

Chapter 1

FUNDAMENTAL SCIENTIFIC ISSUES FOR NANOTECHNOLOGY

Contact persons: G. Whitesides, Harvard University; P. Alivisatos, U. California, Berkeley

1.1 VISION

Nanostructures are the entry into a new realm in physical and biological science. They are intermediate in size between molecular and microscopic (micron-size) structures. They contain a countable number of atoms, and are, as a result, uniquely suited for detailed atomic-level engineering. They are chameleons: viewed as molecules, they are so large that they provide access to realms of quantum behavior that are not otherwise accessible; viewed as materials, they are so small that they exhibit characteristics that are not observed in larger (even 0.1 μm) structures. They combine small size, complex organizational patterns, potential for very high packing densities and strong lateral interactions, and high ratios of surface area to volume.

Nanostructures are the natural home of engineered quantum effects. Microstructures have formed the basis for the technologies that support current microelectronics. Although microstructures are small on the scale of direct human experience, their physics is largely that of macroscopic systems. Nanostructures are fundamentally different: their characteristics—especially their electronic and magnetic characteristics—are often dominated by quantum behavior. They have the potential to be key components in information technology devices that have unprecedented functions. They can be fabricated in materials that are central to electronics, magnetics, and optics. Nanostructures are, in a sense, a unique state of matter—one with particular promise for new and potentially very useful products.

Because they are small, nanostructures can be packed very closely together. Their high packing density has the potential to bring higher speed to information processing and higher areal and volumetric capacity to information storage. Such dense packing also is the cause of complex electronic and magnetic interactions between adjacent (and sometimes, nonadjacent) structures. For many nanostructures, especially large organic molecules, the small energetic differences between their various possible configurations may be significantly shaped by those interactions. In some cases, the presence of surface interface material, with properties different from the nanostructures themselves, adds another level of complexity. These complexities are completely unexplored, and building technologies based on nanostructures will require in-depth understanding of the underlying fundamental science. These complexities also promise access to complex non-linear systems that may exhibit classes of behavior fundamentally different from those of both molecular and microscale structures.

Exploring the science of nanostructures has become, in just a few years, a new theme common to many established disciplines. In electronics, nanostructures represent the

limiting extension of Moore's law and classical devices to small devices, and they represent the step into quantum devices and fundamentally new processor architectures. In molecular biology, nanostructures are the fundamental machines that drive the cell—histones and proteosomes—and they are components of the mitochondrion, the chloroplast, the ribosome, and the replication and transcription complexes. In catalysis, nanostructures are the templates and pores of zeolites and other vitally important structures. In materials science, the nanometer length scale is the largest one over which a crystal can be made essentially perfect. The ability to precisely control the arrangements of impurities and defects with respect to each other, and the ability to integrate perfect inorganic and organic nanostructures, holds forth the promise of a completely new generation of advanced composites. Each of these disciplines has evolved its own separate view of nanoscience; the opportunities for integrating these views and for sharing tools and techniques developed separately by each field are today among the most attractive in all of science.

Nanoscience is one of the unexplored frontiers of science. It offers one of the most exciting prospects for technological innovation. And if it lives up to its promise as a generator of technology, it will be at the center of fierce international competition.

1.2 CURRENT SCIENTIFIC AND TECHNOLOGICAL ADVANCEMENTS

Nanoscience has exploded in the last decade, primarily as the result of the development of new tools that have made the characterization and manipulation of nanostructures practical, and also as a result of new methods for preparation of these structures.

Scaling Laws and Size-dependent Properties of Isolated Nanostructures

It is now well established that such fundamental properties as the melting temperature of a metal, the remanence of a magnet, and the band gap of a semiconductor depend strongly upon the size of the component crystals, provided they are in the nanometer regime. Almost any property in a solid is associated with a particular length scale, and below this length, the property will vary. For instance, the exciton diameter in a semiconductor may be tens or hundreds of nanometers, the distance between domain walls in a magnet may be hundreds of nanometers, etc. This opens the prospect for creating a new generation of advanced materials with designed properties, not just by changing the chemical composition of the components, as has been done in the past, but by controlling the size and shape of the components. This creates great opportunities for fundamental science in condensed matter physics, solid state chemistry, materials science, electrical engineering, biology, and other disciplines.

Tools for Characterization

Scanning probe microscopies have revolutionized characterization of nanostructures, and development of new variants of scanning probe devices continues apace. Older tools, especially electron microscopy, continue to play essential roles. In biological nanoscience, the combination of X-ray crystallography and NMR spectroscopy offers atomic-resolution structural information about structures as complex as entire virus particles.

Fabrication and Synthesis

Tremendous advances are currently occurring in the synthesis and fabrication of isolated nanostructures. These activities range from colloidal synthesis of nanocrystals to the growth of epitaxial quantum dots by strained layer growth. Related activities include the preparation of fullerenes, buckytubes, and other one-dimensional nanostructures, as well as the growth of mesoporous inorganics. Increased activity in the nanoscale design of polymers is also occurring, including the development of dendrimers and complex block copolymers. The techniques of molecular biology have made a very wide range of biological nanostructures readily available through cloning and overexpression in bacterial production systems.

While much has been accomplished in the growth of isolated nanostructures, work has only just begun in the use of self-assembly techniques to prepare complex and designed spatial arrangements of nanostructures. A parallel line of current activity in fabrication of patterned nanostructures rests on the extension of techniques highly developed in the field of microelectronics: photolithography, X-ray lithography, and e-beam lithography. A number of recent developments in synthesis and fabrication offer the potential both to generate new types of structures, and, probably more importantly, to generate these structures at a fraction of the cost of techniques derived from microlithography. Soft lithography, which uses molding, printing, and embossing to form patterned structures in plastics and glasses, has expanded the range of materials that can be used and has suggested routes to previously inaccessible three-dimensional structures.

Computation

Because nanostructures contain few atoms (at least relative to most materials), they are uniquely susceptible to high-level simulation using supercomputers. The capability to treat nanostructures with useful accuracy using computation and simulation will be invaluable both in fundamental science and in applied technologies.

Emerging Uses

Many clear applications for nanotools and nanostructures are already evident and are the targets of existing technology development programs:

- Giant magnetoresistance (GMR) materials have been introduced into commercial use with remarkable speed, and their acceptance suggests the importance of magnetic materials with nanometer-scale spin-flip mean free path of electrons.
- Numerous nanodevices and nanosystems for sequencing single molecules of DNA have been proposed; these structures, if successful, will be invaluable in the Human Genome Project and other large-scale genomics programs. Indeed, it seems quite likely that there will be numerous applications of inorganic nanostructures in biology and medicine, as markers.
- Similarly, there exists a range of ideas for high-density information storage, based, for example, on concepts such as nano-CDs and on nanostructured magnetic materials, including materials showing giant and tunneling magnetoresistive effects; these promise to provide future systems for memory with ultrahigh densities.

- New types of components for information processors based on quantum mechanical principles (resonant tunneling transistors; single electron transistors; cellular automata based on quantum dots) are being explored actively at the level of research; these types of processors appear to fit well in the burgeoning field of quantum computation.
- New protective coatings, thin layers for optical filtering and thermal barriers, nanostructured polymers, and catalysts are already coming to the market. Nanostructured coatings are showing good corrosion/erosion resistance as possible replacements for the environmentally troublesome chromium-based coatings.
- Aerogels—highly porous, sponge-like materials with a three-dimensional filigree of nanostructures—have promise in catalysis and energy applications.

1.3 GOALS FOR THE NEXT 5-10 YEARS: BARRIERS AND SOLUTIONS

Numerous important areas require active research and development. The objectives of current research are to be able to understand the properties of isolated nanostructures; to make arbitrary structures with atomic-level precision; to do so rapidly, in large numbers, and inexpensively; and to design these structures to have desired properties using appropriate computer tools. Nanoscience is far from this objective, but it is moving rapidly in every component of the problem.

Fundamental Properties of Isolated Individual Nanostructures

Individual nanostructures in isolation are the building blocks of nanotechnology. Individual structures are studied because we do not yet know the fundamental limits to the preparation of *identical* nanostructures and because each nanostructure can interact differently with its environment. Underlying the fundamental properties of nanostructures are two broad themes. First, the size-dependent properties of materials in the nanoscale regime are predicted to vary qualitatively according to scaling laws; comparison to these simple scaling laws remains an important activity. Second, the properties of isolated nanostructures have a significant statistical variation, fluctuating in time, and it is important to observe and understand these variations.

Many key questions relate to the structure, or arrangement of atoms, in a nanostructure. The relative stability of different structural phases is altered in the nanometer regime, affected by both kinetic and thermodynamic factors. Variations may arise for many reasons, including surface energies, absence of defects, or electronic quantum size effects. There is a compelling need to map out the kinetics and thermodynamics of phase transformations in nanostructures. For any picture of the physical properties of nanostructures to be complete, the structure of the surface must also be determined. Due to their finite sizes, the structure and composition of the surfaces of nanostructures may have particular importance for their chemical and physical properties. The surfaces of nanostructures are likely to vary significantly from the well-known structures of bulk surfaces, and entirely new experimental techniques for measuring these reconstructions need to be developed. The ability not only to measure, but ultimately to systematically control, the surface and interior structures of nanoscale materials will be an ongoing field of research over the next decade.

Recent developments have permitted the observation of optical, electrical, magnetic, chemical, thermal, mechanical and biological properties of isolated, individual nanostructures. These techniques, which have facilitated developments such as single-electron transistors, scanning probe microscopies, and single-molecule spectroscopy, have revolutionized our understanding of nanostructured materials. The early studies point the way to a long-term agenda: develop new probes of fundamental properties that can work with nanometer spatial resolution and ever-improved temporal resolution and sensitivity.

Early work also reveals that nanoscale systems can be fluctuational by nature. Much work is needed to understand their fluctuations and to learn what the fundamental limits are. As an example, an important question in quantum computation concerns whether it is possible to prepare well-defined superposition of quantum states in nanostructures without rapid dephasing.

Fundamental Properties of Ensembles of Isolated Nanostructures

Nanostructures may be used in a wide range of contexts; most of these are ones in which ensembles of nanostructures are assembled into a complex, functional arrangement. Many properties of nanoscale building blocks vitally depend upon the size, the shape, and indeed the precise arrangement of all the atoms within. Thus, a high priority must be placed upon understanding the fundamental limits to the preparation of identical nanostructures. To this day, the processes of nucleation and growth are incompletely understood, and we do not know what is the largest number of atoms that can be assembled into a precisely defined molecular structure. Even if a system is prepared according to an ideal chemical process, there inevitably will be variations. There is a need to understand further which desirable properties are retained or even simplified by averaging out such variations, and which properties are lost.

Assemblies of Nanoscale Building Blocks

The construction of functional assemblies of nanostructures depends upon a sound understanding of the intrinsic couplings between nanostructures. Charge separation and transport, tunneling, through-space electromagnetic coupling, and mechanical and chemical interactions between nanostructures need to be measured and theoretically described further than has been done to date.

A combination of electron beam (and perhaps X-ray) lithography, scanning probe writing and fabrication, soft lithography, self-assembly, and catalytic growth together offer a rich menu of new and old fabrication techniques to use in patterning nanostructures. With the exception of e-beam and X-ray lithography, these techniques are all early in their development cycle and have substantial promise for growth. The next decade will see these techniques developed and integrated into a suite of methods for the fabrication of nanostructures and nanosystems.

The synthesis of bulk materials—colloids, magnetic structures, zeolites, buckytubes and analogs, aerogels, and many others—is also an area where there is potential for great innovation. In most of these materials, the physics underlying their behavior is understood only incompletely; there is an opportunity now to discover many new

behaviors resulting from confinement of electrons or photons, from high structural perfection, from high ratios of surface to volume, or from some other aspect of small size.

In relevant but independent research in molecular biology, techniques of genetic manipulation, combined with technologies for protein production, provide the way to make small quantities of almost any protein of interest. The genome projects will extend this capability. Progress in biotechnology will increase the ease with which large quantities of genetic materials can be generated.

A key issue is understanding the integration processes of various isolated nanostructures and assemblies of nanostructures.

Evaluation of Concepts for Devices and Systems

Among the most critical impediments to thinking seriously about nanostructure-based systems are the difficulties in understanding how they are to be interconnected and addressed and in understanding what kinds of new functions are achievable. For instance, in nanoelectronics, there are a number of solutions that have been suggested for some of these issues—ranging from using buckytubes as nanowires to addressing individual components via ganged scanning probe devices, or even optically—but there has been almost no serious work directed toward the problems of systems fabrication. Among the numerous questions that must be solved are: what to use as wires; how to design and fabricate devices; and what the architectures of systems should be.

Research is currently focused on exploring the fabrication and characterization of single devices at the level of single electron transistors or resonant tunneling devices. There is much less effort (and certainly much less than is needed) devoted to asking fundamental questions about how electrical current is to be carried from a contact pad to a device in a densely packed array, fault- and defect-tolerant designs, device isolation, the operation of large arrays of cooperative devices, and other fundamental questions dealing with the problem of making an array of nanostructured quantum devices that performs some complex function. Similar to the nanoelectronics issues, resolving the aspects related to integration at nanoscale is essential in dispersions, nanocomposites, sensors, and other areas.

Nanomanufacturing

Developing techniques for fabricating nanostructures inexpensively in very large numbers—that is, manufacturing them—is an area that requires substantial effort: nanoscience will not be fully successful until it has provided the base for manufacturing technologies that are economically viable. It is probable that methods developed for microfabrication in the >100 nm size range will not work in the 20 nm range. It will thus probably be necessary to develop an entire new suite of manufacturing methods for nanostructures. There is reason to believe that self-assembly and soft lithography will be able to make substantial contributions to this important problem, but other fundamentally new methods will also be needed.

Connecting Nanoscience and Biology

One of the opportunities in basic science is to search for synergies between nanoscience in biology and nanoscience as developed in the contexts of computation and information science and solid-state physics and chemistry. There is no question that understanding the structure and function of biological nanostructures will stimulate fabrication of nonbiological materials; it is possible that biologically derived structures may also be useful in assembly of systems of nanodevices. In return, nanofabrication can provide analytical tools for investigating biomolecules (in genomics, proteomics, and high-throughput screening for drug leads) as well as for exploring the interior structure and function of cells. One objective of nanoscience should be to build robust intellectual bridges between its currently scattered disciplinary components, but especially between nanoelectronics and molecular biology.

Molecular Electronics

Molecular electronics offers an attractive opportunity for basic science in nanosystems. Organic molecules are probably the smallest systems that can be imagined for many possible functions, but they have the disadvantage, from the point of view of possible use in nanoelectronic systems, that they are usually poor conductors of electricity. A number of systems have been investigated in which experimental results suggest that organic molecules can act as molecular wires; there are hints that they may also serve as components in more complex systems. The science base in molecular electronics is very early in its development, and it is not yet clear whether organic molecules—even if they do conduct electricity—have the other properties they would need to be the core components of a large-scale nanoelectronics technology. Defining the real promise of molecular electronics should be an objective of research.

Nanostructures as Model Systems for Earth and Planetary Science

Nanoscale components are fundamental building blocks for solid state chemistry. Thus, further study of nanostructures can lead to improvements in our understanding of fundamental processes in earth and planetary science. Improved understanding of interstellar dust, the formation mechanisms of minerals, and the processes of weathering can all result from fundamental studies of nanostructures.

1.4 SCIENTIFIC AND TECHNOLOGICAL INFRASTRUCTURE

Tools for Synthesis and Fabrication, and for Characterization

To work in nanoscience, it is a prerequisite to be able to fabricate and characterize nanostructures: to make rabbit stew, one must first catch a rabbit. Making the important tools for fabrication and characterization available to user communities is an imperative; throughout the nation, research in nanoscience is still limited by limited access to tools. Certain instruments, especially electron microscopes, are sufficiently expensive that they should be operated within consortia; others, especially state-of-the-art scanning probe devices, should be distributed to qualifying individual research groups. The character and cost of the facilities needed for fabrication generally depend on the technique being used. For the more expensive facilities—for example, high-resolution e-beam writers,

good clean-room facilities, and mask-making facilities—a substantial, early investment is needed to prevent fabrication delays.

Flexible Research Structure

Nanoscience is an area in which there is no single way to do research: both single-investigator, peer-reviewed research and programmatic research involving groups of investigators from different disciplines and organizational structures have roles to play. It is important not to narrow the options for modalities of research support at this stage in the development of the field.

Training the Next Generation of Nanoscientists

Nanoscience has emerged into prominence only in the last 5-10 years. It is not supported in universities by existing departments: nanoscientists come from chemistry, physics, biology, electrical engineering, and others, and tend to think of themselves in terms of their historical disciplinary affiliations. Building educational programs that focus on nanoscience and nanotechnology as a distinct field—whether addressing device physics or structural biology—would provide a profound boost to the advancement of nanoscience by making it visible and intellectually attractive to the brightest young people and by promoting transfer of information between disciplines.

1.5 R&D INVESTMENT AND IMPLEMENTATION STRATEGIES

Because nanoscience is an area in which a range of research styles flourish, it is important to keep support distributed among a number of sources; it should not, at this juncture, be concentrated in one Federal agency. The National Science Foundation (NSF) and the Department of Defense Advanced Research Projects Agency (DARPA), for example, serve fundamentally different functions in nanoscience, and consolidation of these functions into one agency could slow progress in the field dramatically. One of the challenges of an area of national importance but in which Government support is distributed to various agencies, is to coordinate Government-sponsored activities so that the whole is greater than the sum of the parts. NSF is the plausible agency to lead the coordination effort.

Reporting

To maintain a high focus on nanoscience/technology and to ensure careful reporting, NSF should be charged with providing an annual appraisal of the field to the Office of Management and Budget (OMB) and other interested parties such as various House and Senate committees, industrial users, etc. Appropriate reporting and interagency discussion would help to maximize productive transfer of processes and materials among groups, regardless of the source of support.

Emphasis in Support

Nanoscience is still in its infancy. The emphasis in Federally funded research should be on precompetitive fundamental science and engineering. The object of the work should be to develop flexible, innovative methods of making, characterizing, applying, and manufacturing nanosystems. In nanoscience, as in many fields, technology transfer

represents a difficult step. In other fields of technology—especially biotechnology and information technology—the venture community has played a major role in technology transfer. Developing intellectual property and financial policies that make nanoscience an attractive investment would accelerate the development of commercial technologies.

1.6 PRIORITIES AND CONCLUSIONS

Interest in nanoscience is burgeoning, largely due to its enormous practical potential. Yet it is very clear that nanoscience has provided a new way of thinking that has the potential to promote truly exciting developments in fundamental science as well. Long-standing questions in condensed matter physics and chemistry, in biological science, in materials science, and in mechanical engineering will receive renewed attention as a result of the exciting developments in nanotechnology.

Priorities

- a. Build a broad program of R&D in nanoscience that will include research universities, relevant industry, and some of the national laboratories. Important public policy objectives in this field should include building a “community” focused on nanoscience/technology and providing stable support for this community at a level high enough to allow the participating groups to reach a critical mass.
- b. Develop other mechanisms for bridging the gaps between communities interested in nanoscience, including both the physical and biological sciences.
- c. Develop policies explicitly designed to attract large companies as participants in programs of Federally funded groups. Without the large-company participation, technology development programs in nanoelectronics will probably fail at the stage of research planning and product definition.
- d. Develop a strategy for informal coordination of R&D among participating Federal agencies, centered in NSF.
- e. Maintain an active series of reports to OMB and Congress, both to aid in educating policymakers about the progress, opportunities, and failures of the field, and to provide a general education about nanoscience at senior levels in the Government.
- f. Provide Federal funds to push science that seems to offer the potential of developing into profitable technology rapidly to the point of manufacturable prototypes using focused, DARPA-style programs.
- g. Address the problems of public perception of threats from nanoscience with active programs to reduce any possible threats and educate the public.

1.7 EXAMPLES OF CURRENT ACHIEVEMENTS AND PARADIGM SHIFTS

1.7.1 Quantum Dot Formed by Self-assembly (Ge “pyramid”)

Contact person: R.S. Williams, Hewlett-Packard Co.

Figure 1.1 is a scanning tunneling microscope (STM) image of a pyramid of germanium atoms on top of a silicon surface. The pyramid is ten nanometers across at the base, and it is actually only 1.5 nanometers tall (the height axis in the image has been stretched to

make it easier to see the detail in the faces of the pyramid). Each round-looking object in the image is actually an individual germanium atom.

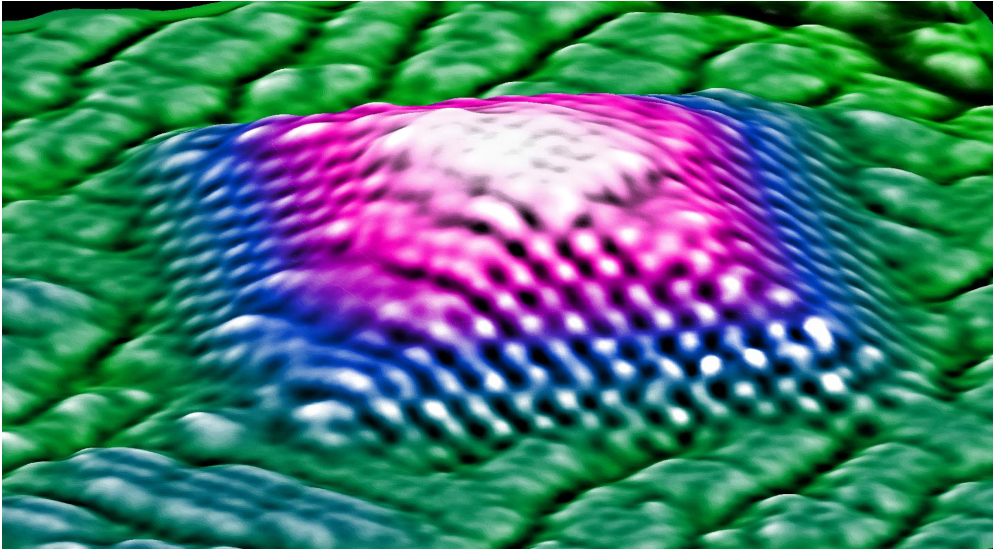


Figure 1.1. STM image of quantum dot formed by self-assembling (Ge “pyramid”) (courtesy Hewlett-Packard; image acquired by G. Medeiros-Ribeiro, Hewlett-Packard Labs).

The pyramid forms itself in just a few seconds in a process called “self-assembly.” If the proper number of germanium atoms is deposited onto the correct type of silicon surface, the interactions of the atoms with each other causes the pyramids to form spontaneously. The propensity of some materials to self-assemble into nanostructures is currently a major area of research. The intent is to learn how to guide or modify self-assembly to get materials to form more complex structures, such as electronic circuits.

Manufacturing processes based on guided self-assembly of atoms, molecules, and supramolecules promise to be very inexpensive. Instead of requiring a multibillion-dollar manufacturing facility, electronic circuits of the future may be fabricated in a beaker using appropriate chemicals, and yet they may be many thousands to millions of times more capable than current chips. Just twenty years ago, few scientists even dreamed it would be possible to see such a detailed picture of the atomic world, but with the advent of new measuring tools, the scanning probe microscopes developed in the mid-1980s, seeing atoms is now an everyday occurrence in laboratories all over the world.

1.7.2 Quantum Corral

Contact person: D. Eigler, IBM

Figure 1.2 is a scanning tunneling microscope image of a “quantum corral.” The corral is formed from 48 iron atoms, each of which was individually placed to form a circle with a 7.3 nanometer radius. The atoms were positioned with the tip of the tunneling microscope. The underlying material is pure copper. On this copper surface there are a group of electrons that are free to move about, forming a so-called “two-dimensional electron gas.” When these electrons encounter an iron atom, they are partially reflected. The purpose of the corral is to try to trap, or “corral” some of the electrons into the circular structure, forcing the trapped electrons into “quantum” states. The circular undulations in the interior of the corral are a direct visualization of the spatial distribution

of certain quantum states of the corral. Experiments such as this give scientists the ability to study the physics of nanometer-scale structures and to explore the potential application of these small structures to any of a number of purposes.

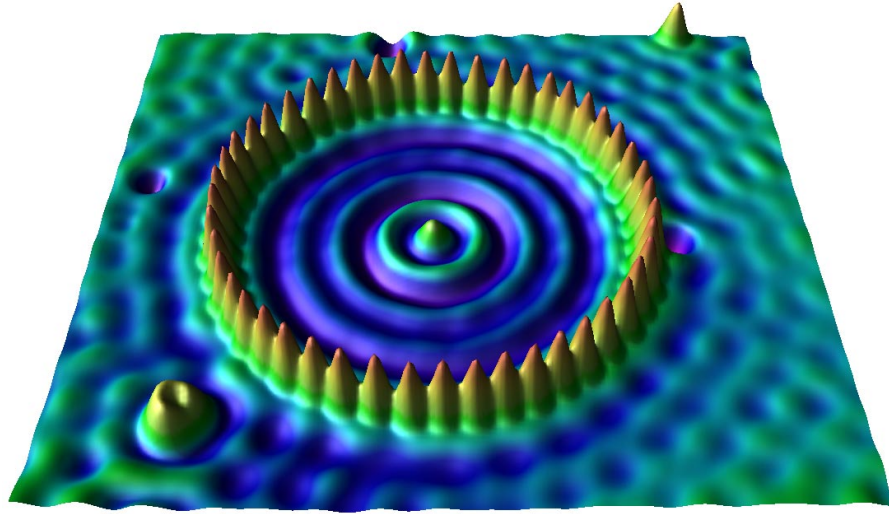


Figure 1.2. STM image of a “quantum corral” (courtesy IBM Research Division).

1.7.3 Magnetic Behavior at Nanoscale

Contact person: P. Alivisatos, U.C.-Berkeley

Figure 1.3 is a transmission electron microscope (TEM) image of an elegant example of natural nanotechnology that occurs in magnetotactic bacteria. These are bacteria that contain within them a “compass” that allows them to move in a particular magnetic direction. The compass consists of a series of magnetic nanoparticles arranged in a line.

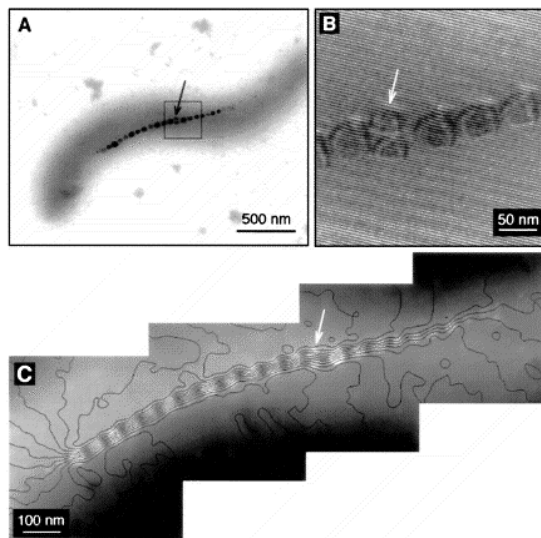


Figure 1.3. TEM image showing natural nanotechnology in magnetotactic bacteria (*magnetospirillum magnetotacticum* strain MS-1). Chains of nanocrystals used for navigation illustrate nature’s exploitation of a fundamental scaling to achieve maximum and most efficient use of magnetization (reprinted with permission from Dunin-Borkowski et al. 1998, ©1998 American Association for the Advancement of Science).

Each particle is as large as it can be and still remain a single magnetic domain, 25 nm. Larger particles have a type of defect, a magnetic domain wall, that lowers their coercivity. In the bacteria, these magnetic particles aggregate spontaneously into chains. The resulting compass uses a minimum amount of material to achieve the desired property, alignment along Earth's magnetic field.

Artificial nanotechnology researchers can learn much from what already occurs in nature. The time required for a magnetized specimen to lose memory of its direction of magnetization depends exponentially upon the volume, provided the crystal is still in the nanometer regime. Thus, the same physics imposes a lower limit of a few tens of nanometers to the size of an iron oxide particle that could be used in a magnetic memory unit that operates at room temperature.

1.7.4 Ordered Monolayer of Gold Nanocrystals

Contact person: R. Andres, Purdue University

Figure 1.4 is a transmission electron microscope image of an ordered monolayer of gold particles 5 nm in diameter supported on a thin carbon membrane. The round-looking objects are well-faceted single crystals of gold atoms. These nanocrystals have the shape shown in the bottom right inset and are aligned as a hexagonal array as illustrated by the expanded view shown at the bottom left. Each gold particle is mechanically and electronically separated from its nearest neighbors by organic molecules, which give structural integrity to the monolayer and serve as a controlled tunnel barrier for electron transport between the particles. This ordered monolayer forms spontaneously on a water surface and can be transferred intact to a wide range of flat solid substrates. If instead of transferring the entire monolayer, a method can be developed to transfer only a selected pattern of narrow ribbons, it would provide an elegant solution to the problem of interconnecting electronic devices having smaller and smaller dimensions.

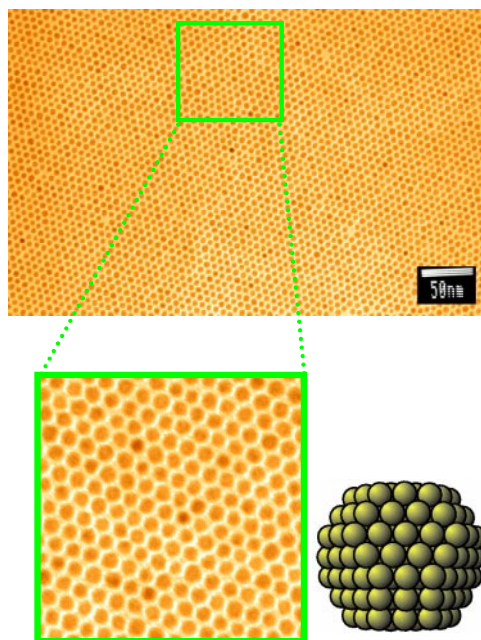


Figure 1.4. TEM image of an ordered monolayer of gold nanocrystals.

1.7.5 Nanostructured Polymers

Contact person: S. Stupp, Northwestern University

Figure 1.5 depicts a supramolecular nanostructure formed by the ordered self-assembly of triblock copolymers. The polar liquid-crystalline parts of the molecules (bottom) arrange themselves in an ordered lattice, while the bulky, aromatic-hydrocarbon units (top) form an amorphous cap. These nanosized mushroom-shaped units further self-assemble into polar sheets whose top surfaces (mushroom caps) are hydrophobic and whose bottom surfaces (mushroom stems) are hydrophilic. Such self-assembled nanostructures are under investigation as anti-icing coatings for aircraft, lubricating layers for microelectronics, anti-thrombotic agents for arteries, etc.

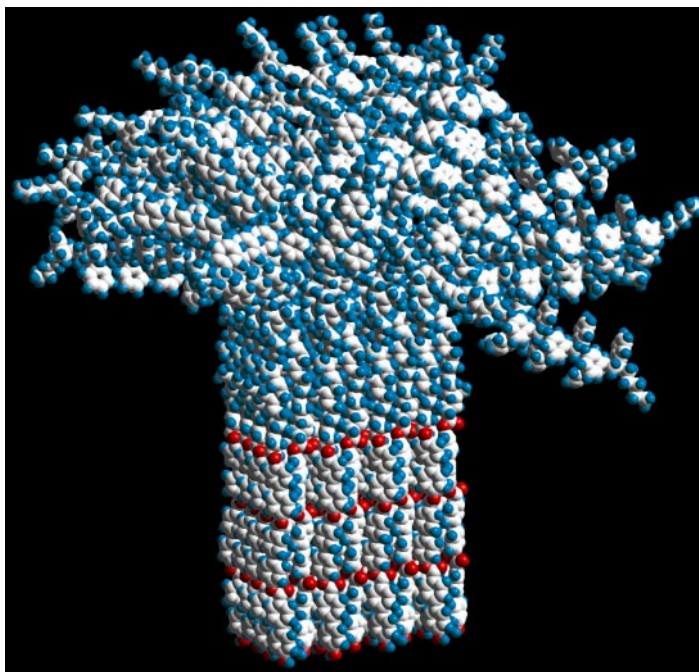


Figure 1.5. Supramolecular nanostructure formed by the ordered self-assembly of triblock copolymers (reprinted with permission from Stupp 1997, ©1997 American Association for the Advancement of Science).

1.7.6 Super Strong Materials by Nanostructuring

Contact persons: H. Kung and T.C. Lowe, Los Alamos National Laboratory

Traditionally, the mechanical strength, σ , of crystalline materials is believed to be largely controlled by the grain size d , often in the manner described by the Hall-Petch relationship, $\sigma = kd^{-1/2} + \sigma_0$. As the structural scale reduces to the nanometer range, researchers have found that the materials exhibit different scale dependence and there is a limit to the conventional descriptions of yielding (Misra et al. 1998). In addition to the high strength, the intrinsically high interface-to-volume ratio of the nanostructured materials may enhance interface-driven processes to extend the strain-to-failure and plasticity. A recent study on nanostructured Cu/Nb composites shows a complete suppression of brittle fracture when the wire was tensily tested at liquid He temperature (Han et al. 1998). This is an amazing finding, since bcc metals (such as Nb) are known to fracture in a brittle fashion at 4.2 K. The nanostructured Cu/Nb composites exhibit

significant strain hardening and ductility before fracture at a tensile strength of ~ 2 GPa and a strain of 10.

These results show that by reducing the structural scale to the nanometer range, one can extend the strength-ductility relationship beyond the current engineering materials limit, which is illustrated by the broad curve in the schematic diagram on the right side of Figure 1.6. A limitation of current engineering materials is that gain in strength is often offset by loss in ductility. The nanocomposite results suggest that by reducing the structural scale and by fully understanding the deformation physics governing the plasticity processes in nanostructured materials, we can produce materials with a combination of high strength and ductility (top right-hand corner of Figure 1.6).

Due to their extremely complex nature and ultrafine structural scale, the characterization of deformation physics of nanostructured materials requires a close integration of state-of-the-art experimentation with atomistic modeling. Three-dimensional molecular dynamic (MD) simulations with up to 100 million atoms can now be performed with realistic interatomic potentials based on the embedded-atom method (Zhou et al. 1998; Holian and Lomdahl 1998). This opens up possibilities for unprecedented direct comparison between theory and experiments that will greatly enhance our understanding of the fundamental physics of materials with strength close to the theoretical limits.

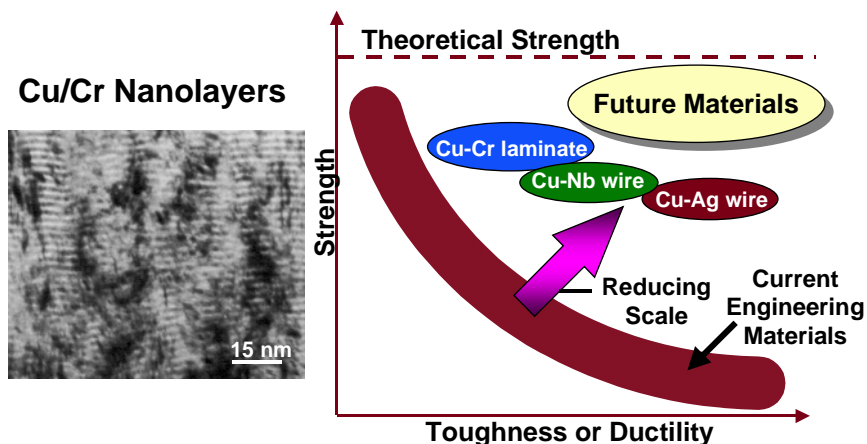


Figure 1.6. High resolution TEM image (left) of Cu/Cr nanolayers and diagram (right) of how reducing the scale of wire (materials) structure will affect the “toughness” and ductility of the materials. Nanostructured materials of the future will be able to transcend the limits of strength and ductility of current engineering materials.

1.7.7 Quantum Computing

Contact person: H. Everitt, U.S. Army Research Office

One of the primary justifications for investment in nanotechnology stems from the desire to continue “Moore’s law” which, in one form, states that the feature sizes of microelectronic devices shrink by half every four years. At this rate, feature sizes will be less than 10 nanometers by 2020 and atomic scale by 2035. In fact, Moore’s law will halt before then, about 2012, because of quantum mechanical effects that will prevent us from continuing to improve performance of logic devices simply by shrinking them. At that

point, new information processing methodologies will be required if we are to continue to advance our ability to compute.

Perhaps the most promising approach to getting beyond Moore's law is that of quantum computing. Originally proposed by Richard Feynman in the early 1980s, the idea is to take advantage of quantum mechanics, rather than be limited by it, to develop processors that simulate physical phenomena more naturally and exponentially faster than a digital computer can. Whereas a digital bit may only store information in the form of a sequence of "0s" and "1s," a quantum bit may be in a superposition state of "0" and "1," that is, representing both values simultaneously until a measurement is made. A sequence of N digital bits can represent a single number between 0 and $(2^N)-1$, while N quantum bits can represent all 2^N numbers simultaneously. A quantum computer with only 300 quantum bits can represent a system with $2^{300} \sim 10^{100}$ elements, a number greater than the number of atoms in the universe! A quantum computer could solve problems much more complex than a digital computer ever could.

Quantum algorithms have been developed to factor large numbers exponentially faster than digital computers could and to search N -element databases at a rate $N^{1/2}$ faster than a digital computer could. However, to date only simple quantum logic operations on a few, atom-based quantum bits have been demonstrated, and it is clear that this approach will not lead to large scale quantum computation. Nanotechnology may solve the problem of fabricating multiple quantum bits just as it brings us to the end of Moore's law. Arrays of semiconducting or superconducting quantum dots ("artificial atoms") are within reach of today's nanotechnology. Quantum dots can be used for quantum bits if (1) they are nanometer sized to exploit quantum mechanical effects, (2) identical to every other quantum dot in the array, and (3) isolated from the environment to preserve the quantum effects. Demonstrations of single quantum dot quantum bits may only be a few years away; if so, nanotechnology will provide the means to fabricate arrays of thousands of quantum bits, and the first large scale quantum computers may not be far behind.

It has been claimed that a classical computer could take as long as the age of the universe to factor a 200-digit number into its two prime cofactors. This is the basis of modern cryptography: the cofactor is the key; the 200-digit number is broadcast openly with the foreknowledge that the number won't be factored in time to be useful to an eavesdropper. It is possible that a quantum computer could factor that number in minutes, rendering today's most sophisticated cryptographic schemes vulnerable and obsolete.

1.7.8 Three-Dimensional Structures for New Circuitry

Contact person: M. Reed, Yale University

Figure 1.7 depicts a collection of nanoparticles about 5 nm in diameter (gold particles in gold and semiconductor particles in green) with attached functionalized endgroups (colored rods on particles) and buckyballs and nanotubes (black) on a substrate with gold electrodes. This is a rendition of a self-assembled molecular circuit produced by self-assembly of the molecules and the ~5 nm gold nanoparticles using a thiol (S) chemistry process in a beaker.

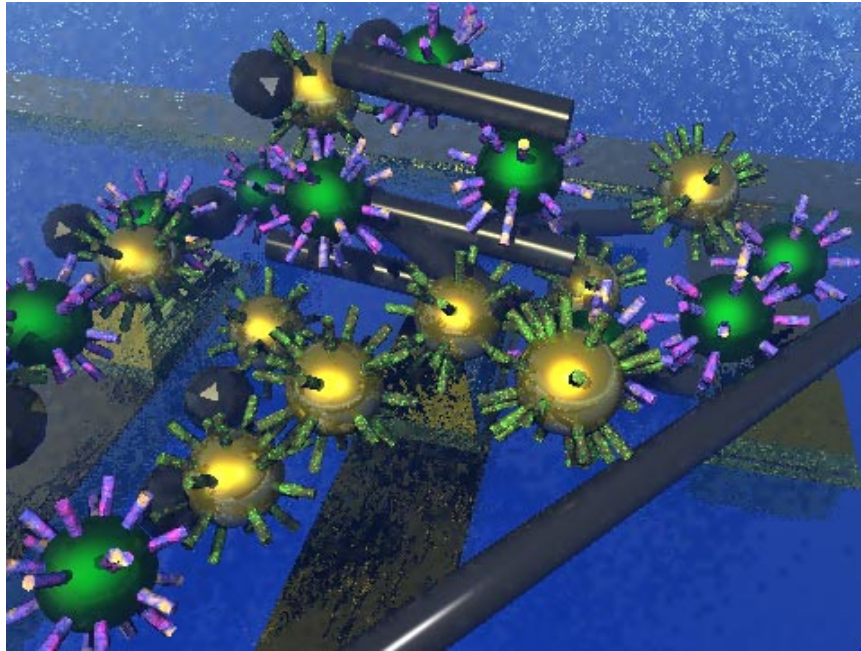


Figure 1.7. Collection of nanoparticles of about 5 nm dia. (©1999 Mark Reed. All rights reserved).

1.8 REFERENCES

- Dunin-Borkowski, R.E., M.R. McCartney, R.B. Frankel, D.A. Bazylinski, M. Posfai, and P.R. Buseck. 1998. Magnetic microstructure of magnetotactic bacteria by electron holography. *Science* 282:1868-1870.
- Han, K., J.D. Embury, J.R. Sims, L.J. Campbell, J-J. Schneider-Muntau, V.I. Pantsyrnyi, A. Shikov, A. Nikulin, and A. Vorobieva. 1999 (in press). The fabrication, properties and microstructures of Cu-Ag and Cu-Nb composite conductors. *Materials Sci. and Eng. A*.
- Holian, B.L. and P.S. Lomdahl. 1998. Plasticity induced by shock waves in nonequilibrium molecular dynamics simulations. *Science* 280:2085-2088.
- Misra, A., M. Verdier, Y.C. Lu, H. Kung, T.E. Mitchell, M. Nastasi, and J.D. Embury. 1998. Structure and mechanical properties of Cu-X (X = Nb, Cr, Ni) nanolayered composites. *Scripta Mater.* V 39:555-560.
- Stupp, S.I., V. LeBonheur, K. Walker, L. S. Li, K. E. Huggins, M. Keser, and A. Amstutz. 1997. Supramolecular materials: Self-organized nanostructures. *Science* 276:384.
- Zhou, S.J., D. Preston, P.S. Lomdahl, and D.M. Beazley. 1998. Large-scale molecular dynamics simulations of dislocation intersection in copper. *Science* 279:1525-1527.