Grand Challenge Area
Nanostructured Materials by Design

Challenge

Nanoscience involves structures with a limited number of atoms or molecules, larger numbers than traditionally handled by chemistry and smaller numbers than traditionally handled by materials science or solid-state physics. This departure from traditional material sizes can fundamentally change the way nanostructured materials behave, such that their properties frequently cannot be predicted from current models of materials behavior.

One reason for the difference in the properties of nanoscale materials compared to the analogous macroscale, or bulk, material is the large surface area per unit volume. Atoms at surfaces often behave differently from those located in the interior of a grain or particle. In addition, tiny variations in the structure and composition of nanostructured materials can have a dramatic effect on their properties. As a result, many important physical and chemical interactions, like catalysis, take place at surfaces or interfaces and, because of the high surface area and unique properties, are enhanced in nanostructured materials.

Other properties, such as magnetism and electrical and heat conductivity can change substantially as size is reduced to the nanoscale. The differences in these properties stem from surprising collective effects and so-called quantum-size effects that arise from the confinement of electrons in nanometer-sized structures.

Vision

When manufactured into usable products, nanostructured materials manifest the unique properties of their component parts. By gaining understanding and control at the nanoscale, materials scientists will be able to develop novel, high-performance, affordable, and environmentally benign materials. These novel materials could be custom designed for special purposes, having structural, optical, electronic, magnetic, and/or other special properties suited to their intended uses.

Modeling and simulation, aided by the expected continued advances in computational power, will play a major role in the realization of this vision. With the relatively small number of atoms contained in nanostructures, their properties can be predicted with increasingly accurate and fundamental models of atomic interactions. Therefore, theory and experimentation are expected to be highly interactive.

Agency Participation

(lead in bold)

DOD	Improved armor, high strength-to-weight materials, lower life-cycle costs
DOE	Modeling/simulation, energy storage/transmission, friction, wear, corrosion
DOT	Improved materials and systems for transportation infrastructure
FDA	New or improved pharmaceuticals, cosmetics, biologicals, and medical device implant materials
IA	Materials-by-design for intelligence applications
NASA	High-performance, low-weight materials for space
NIST	Standard reference materials, materials property data, materials characterization methods
NSF	Novel structures, synthesis, and processing methods
USDA	Nanostructured materials from agricultural origins, nanocomposite polymers to enhance packaging functionality

Research Example: Molecular Perfection – The Fullerene Ideal (supported by DOD, NASA, and NSF)

Imagine a soccer ball shrunk to one billionth of its normal size. In 1985 researchers at Rice University created a geodesic-sphere-shaped molecule made of 60 carbon atoms (C60), dubbed the "buckyball." It was the first of a new class of molecularly perfect nanostructures now called fullerenes, named after the American architect Richard Buckminster Fuller.

The C60 molecule was soon followed by other fullerenes containing many more atoms of carbon and taking different shapes. One of the most interesting of these is the "buckytube," or carbon nanotube (CNT), an elongated nanoscale tube made entirely out of carbon. A computer model of a CNT is shown in Figure 7.

CNTs have unique properties, which, like those of diamond, arise from its perfect structure. Depending on the precise pattern of the carbon network, a CNT can act as either a highly conductive metal wire only one nanometer in diameter, or as a semiconductor. It has been used to build the first room-temperature transistor ever made from a single molecule, and is widely expected to be the key ingredient in nanoelectronics that will vastly extend the power and shrink the size of computers and other "smart" devices. Carbon nanotubes are also efficient electron emitters, which may lead to their application in affordable flat panel displays.

In addition to their remarkable electrical properties, carbon nanotubes are incredibly strong. Pulled end-to-end, a CNT has a tensile strength about 30 times greater than that of steel, while having only 1/6th its weight, making it the strongest fiber ever made. Researchers at the University of Texas at Dallas, with funding from the Defense Advanced Research Projects Agency in DOD, have woven fabric from fibers spun from a composite of polymers and CNTs. The new CNT-based fiber has a very high breaking strength and can be used to replace materials like Kevlar in bulletproof vests and other applications.

Finally, the thermal conductivity down the length of a single carbon nanotube has been measured to be 50% higher than diamond – previously the material with the highest known thermal conductivity – making it a superb material for piping heat from one place to another. Heat removal is a key issue, for example, in computers and other high-density electronic devices.

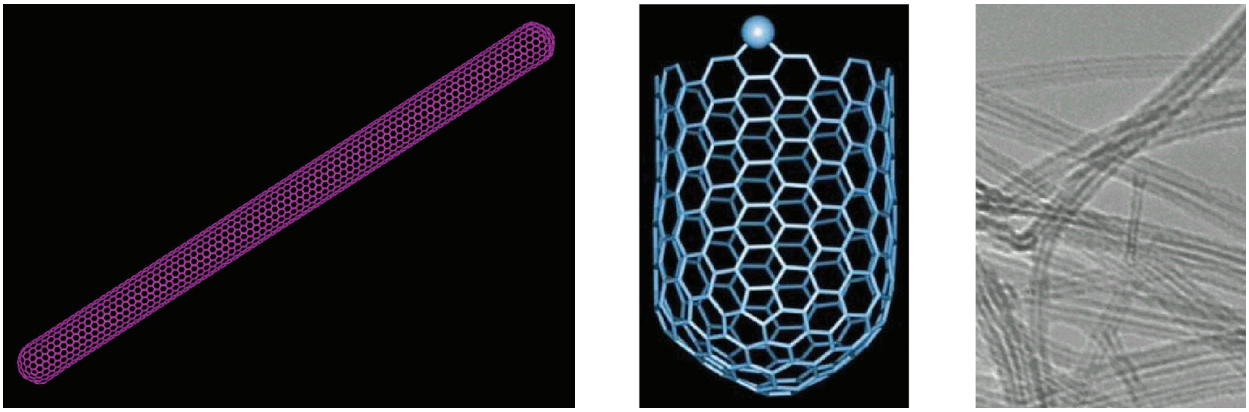

Figure 7. Single-walled carbon nanotubes. (Left) Computer drawing (courtesy Richard Smalley, Rice University). (Center) Enlarged view of computer drawing; (Right) High-resolution electron micrograph of nanotubes (courtesy NASA).