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MOLECULAR MANUFACTURING DEVELOPMENT AND TECHNOLOGY PLANNING

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Abstract

Research and development of molecular manufacturing and related, enabling technologies is proceeding at an accelerating pace. The general capability to synthesize macroscopic objects and devices to atomic specification brings with it some surprising and important consequences, which are outlined in this presentation with an emphasis on aerospace applications. With order-of-magnitude performance improvements that are predicted for materials and devices, molecular manufacturing is now receiving attention at the highest level of government in the United States. Although determining the exact timing of the "assembler breakthrough" remains a speculative exercise, corporations can adopt strategies to avoid being blindsided by nanotechnology development. Industry can cooperate with governmental institutions, educational institutions, professional societies and standards organizations to (a) focus research priorities appropriately, (b) insure the adequate training of scientists, engineers, and technologists, (c) address public safety and environmental concerns, and (d) address national security concerns. Policy formulation will be an ongoing challenge, although new tools can improve the process of critical discussion and debate.

KEY WORDS: Molecular nanotechnology, molecular manufacturing, aerospace materials

1. Introduction

Molecular nanotechnology is an interdisciplinary field combining the scientific principles of molecular chemistry, molecular biology and physics with the engineering principles of mechanical design, structural analysis, computer science, electrical engineering, and systems engineering. Molecular manufacturing is a method for the processing and rearrangement of atoms to fabricate custom products. It would rely on the use of a large number of molecular electro-mechanical subsystems working in parallel. Built to atomic specification, the products of this technology would exhibit order-of-magnitude improvements in strength, toughness, speed, and efficiency, and be of high quality and low cost. **Section 2: Technical Issues** provides an overview of molecular nanotechnology and explores ways in which molecular manufacturing

could be applied to improve aerospace materials. **Section 3: Business Strategy, Education, and Policy Issues** reviews the origins of the field, the current state-of-the-art, forces affecting its development and progress, and the implications of its eventual emergence as the dominant manufacturing technique of the 21st century.

2. Technical Issues

This section provides basic definitions of relevant terms, and draws what hopefully are useful distinctions between molecular nanotechnology and similar areas of study. A brief discussion of biological examples of molecular machines leads to a general discussion on the design of molecular devices. Existing designs represent a set of devices that could comprise a system to build objects to complex atomic specifications. With this capability, one product will be materials 10-100 times stronger and tougher than we have today on a commercial basis. Molecular nanotechnology will also enable a very fine-grained integration of computers and sensors with materials.

Definition of Terms

Molecular nanotechnology is defined as:

Thorough, three-dimensional structural control of materials and devices at the molecular level; the products and processes of molecular manufacturing.

It is useful to clarify the definition of the technology by drawing distinctions between it and some related fields. Molecular nanotechnology is distinguished from solution chemistry by the manner in which the chemical reactions will occur: instead of the statistical process of molecules bumping together in random orientations and directions in solution until a reaction occurs, discrete molecules are brought together in individually controlled orientations and trajectories to cause a reaction to occur at a specific site. Furthermore, this is performed under programmable control.

In biological systems ribosomes build proteins by "grabbing" onto tRNA molecules and transferring their amino acids to a growing polypeptide chain, under the programming specified by mRNA from its DNA template. Unlike biological systems, molecular manufacturing systems:

- (1) could transport raw materials and intermediate products more rapidly and accurately with conveyor belts and robotic arms,
- (2) would control *all* trajectories and orientations of *all* devices in the system, not just the relative orientations at points where reactions occur (ribosomes, tRNA, mRNA, amino acids, and DNA are suspended freely in the cell environment and rely on random collisions for reaction site alignment and diffusion for the transport of raw materials and products),
- (3) would make heavy use of positional assembly (such as a blind robot thrusting a pin into the expected location of a hole) as opposed to matching assembly (a tRNA molecule bumping around a ribosome until it fits into the slot with the

- matching pattern of hills and valleys and positive and negative charges on its surface), and
- (4) would, like auto factories and textile mills, lack the ability to independently evolve (a mutation in a molecular nanomachine would simply render it inoperable).

Microtechnology is also quite different: nanolithography is the patterning and selective etching of bulk material (usually silicon) to create devices with features as small as a few nanometers at their narrowest point. Micromachines such as electrostatic motors and steam engines have been fashioned in this way and we refer to this as a "top-down" manufacturing approach. These devices are inherently limited by the defects present in the original bulk material. Molecular manufacturing, by contrast, is "bottom-up"—building structures by piecing together (essentially defect-free) atoms and molecules.

The term *assembler breakthrough* refers to the point in time when assembler technology is sufficiently advanced for the systems to make copies of themselves.

Synthesis of exact structures would be performed in an environment where no unwanted side reactions could occur and with no contaminants present. The term *machine-phase* has been coined to draw a distinction between this type of environment and solid-, liquid-, and gas-phase systems [1]:

- A machine-phase system is one in which all atoms follow controlled trajectories (within a range determined in part by thermal excitation).
- Machine-phase chemistry describes the chemical behavior of machine-phase systems, in which all potentially reactive moieties follow controlled trajectories.
- Machine-phase conditions can be described as eutactic: Characterized by precise molecular order, like that of a perfect crystal, the interior of a protein molecule, or a machine-phase system; contrasted to the disorder of bulk materials, solution environments, or biological structures on a cellular scale.

Designing Molecular Machines and Devices

The ribosome example shows that specialized molecular mechanical devices work in biological systems. But this system is of little use in the envisioned implementation of molecular nanotechnology. A more general kind of assembler could be used to make different kinds of structures with a wider range of capabilities. One can start by noting that it is more difficult to design mechanical systems with the irregular shapes characteristic of many proteins, and what we would like instead are things that look more like simple, conventional mechanical parts that we can use to build more complex subsystems like robot arms and conveyor transports. As shown in Table 1, biological systems are not devoid of structures with these more traditional mechanical shapes and functionalities.

Since the publication of *Nanosystems* in 1992 [1] and subsequent work, there is now a small library of designs of molecular mechanical parts that can be employed to create an assembler system with general capabilities for the mechanosynthesis of a wide range of materials and

devices. Space and copyright considerations prevent the inclusion of illustrations of these devices in this paper, but many are available on the Internet [4-6]. They include structural components such as tubes, rods, strained shells, and brackets. These *diamondoid* parts (based on the atomic structure of diamond) can serve as stiff, passive members of housings and frameworks to constrain moving parts, or they can serve as moving parts themselves. Substitution of atoms such as O, N, and Si for C results in enormous numbers of possible stable conformations for different desired shapes.

Table 1. A comparison of macroscale and biomolecular components and functions (from reference [2]).

Device	Function	Molecular example (s)
Struts, beams, casings	Transmit force, hold positions	Microtubules, cellulose
Cables	Transmit tension	Collagen
Fasteners, glue	Connect parts	Intermolecular forces
Solenoids, actuators	Move things	Conformation-changing proteins, actin/myosin
Motors	Turn shafts	Flagellar motor
Drive shafts	Transmit torque	Bacterial flagella
Bearings	Support moving parts	Sigma bonds
Containers	Hold fluids	Vesicles
Pumps	Move fluids	Flagella, membrane proteins
Conveyor belts	Move components	RNA moved by fixed ribosome (partial analogue)
Clamps	Hold workpieces	Enzymatic binding sites
Tools	Modify workpieces	Metallic complexes, functional groups
Production lines	Construct devices	Enzyme systems, ribosomes
Numerical control systems	Store and read programs	Genetic system

Moving parts have also been either designed or outlined to some reasonable degree; these include sleeve bearings, nuts and screws, rods in sleeves, constant force springs, axle bearings, spur gears, helical gears, rack-and-pinion gears, roller bearings, bevel gears, worm gears, belt-and-roller systems, cams, planetary gear systems, dampers, detents, clutches, and ratchets. For example, an analysis of molecular sleeve bearings has shown that energy barriers to rotation can be so small as to be virtually frictionless, even when the bearing is heavily loaded perpendicular to the axis.

A similar analysis for molecular gears showed that energy barriers to gear tooth slippage are large (>500 maJ) with moderate numbers of teeth (more than 20), while energy barriers to corotation are small (<0.01 maJ). These gears are projected to be highly efficient at transmitting power. For a gear system operating at a shear force of 1nN, phonon scattering and thermoelastic

drag losses are estimated to account for only three thousandths of a percent of the transmitted power.

Subsystems of intermediate complexities have been either designed or outlined with supporting calculations. These include:

- Mechanical measurement devices
- Stiff, high gear ratio mechanisms such as harmonic drives and toroidal worm drives
- Seals and pumps for fluid transport
- Vacuum systems to remove contaminants
- Cooling systems with fractal plumbing
- Electromechanical transducers and actuators
- Electrostatic nanomotors

Electrostatic nanomotors could be used to drive molecular conveyor belts for material transport and to turn worm drives as part of robotic positioning arms (useful for positional synthesis). Calculations [1] show that a motor with a radius of 195 nm and an applied voltage of 10 V, the angular frequency would be about 5×10^9 radians per second and the rim speed 1000 m/s. The power density is high: 10^{15} watts/m³, limiting the number of motors in a given volume due to cooling constraints. Bearing drag is estimated to be small, ~1.3 pW, but the sliding tunneling contact may exert a drag associated with electron transfer that could dominate the power losses in the motor.

Nanomechanical Computational Systems. Molecular mechanical computational devices have been designed by Drexler [1]. Carbyne rods in tension could be used to transmit signals by moving back and forth axially, and molecular groups (based on a pyridazine ring) attached to the rods could serve as gates and probes. Depending on the gate's position, it could either block or allow the probe knob to pass by. In this type of arrangement the logic gate is the equivalent of a transistor. Estimates of the performance of a RISC (reduced instruction set computing) machine based on rod logic yield the following:

- Switching times are on the order of 0.1 ns
- The energy dissipation is $\ll kT_{300}$
- Combinational logic systems can achieve four register to register transfers in 1.2 ns
- Nanomechanical RISC machines can achieve clock speeds of ~1 GHz, executing instructions at ~1000 MIPS
- A CPU-scale system containing 10^6 transistor-like interlocks could fit within a 400 nm cube; at 1 GHz it would dissipate 60 nW, performing $>10^{16}$ instructions per second per watt
- A forced convection system with fractal plumbing could effectively remove about 100 kW from a one centimeter cube at 273 K. This would allow $\sim 10^{12}$ CPU scale systems with 10^6 transistors each to operate within that volume.

This 10^{12} CPU system would run at about 10^{15} MIPS. By comparison, personal computers run at about 100 MIPS, supercomputers run at about 10^6 MIPS, and the human brain runs at about 10^9 MIPS. So one of these molecular computational systems would have the computational

equivalent of a million human brains in the volume of a cubic centimeter (in terms of logic operations per second—programming is another matter). Fast molecular tape memory similar to RNA is also possible. It would have a storage density on the order of 5×10^{21} bits per cubic centimeter. That is sufficient density to store the information content of the Library of Congress within the dimensions of a sheet of office paper.

Molecular Sorting, Processing, and Assembly. To build parts to atomic specification it will be necessary to have a high level of control over the transport and positioning of molecular building blocks. One possible scheme has reagent moieties transported up through the center of a hollow manipulator arm to a working tip for positional synthesis. One such device has been designed to a moderate level of detail [5]. The arm's design stiffness of 25N/m helps to hold positional errors to below one in 10^{15} . Applying 1 nN of force at the tip would deflect the arm only 0.04 nm.

Parts could be made more rapidly (but less flexibly) with molecular mills, which are well suited to making standard components at high rates. For example, one device might be designed to attach one hydrogen atom to a specific position on the surface of molecular bearings as they move by on a conveyor belt. Mills of this sort could be employed to make blocks of systems up to $1\mu\text{m}$, at which point manipulators could fabricate larger components using these blocks. (Manipulators could also be used to fabricate items of smaller sizes, more flexibly though less rapidly than mills.) By convergent assembly, these many smaller parts could be assembled to form fewer larger parts. A 1 kg structure would contain about 10^{15} blocks made from about 10^6 separate systems.

A desktop manufacturing system could use a cheap fuel such as acetone (about 10¢/kg), weigh about one kilogram, produce high purity products at a rate of 1 kg/hr, have a waste product of high purity water, and generate excess power along with waste heat (from release of energy from feedstock molecules).

Theoretical Properties of Materials

The materials we make are fraught with defects on several scales:

- at the intramolecular or intragranular level, where an atom in a molecule or grain may be missing, out of place, or may be substituted with the wrong kind of atom
- at the intermolecular (or intergranular) level, where molecules (or grains) that could be favorably matched (aligned) with their neighbors, aren't; and where contaminant atoms, molecules, or films can poison the intergranular boundaries
- at the microscale where large clusters of molecules (such as fibers) or individual grains may be unsuitably sized or aligned; and where microtears, pits, fissures, and cracks can degrade material performance
- at the macroscale where we have visible flaws

These defects exact a major toll on materials properties and performance. Calculations of the theoretical properties of perfect crystals (and experimental verification) show that if metal and

ceramic parts could be made from pure, perfect crystals, their strength would be between 10 and 50 times that of the strongest form of the same material made using today's routine commercial practices. This is illustrated in Figure 1. Use of novel, highly alloyed, and composite 'perfect' materials would push that factor over 100 times the strength of today's commercial materials. Theoretical elastic strains are also very high—on the order of 10%.

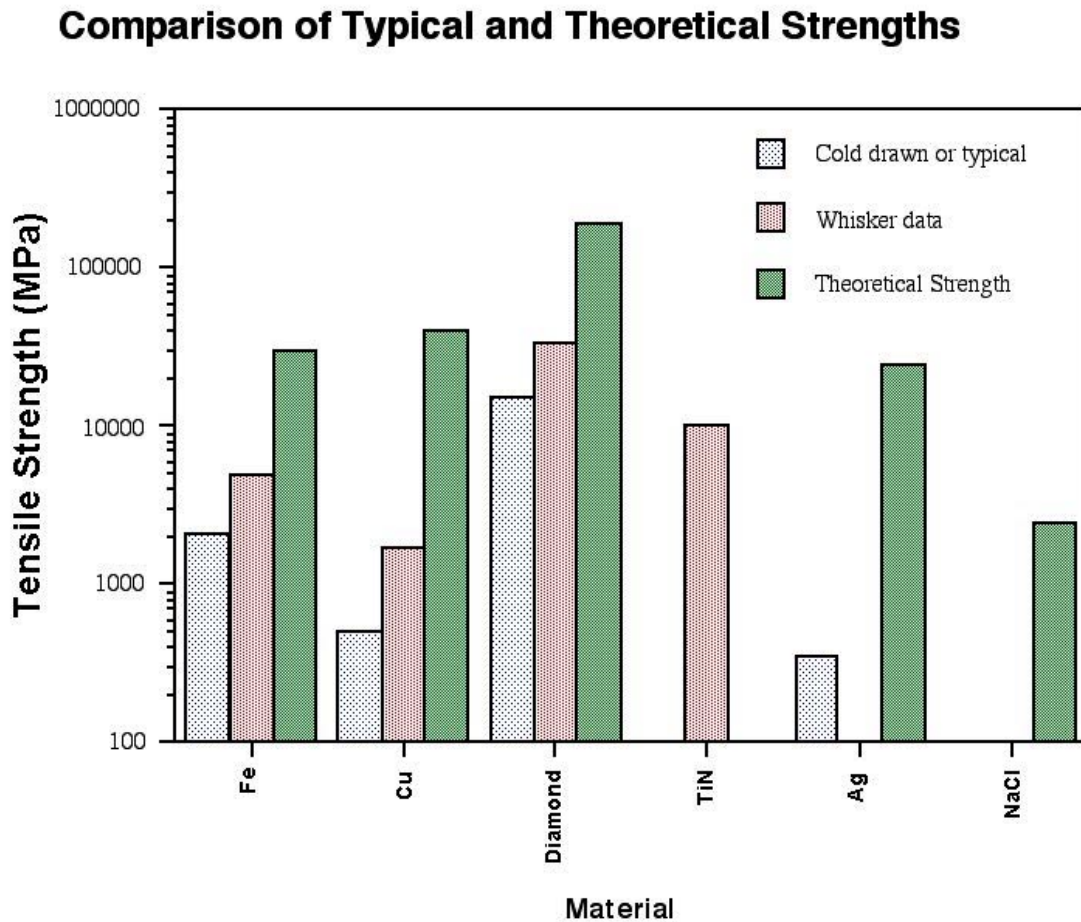


Figure 1. If materials could be made pure and atomically perfect, they would be 10-50 times stronger than today's strongest (though most brittle) form of the same substance. Suitable alloying of the atomically perfect material would increase that differential by more than 2X.

Other properties would also benefit from molecular nanotechnology. For example, there are reports of exceptional corrosion resistance when iron is purified to 99.995%; that material is also reportedly ductile down to 4.2K [7]. Greater improvements can be expected with the elimination of defects as sites for corrosion attack, and with surfaces constructed to atomic smoothness and appropriately terminated to inhibit chemical reactions. The use of oxides and intermetallics could be greatly expanded in oxidation- and corrosion-resistant applications without the current problems of embrittling impurities, defect structures, and grain boundaries.

Although no material or device of macroscopic dimensions can be made indefinitely defect-free (because of the damaging effects of pervasive high energy background cosmic radiation),

molecular nanotechnology will provide us with the capability to produce bulk solids to as near perfection as our environment will allow. No existing process can make this same claim.

Applications of nanotechnology to aerospace materials

Clearly, there would be significant advantages to having materials that are 100 times stronger than we have now. Objects made from these materials could be up to 100 times lighter, using 100 times less of the same substance. By substituting diamondoid composite material this factor could be increased to about 250. As a result, ultralight cars, trucks, trains, aircraft, and spacecraft would use far less energy, especially with atomically smooth surfaces to reduce internal friction and air resistance losses.

Space transportation costs could be reduced considerably with the products of nanotechnology. Comparing structural components made from titanium versus a diamondoid composite material, McKendree [8] estimated that single stage to orbit transportation costs would drop (in one scenario) from \$16,000/kg to \$3.54/kg. Substituting diamondoid materials for aluminum, Drexler [9] estimated that a vehicle with a gross lift-off mass of only ~3000 kg could deliver a 500 kg payload (four people with luggage) to orbit. The dry, empty mass of the vehicle would be only ~60 kg. Though the cost per flight savings would not be quite as dramatic with commercial and military aircraft, it would still be considerable.

For high temperature engine components that use superalloys for creep and oxidation resistance, density could be reduced and strength greatly increased by substituting (for example) atomically perfect alumina (or a toughened composite) for Haynes 188. At 1200°C, the theoretical strength to density ratio of atomically perfect alumina is estimated to be 1.3 MPa·m³/kg, or about 150 times that of Haynes 188 (a common material for this application). The oxidation resistance of alumina would obviously be far superior to the cobalt-base material, and the creep resistance should also be significantly better.

Friction effects that increase aerodynamic drag and reduce engine efficiency can be modified with the use of atomically smooth surfaces. Laminar flow control (LFC), which would lead to efficiency improvements on the order of 10%, has been demonstrated to work when leading surfaces are highly polished, but there has been no practical method to maintain the polish under normal operating conditions. Active surface solutions to LFC can also work, but are not tolerant of minor surface damage and dirt encountered in typical operating environments. Atomically smooth diamondoid coatings that are fully terminated (saturated) with fluorine would be relatively immune to environmental contamination.

An intriguing idea is that of an active, programmable material [10]. The concept is to have a material made of small cellular units that connect to each other with screw-type mechanisms. Computers would direct the cells, powered with small electrostatic motors, to adjust their relative spacing with the screws. By selecting which screws would tighten and which would loosen, the shape of a item could change to conform to the needs of the user. J. S. Hall has provided some striking illustrations of this concept [11]. In aerospace systems, one application would be to dynamically adjust the shape of a wing at either the macroscopic or microscopic level to improve aircraft performance by adjusting for turbulence.

The usage pattern of transportation systems is likely to change dramatically. With desktop manufacturing employing locally available materials to create complex objects, there will be little need to transport raw materials, intermediate materials, or finished products back and forth across the planet. Instead, the information (software) necessary to create a new product could be downloaded from the Internet (purchased, for commercial products) to the desktop manufacturing system. The product would then be made on site (e.g., at home) using simple hydrocarbons and other feedstock. Most of the commercial transportation that we now use would then become unnecessary. Increased personal travel could conceivably replace much of the displaced commercial transportation component, though the demographics would be different (e.g., fewer trucks).

Conclusions for this section

- (1) Engineering calculations based on proven molecular modeling techniques show us that molecular mechanical systems can be designed with general capabilities to manipulate individual molecules and build materials and devices to atomic specification.
- (2) Biological examples show us that molecular mechanical systems work in practice, with high levels of reliability.
- (3) Calculations of theoretical properties and measurements of near-perfect whiskers show us that, with the capabilities of molecular nanotechnology, we can expect materials that are at least 10-50 times stronger than today's commercial products.
- (4) Molecular nanotechnology will enable a very fine-grained integration of computers and sensors with materials (intelligent materials systems). The additional integration of electromechanical devices will blur the distinction between materials and machines. Materials will be viewed as active systems with programmable shapes and properties.

3. Business Strategy, Education, and Policy Issues

Strategic Planning

A key property of a molecular manufacturing system is that such a system would be capable of making a copy of itself—down to virtually every atom. Reprogramming of the copy, via a "hardware compiler," would then allow the production of other objects using locally available materials. Thus, it will be possible to replicate inexpensive desktop factories for the production of most products to atomic specification. Once developed, we anticipate that these systems would become dispersed to individuals on a global basis in short order.¹ This represents a substantial change from existing manufacturing systems that rely on widely dispersed and highly specialized conversion steps from raw materials into finished products. Outside of information technologies, there are few if any business models for the production of finished goods directly from raw materials.

¹ Economist David Freedman expects that an assembler system providing basic necessities would be available free to all, while a system with more capabilities could be purchased.

Because businesses can be affected in so many different ways, and different companies have a wide variety of strengths and business objectives, strategic planning for the emergence of molecular nanotechnology is best approached on an individualized basis. That said, there are some general strategies that make sense:

1. *Corporate awareness.* A company should have a specific program in place to track developments in molecular nanotechnology. This can be accomplished through internal resources, or outsourced, or a combination of the two—but however this is done it is important to have good filters in place. There is so much similar-sounding information on various flavors of nanotechnology that it is not always clear what is a likely path to the technology described in this paper and what is merely tangential. Interpreting how this information could pertain to a company beyond the assembler breakthrough is a speculative, though not necessarily hopeless endeavor. Good places to start are with the Foresight Institute (www.foresight.org) and the Institute for Molecular Manufacturing (www.imm.org).
2. *Intellectual property.* Depending on the nature of one's business it might make sense to review both existing patents and patent work-in-progress from a post-assembler breakthrough perspective. Decisions on how to proceed with ongoing work are likely to be influenced by perceptions on how close we are to the assembler breakthrough. Those process technology patents not based on assembler systems will become worthless beyond that point. We cannot overemphasize how sharp the transition to assembler-based manufacturing could be. Patents on certain materials could retain value, but unexpected combinatorial possibilities enabled by molecular manufacturing could also circumvent the design space defined by a patent.
3. *Service economy.* In some cases, transitioning from a manufacturing-oriented business to a service-oriented model could help a company defend itself from post-assembler-breakthrough obsolescence.
4. *New research.* Initiating research to develop molecular nanotechnology is the most direct approach to try to ensure that a company survives, and is probably more likely to succeed than defensive ploys. If the Zyvex (www.zyvex.com) business model turns out to be correct, a large and expensive effort is not necessary if the right combination of intellectual talent can be assembled.

For completeness, the *doomsday strategy*—suggested to the author by one company's president—bears mentioning. It goes something like, 'Our business could never transition to assembler-based manufacturing, so we will ignore it until it takes over. Then we fold our business.' The investment community will likely take ample care of this sort of company long before the assembler breakthrough comes along.

Education, Regulatory, and Policy Issues

There are reasons to be concerned about this technology and although we advocate increased involvement by the materials community, we only do so with the caveat that any development must be performed in a responsible manner—subject to guidelines, consensus standards, and any appropriate laws. The ability to control the structure of matter with such thoroughness is a responsibility not to be taken lightly.

Considering that the concept of molecular manufacturing has been in the open literature since 1981 and in TMS and ASM publications since early 1990 [12-15], it is curious that no materials society has developed a formal position on the implications of constructing macroscopic products to atomic specification. Now that the importance of this field has been brought to the forefront in the U.S. with the National Nanotechnology Initiative [16] we need to put molecular manufacturing on the materials policy agendas of our technical societies. Suggested initiatives are:

- Evaluate the relative value of molecular manufacturing research along with other initiatives and recommend priorities to our government
- Help define the role of materials engineers and scientists in developing molecular manufacturing systems
- With other technical societies, develop guidelines for safe systems and participate in policy development. The Foresight Institute has already issued an initial set of guidelines for consideration [17]. A regulatory framework has been proposed, but needs to be critiqued with a diversity of viewpoints [18]. A new online tool known as <http://crit.org> can be used to improve the process of critical discussion and debate.
- Work with other technical societies to encourage interdisciplinary collaboratives
- Collaborate and participate with the Foresight Institute in their annual conference on Molecular Nanotechnology
- Outline materials science and engineering curricula to enable students to effectively contribute to the development of molecular manufacturing
 - For those who don't yet see molecular manufacturing as inevitable, this sort of training is not inconsistent with what we should be teaching anyway as it would stress fundamentals like materials design at atomic and meso scales, computational materials science, and chemical bonding and potential surfaces
 - We must not forget to foster an understanding of the consequences and maintain a perspective on the social aspects of the technology

Conclusions for this section

- (1) The nature of our economy will be radically transformed with assembler-based manufacturing. Businesses can adopt strategies to prepare for the coming changes, although specific tactics depend on the nature of the business, its goals, and its strengths.
- (2) A technology that provides atomically fine-grain control over the structure of large quantities of matter has important implications for computer science, energy, the environment, medicine, and national security. With the National Nanotechnology Initiative being established, now is an excellent time for materials societies to take a

leadership role in the development of molecular manufacturing through interdisciplinary collaborations, policy formulation, and educational initiatives.

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Biography

Dr. Forrest is a consultant in advanced materials technology with Baverstam Associates, with over 15 years of metallurgical experience in plant operation and research positions in the steel industry. His doctoral research at the Massachusetts Institute of Technology involved the physical and mathematical modeling of electromagnetically driven fluid flow. Dr. Forrest has been active in the emerging field of molecular nanotechnology since 1985. He has prepared technology assessments in this area for Digital Equipment Corp. and Allegheny Ludlum, and has actively promoted interest in molecular manufacturing within the materials community. In 1995 he was appointed Acting President of the Institute for Molecular Manufacturing, a non-profit organization dedicated to advancing the development of molecular nanotechnology by directly funding critical research.