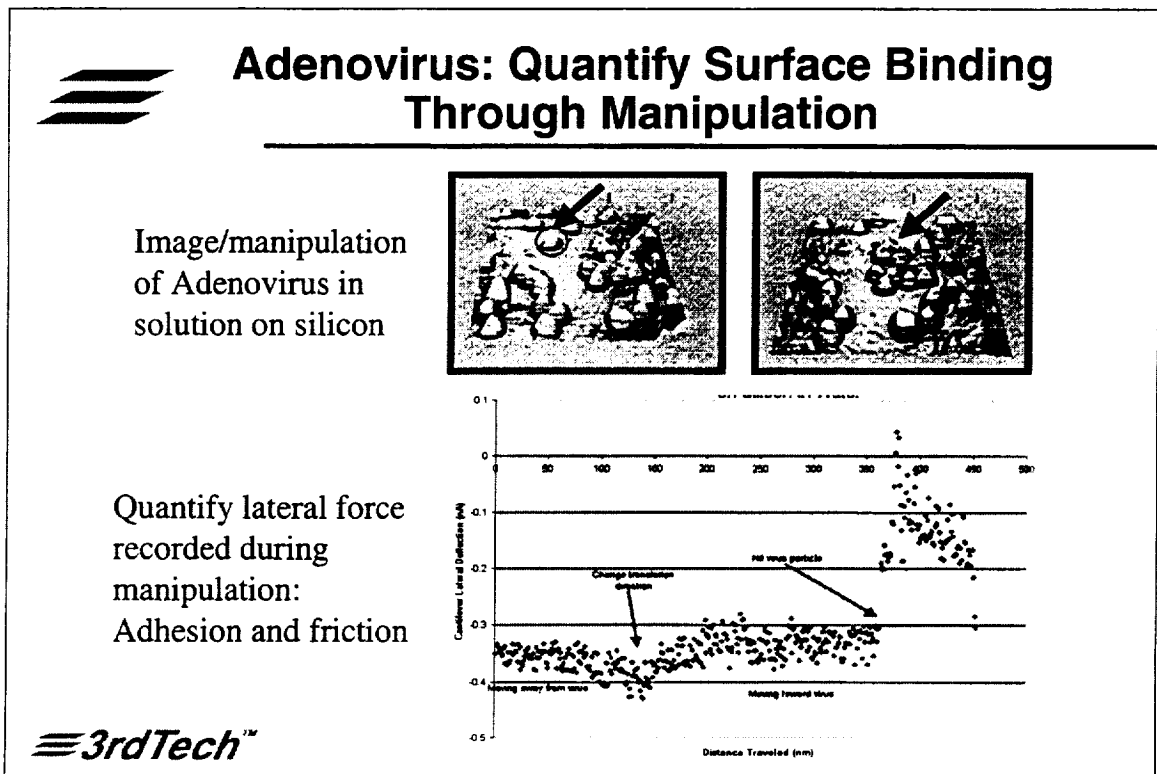
Negishi, A., Matthews, W. G., McCarty, D. M., Samulski, R. J., Rohrer, D., Henderson, A., Taylor, R. M. and Superfine, R., "Three-Dimensional Icosahedral Structure of Adenovirus Using AFM," *Biophys. Journal* (submitted).



Adenovirus Surface Binding

Here we investigated the stickiness of the adenovirus. By doing repeated contact mode manipulations, we can measure the lateral force it takes to slide a virus across the sample surface, which, in this case, is silicon. The graph shows an initial peak in the force which detaches the virus from the surface, and then shows a steady-state sliding force.

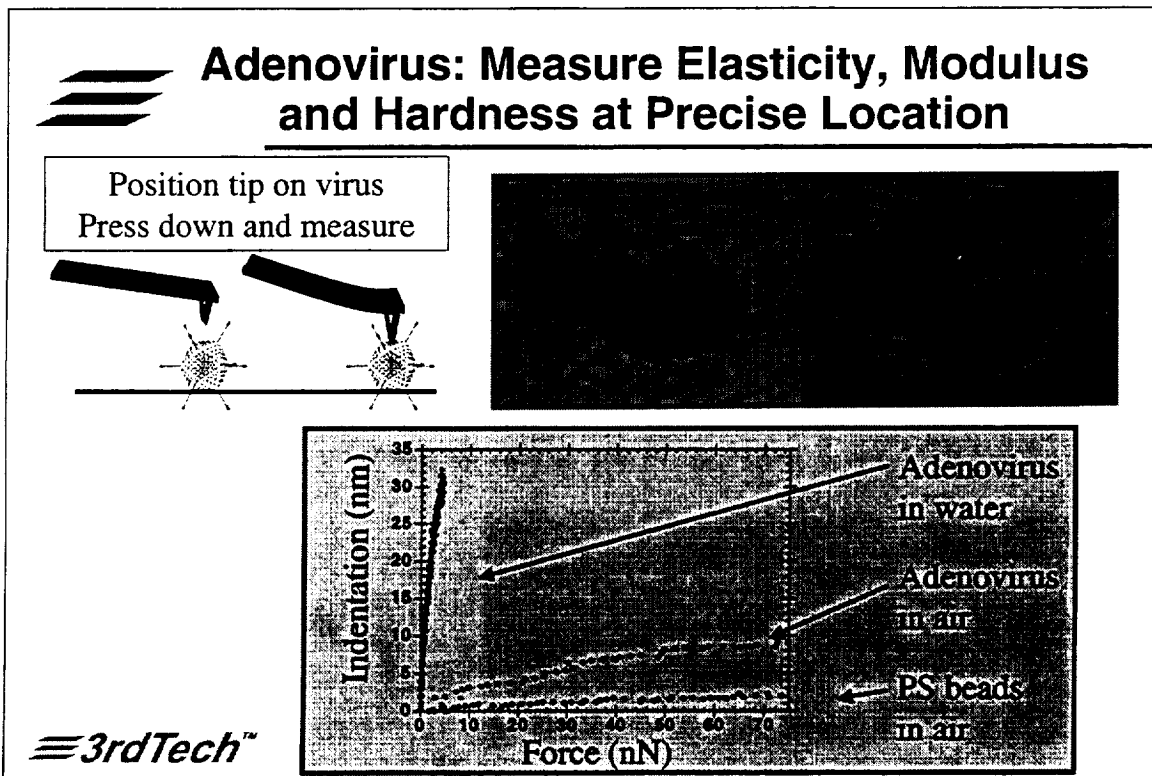
Negishi, A., Matthews, W. G., McCarty, D. M., Samulski, R. J., Rohrer, D., Henderson, A., Taylor, R. and Superfine, R., "Probing the Structural Properties of Adenovirus Using the Atomic Force Microscope," *Biophysical Society 43rd Annual Meeting, Feb. 13-17, 1999, Baltimore, MD, Biophys. Journal*, 1999, Vol. 76, A27.



Adenovirus Elasticity

Scientists have also measured the “squishiness” of adenovirus using the NanoManipulator Interface. Because the scientists could feel their sample with the Phantom, they could position the AFM tip exactly on top of a virus. Then the NanoManipulator made an automatic switch to perform a force-spectrum. The image on the right shows an adenovirus with a dimple in the top from an AFM tip. They did this both in water and in air, and found that adenoviruses are much less rigid in water. The researchers’ pathology collaborators had assumed that adenoviruses were always hard and had to force their way through cell structures. These measurements helped them realize the possibility that the viruses deform to get through those tiny spaces.

Matthews, W. G., Negishi, A., Seeger, A., Taylor, R., McCarty, D. M., Samulski, R. J. and Superfine, R., “Elasticity and Binding of Adenovirus in Air and in Liquid,” *Biophysical Society 43rd Annual Meeting, Feb. 13-17, 1999, Baltimore, MD, Biophys. Journal, Vol. 76, 1999, A265.*



Application 2: Carbon Nanotubes

Another major area of research at UNC-CH is carbon nanotubes.



Application 2: Nanotubes

Size range from .8nm to >50nm diameter

- **Mechanical Properties:**

Stiffest material in nature

- **Electrical Properties:**

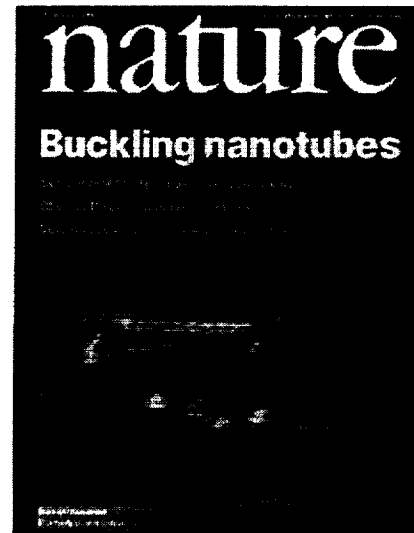
Ideal conductors, semiconductors, metals

- **Friction:** model system for basic science

- **NanoElectroMechanical Systems (NEMS)**

Atomic scale gears

Actuating devices

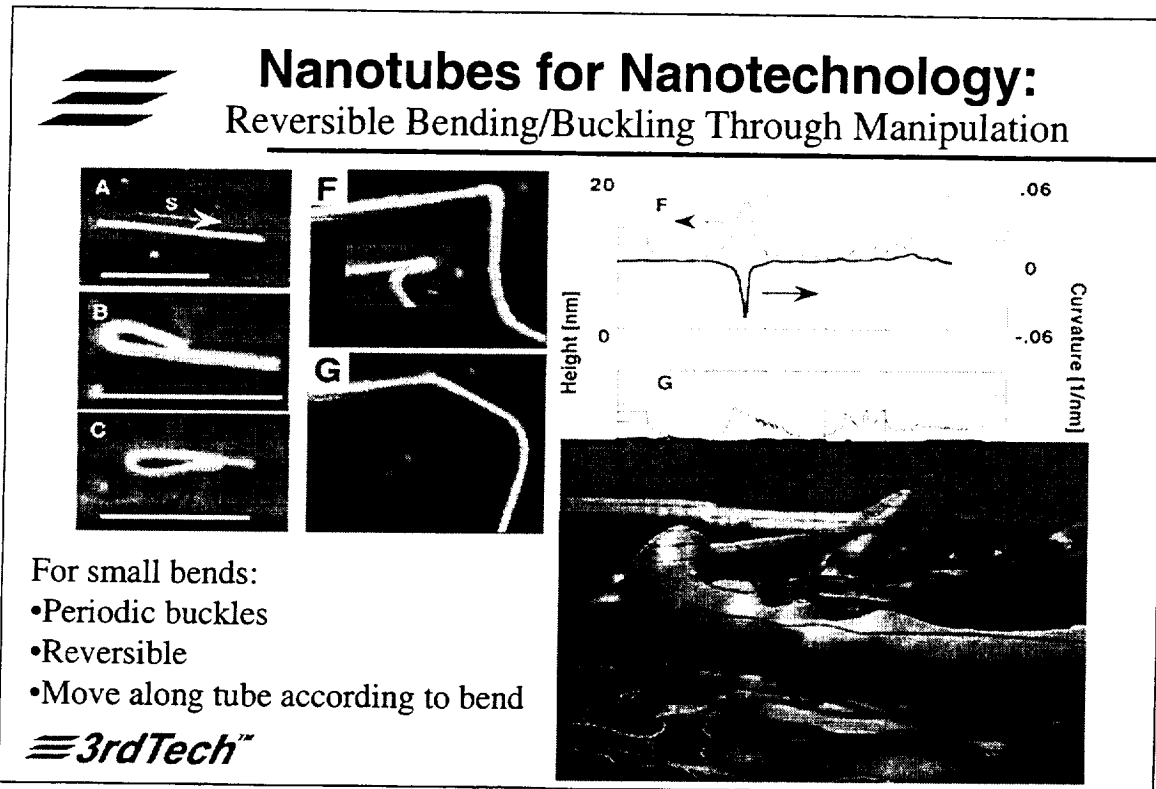


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Nanotubes: Bending and Buckling

Using the NanoManipulator, it is easy to bend nanotubes. Researchers performed many manipulations of multi-wall carbon nanotubes and found that for small bends, the periodic ripples observed matched the behavior of a 1 cm aluminum tube, and of some theoretical simulations of single-wall tubes. They also found that small bends were completely reversible, but large bends or kinks caused a weak point that tended to kink again.

Falvo, M. R., Clary, G. J., Taylor II, R. M., Chi, V., Brooks Jr., F. P., Washburn, S. and Superfine, R., "Bending and Buckling of Carbon Nanotubes Under Large Strain," *Nature*, Vol. 389, No. 6651, Oct. 1997, pp. 582-584.

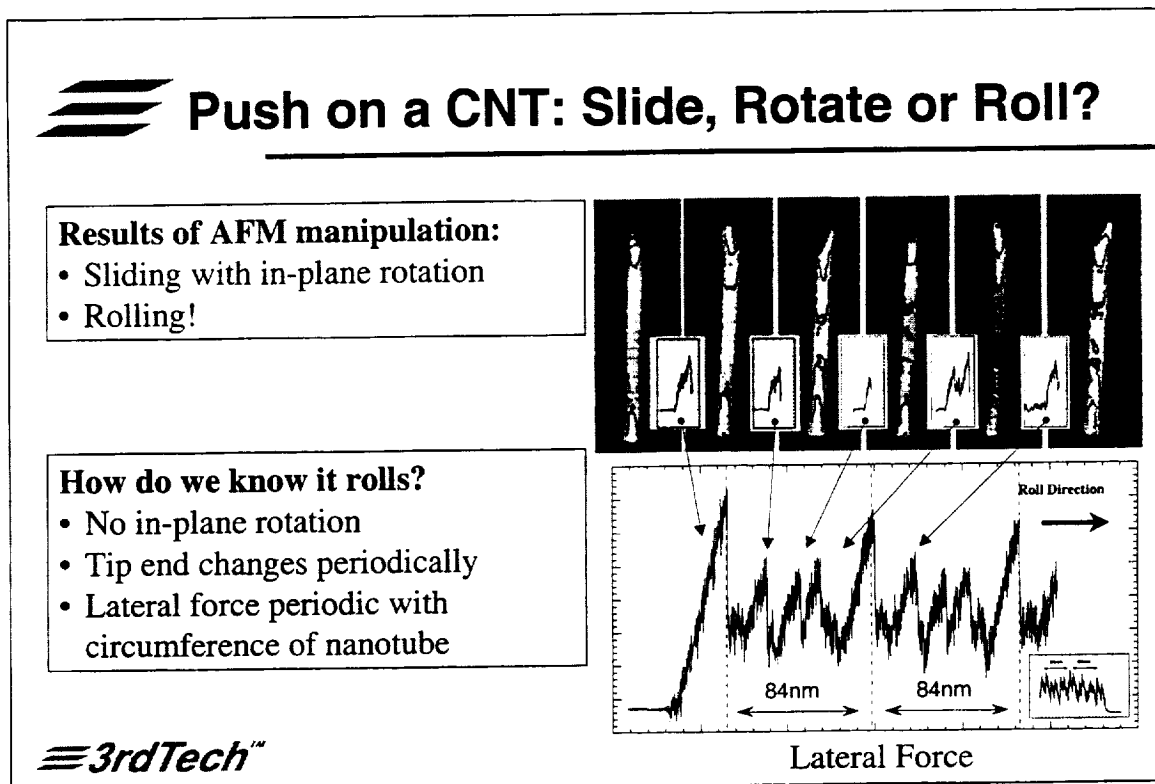


Nanotubes: Slide or Roll?

Researchers also examined large multi-wall nanotubes on a graphite substrate. Most of the time, the nanotubes rotated in the plane of the substrate when pushed off-center. But in certain orientations, the tube required much more force to move, and it did not pivot. Instead, it maintained a specific orientation. The end of the tube pictured was originally thought to be an imaging artifact, but when the experiment file was later re-examined using the automatic lab notebook, they discovered that it was an indication that the tube was rolling. The periodic change in force also matched the circumference of the tube.

This is an example of a finding that might have been missed without the ability to re-analyze data.

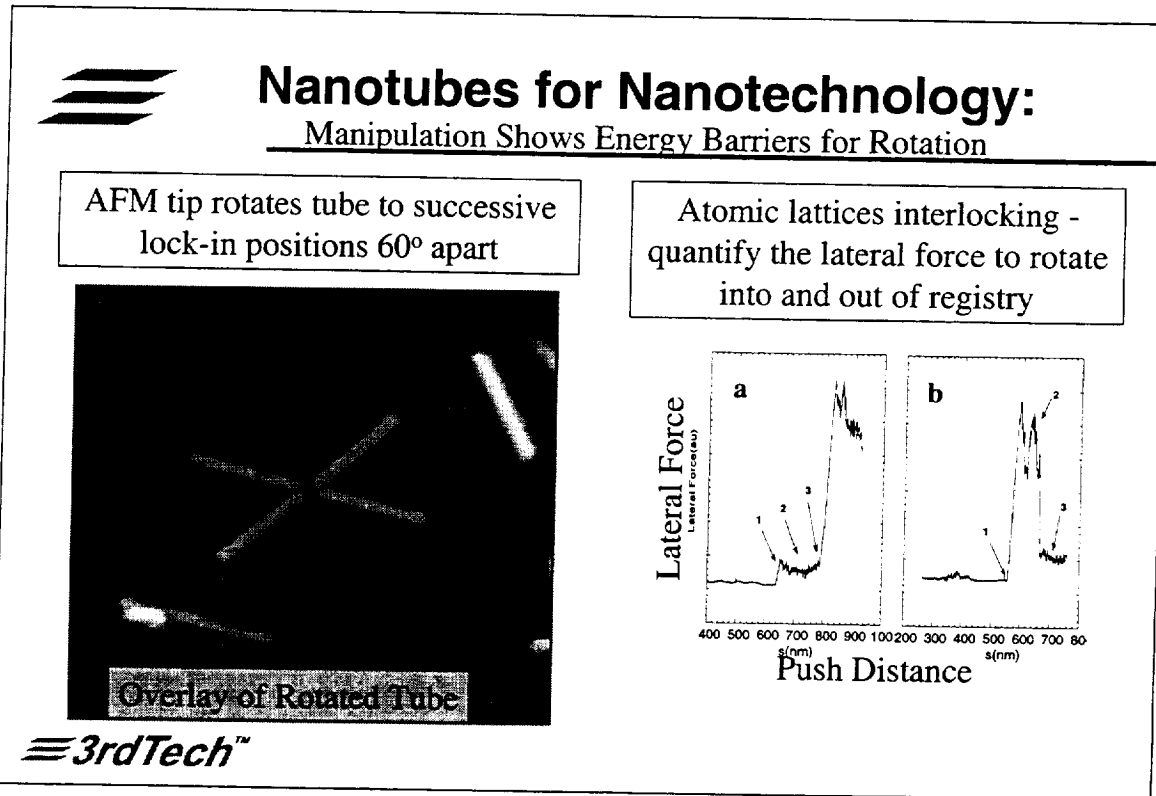
Falvo, M., Taylor II, R. M., Helser, A., Chi, V., Brooks Jr., F. P., Washburn, S. and Superfine, R., "Rolling and Sliding on the Nanometer Scale," *Nature*, Vol. 397, Jan. 1999, pp.236-238.



Nanotubes: Graphite Lattice Interlocks

Further manipulations indicate that each tube locks in at three different orientations, 60 degrees apart, on a graphite substrate. This corresponds to the symmetry of the graphite lattice. The researchers also measured the increase in lateral force when the tube went into registry with the graphite lattice.

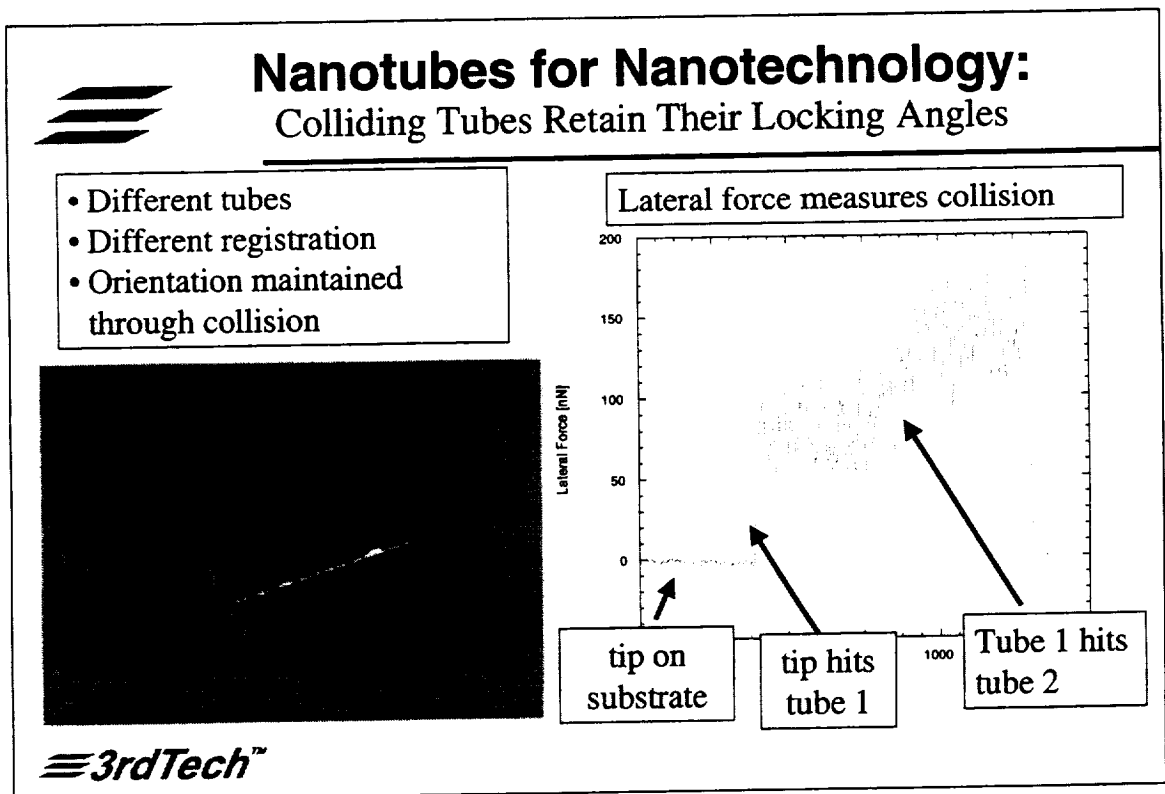
Falvo, M. R., Steele, J., Buldum, A., Schall, D., Taylor, R., Lu, J. P., Brenner, D. and Superfine, R., "Atomic Lattices Can Act Like Gears," *Nature* (submitted).



Nanotubes: Locking Orientations

Different tubes have different locking orientations. These tubes have different helicity, so when their lattices mesh with the graphite substrate, they have different orientations. Using the NanoManipulator, researchers could even roll one tube into the other and roll them both while the tubes maintained their orientations. This showed that the two tubes have different locking orientations on the same region of graphite.

Scientists are still investigating why the force required to roll a tube in registry is much higher than the force to slide a tube which is not in registry.




Nanotubes: NEMS

The UNC group has also experimented with arranging nanotubes to learn more in preparation for building nanotube structures. Here they push one tube on top of two others to form a bridge.

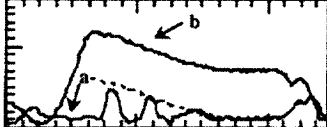


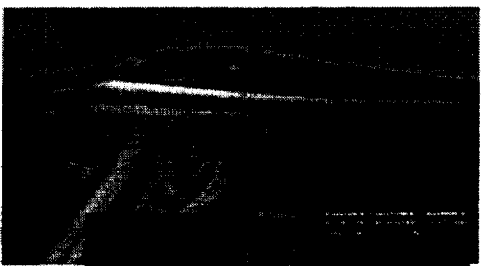
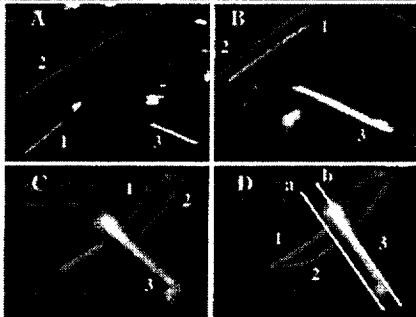
Nanotubes can also be manipulated and connected to electrical contacts for electromechanical devices consisting of one or multiple tubes.

Paulson, S., M. R. Falvo, N. Snider, A. Helsen, T. Hudson, A. Seeger, R. M. Taylor, R. Superfine, and S. Washburn, "In situ Resistance Measurements of Strained Carbon Nanotubes," *Applied Physics Letters*, Vol. 75, No. 19, Nov. 1999, pp. 2936-2938.



Nanotubes for Nanotechnology: Next Step: 3D Structures and NEMS Devices

AFM manipulation rearranges tubes into bridge




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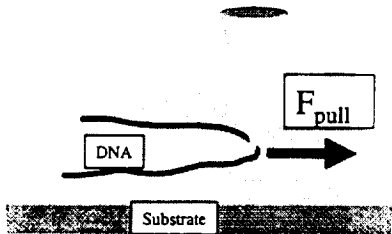
Application 3: DNA Manipulation

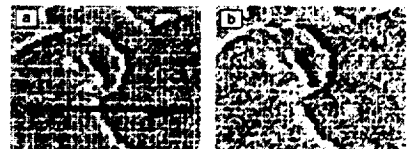
Here we have an example of a manipulation and a force measurement on a very small and delicate sample. The DNA is only a few nanometers high, and the lateral forces measured are very noisy. The average behavior of the force for this manipulation indicates a rupture force for the DNA of about 500 pico-Newtons.

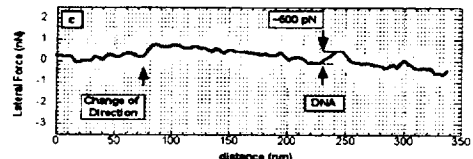
Guthold, M., Matthews, W. G., Taylor, R. M., Erie, D., Brooks, F. P. and Superfine, R., "Quantitative Manipulation of DNA in Liquid with the NanoManipulator Scanning Force Microscope," *Biophysical Society 43rd Annual Meeting, Feb. 13-17, 1999, Baltimore, MD, Biophys. Journal, Vol. 76, A351, 1999.*



Application 3: DNA - Mechanical/Protein Interactions








Distance (nm)	Lateral Force (pN)
0	0
50	0
75	0
100	0
150	0
200	0
220	-600
250	0
300	0
350	0

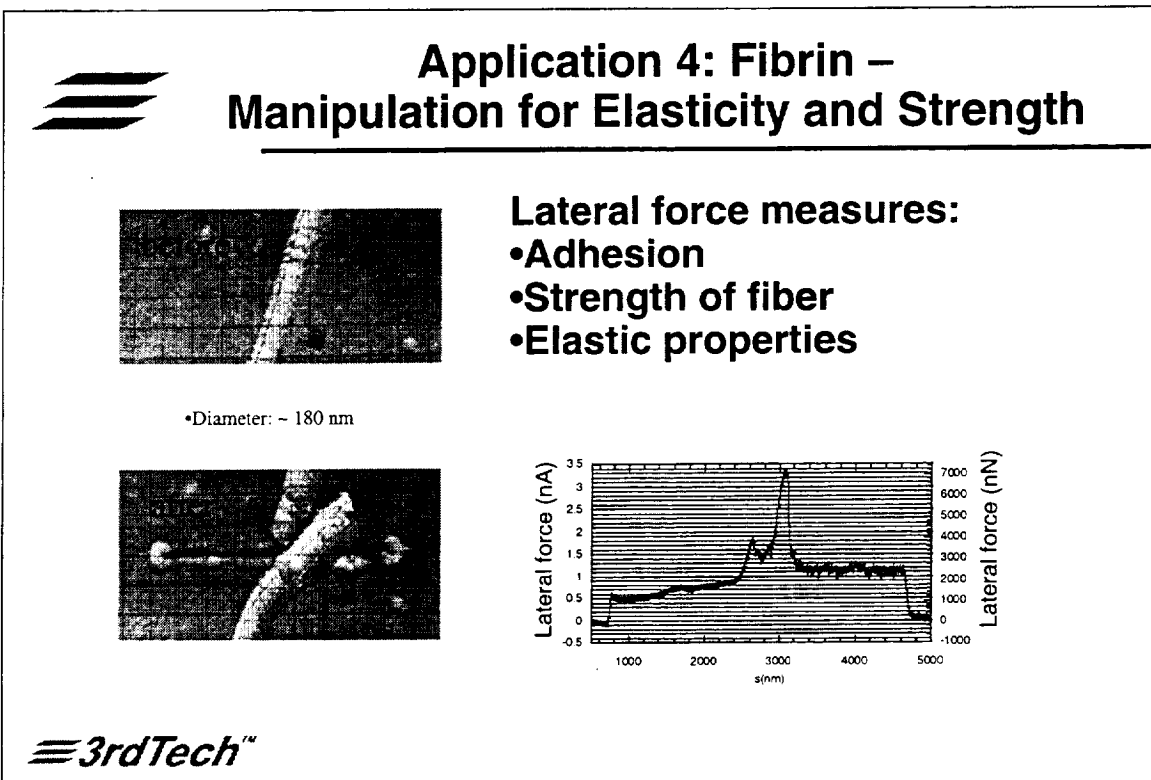
Protein Nucleic Acid Complexes: High Resolution Imaging
DNA/Chromosome: Precision Selection and Dissection



Application 4: Fibrin Manipulation

Fibrin is the fiber that forms when blood clots. The difference between fibrin from people with hemophilia, and from those without, can help scientists understand the disease. Researchers found that when a fiber is pushed with an AFM tip, it stretches and then ruptures. This particular manipulation shows that the fiber will also spring back towards its original position after the AFM tip passes.

Guthold, M., Falvo, M., Matthews, W. G., Paulson, S., Negishi, A., Washburn, S., Superfine, R., Brooks, F. P. and Taylor, R. M., "Investigation and Modification of Molecular Structures Using the NanoManipulator," *Journal of Mol. Graphics Mod.*, Vol. 17, 1999, pp. 187-197.



Summary

The NanoManipulator combines 3D graphics, force-feedback, virtual tips and complete experiment recording to greatly increase the value of an SPM. The device has been used extensively by scientists at the University of North Carolina at Chapel Hill.

Now, with the commercialization of the NanoManipulator, scientists at other research centers and universities can have access to these same capabilities.

3rdTech, Inc. will be working with the researchers at UNC-CH on an ongoing basis – exchanging ideas and using their problems as driving problems for enhancing the NanoManipulator. 3rdTech will also be analyzing the needs of researchers in nanotechnology for the development of future interactive tools.



Summary

- The NanoManipulator System is a powerful new tool for research in nanotechnology
- It enables unique capabilities for SPMs
 - 3D visualization
 - Force-feedback
 - Record/replay/re-analyze
- Available commercially for the first time

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Further Information

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Web: www.3rdtech.com

Further Information: info@3rdtech.com



Further Information

- Come see, and feel, the NanoManipulator System.
- We are tool builders. What tools do you need?
- Company and product information:
 - <http://www.3rdTech.com>
- Previous research:
 - <http://www.cs.unc.edu/Research/nano/>
- Thanks: UNC-CH Physics and Computer Science for images and information.

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