Advisory Technical Awareness Council
The Advisory Technical Awareness Council will advise and alert the Board of Trustees and ASM membership by: identifying global trends and developments in materials, including technology, commerce, government, societal perceptions, and education; assessing for the society the impact of these trends on the welfare of ASM membership; and recommending the initiation of projects and tasks addressing the above.

ATAC White Paper
4 Jan 2005

Molecular Manufacturing Will Change Materials Technology

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Molecular manufacturing is a technology that is being developed to build large objects atom-by-atom, quickly and cheaply, with virtually no defects. Molecular machines are being built now, and molecular manufacturing is projected to mature with the next ten years. This white paper provides a brief background on this technology, summarizes recent key advances, provides an estimated timeframe for emergence based on quantitative trendlines, and outlines implications for ASM International's membership.

Background

Although the term "nanotechnology" is now used to describe a broad and diverse range of technological areas, it was originally used to describe a novel method of manufacturing first articulated by Richard Feynman: that molecular machines should be able to build substances by mechanically placing each atom into position exactly as specified [1]. More recently, Eric Drexler, Ralph Merkle, Robert Freitas, and others have provided a compelling vision of how massively parallel arrays of molecular assemblers could build large, atomically precise objects cheaply and quickly [2-6]. The envisioned products of these molecular manufacturing systems include [6]:

- powerful desktop computers with a billion processors
- abundant energy with inexpensive, efficient solar energy systems
- cures for serious diseases using nanorobots smaller than cells
- new materials 100 times stronger than steel
- a clean environment with nanomachines to scavenge pollutants
- more molecular manufacturing systems (they could build copies of themselves)

Since 1986 this vision of molecular nanotechnology has captured the public's imagination and is now an integral part of popular culture. References to these sorts of nanomachines are standard fare in many well-known science fiction books, movies, and television shows. Encyclopedias and children's books feature colorful and atomically-accurate designs of molecular gears and bearings, as well as artist's renditions of (often fanciful) nanomedical devices cleaning a blocked artery or killing a virus. Today's generation is fully expecting some form of this vision to be realized in their lifetime.

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By contrast, the scientific community has been less than embracing of these ideas. The most vocal critics claim that this technology is either so distant in the future that we need not concern ourselves, or fundamentally impossible and will never happen. The engineering community has been for the most part silent about the controversy, which is a significant omission[2] because the proposed technology has very little to do with new science and everything to do with engineering analysis, design, and construction.

This assessment focuses on specific advances that demonstrate quantifiable progress toward the development of molecular manufacturing systems:

- The process of robotically positioned molecular assembly is possible, because it was demonstrated in 1999.
- Non-biological molecular machines are possible, because they have been built and tested.
- Molecular gears and bearings are feasible, because models based on molecular dynamics and molecular mechanics show they will work.

Molecular machines can be fashioned from known structures using available technologies. Figure 1 illustrates how current advances in molecular technologies provide the foundation for positional molecular assembler machines: structural members, sliding and rotating parts, motors, and positioning and joining technology. Carbon nanotubes, which have been commercially available for several years, can serve as strong, stiff, structural members. They can be joined together using electron beams. Individual molecules can be positioned and joined to structures with a scanning tunneling microscope. Nested carbon nanotubes can serve as both cylindrical bearings and telescoping arms. An electrostatic nanomotor has also been synthesized and tested. Crude, less capable assemblers, coupled with continuing advances to make molecular mechanical parts, will lead to more highly advanced molecular assembler systems with broader capabilities.

[2] It also represents an opportunity for engineering societies such as ASM to fill the vacuum in the molecular manufacturing knowledge base.

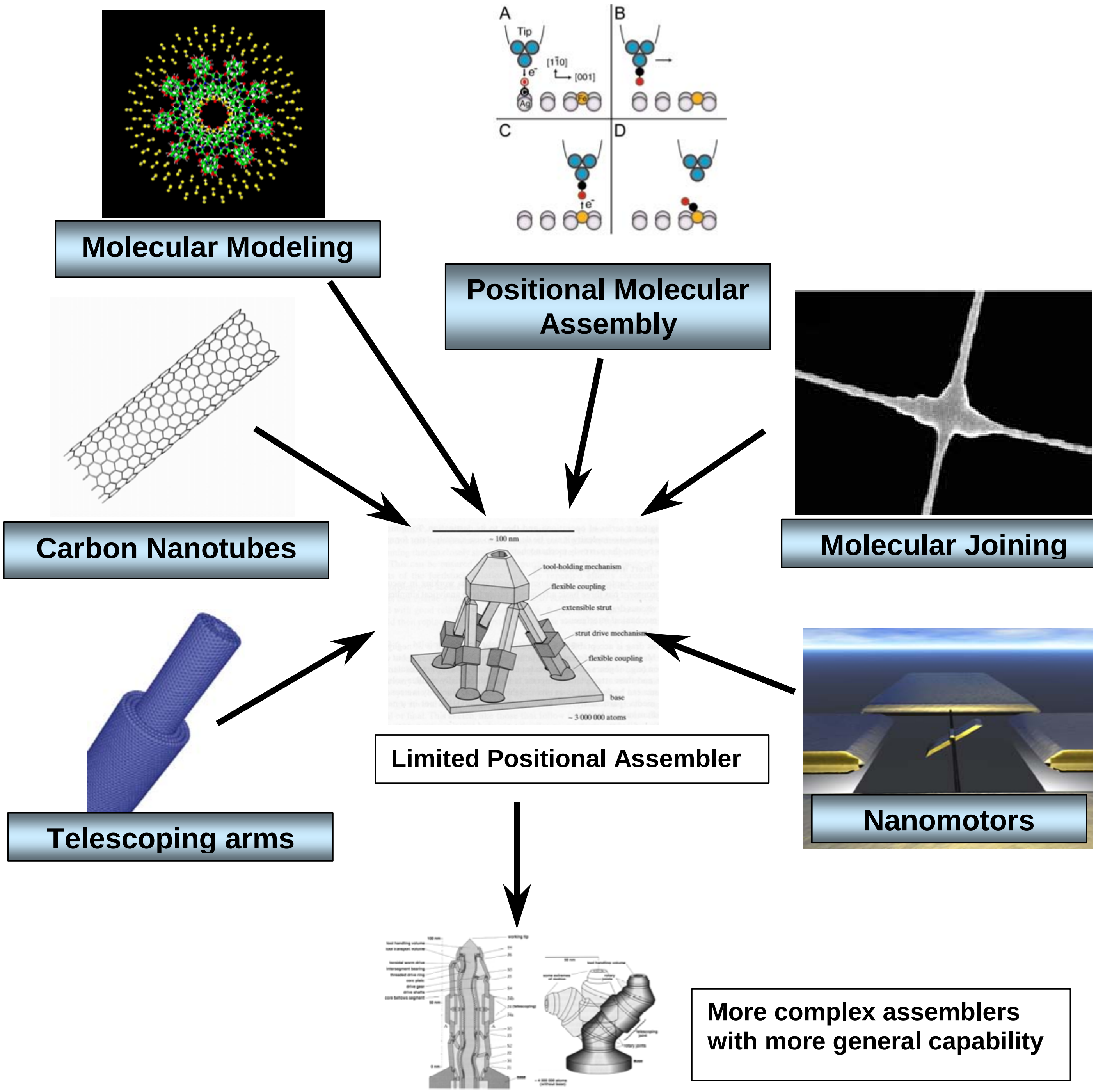
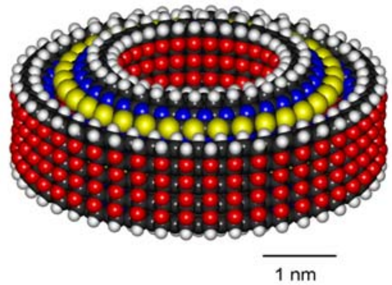
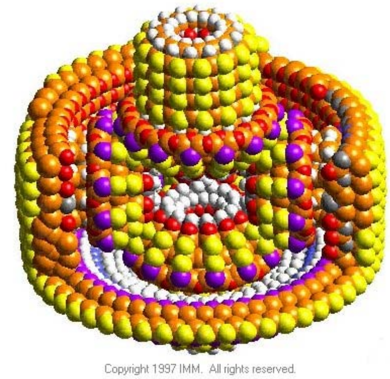
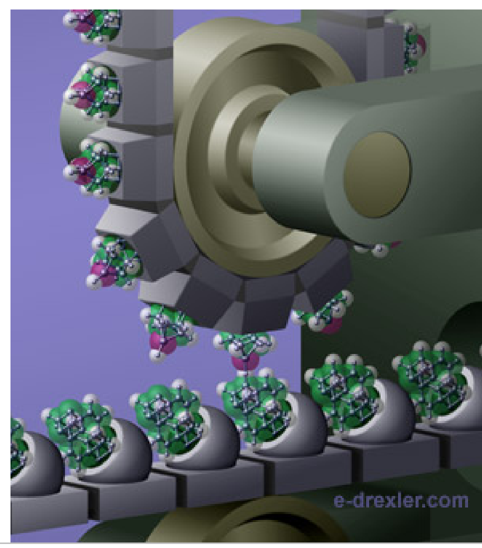
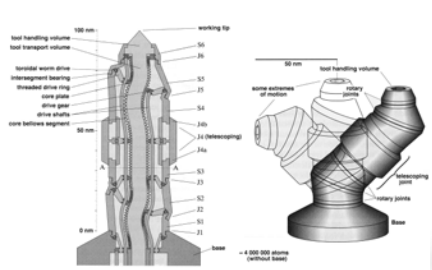
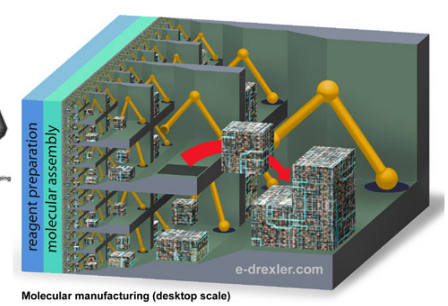


Figure 1. An illustration of the technological advances that are leading to the development of molecular robotic positioning and assembly systems.

A few of the key concepts are summarized in the sidebar "Molecular Manufacturing Concepts." The first set of illustrations shows a cylindrical bearing and a differential gear. The design and performance of these mechanical parts have been studied in detail, and show that high efficiencies are possible when complementary atomic surfaces are properly matched. The second illustration shows a schematic of a conveyor transport system and the transfer of hydrogen atoms from molecular feedstock onto parts being assembled.

Molecular Manufacturing Concepts	
Electromechanical systems will be constructed at the molecular scale, including: support structures, rods, shafts, gears, bearings, conveyors, nanomotors, and manipulators. With proper design and built to atomic specification and precision, sliding surfaces would have low friction and gears and nanomotors would have high power conversion efficiency. A molecular sleeve bearing is shown on the left, and a cutaway view of a molecular differential gear is shown on the right. The designs employ C, H, O, S and N atoms; energy minimizations were performed using molecular mechanics software to calculate the atomic positions. *Sources: K. E. Drexler and the Institute for Molecular Manufacturing.*	 
Molecular mills could be employed to facilitate rapid assembly. In this illustration, hydrogen atoms (white) are being transferred from molecules on the upper conveyor belt (partial atomic detail) to molecules on the lower conveyor belt as they move from left to right. *Source: K. E. Drexler, www.e-drexler.com*	
At the nanoscale, megahertz rates of atomic placement are typical: estimates of system performance show that a four million atom manipulator arm (left) could make a copy of itself in less than 10 seconds. A convergent assembly system employing similar arms (right) would house successive assembly stations to build up parts from basic components (left side) to more complex modular assemblies (center) to finished products. *Sources: K. E. Drexler, Nanosystems [5] and www.e-drexler.com.*	 

An exemplar 1 kg desktop assembler would produce atomically exact products at a rate of 1 kg/hr, would have a waste product of 1.5 kg/hr of high purity water, and generate 3.6 kW/hr excess power along with 1.1 kW/hr of waste heat (from the release of energy from breaking bonds of inexpensive feedstock molecules). As in biological systems, the property of self-replication is necessary to create a large number of machines (that can grow in number at an exponential rate) in order to process kilogram to kiloton quantities of material in useful timescales. One product of the desktop assembler would be a copy of itself. *Source: K. Eric Drexler (www.e-drexler.com)*

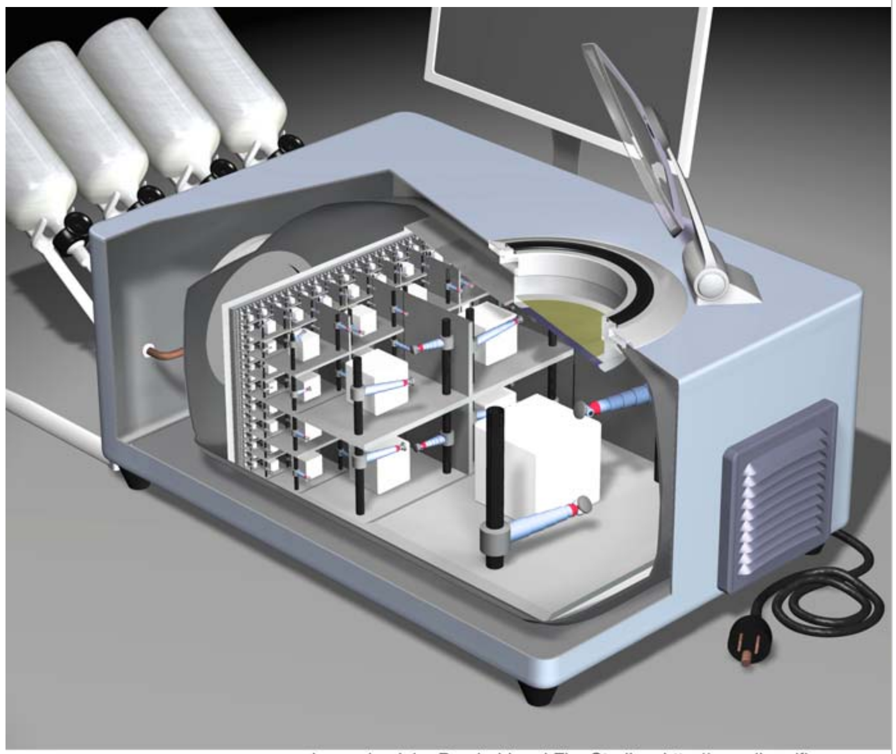


Image by John Burch, Lizard Fire Studios, http://www.lizardfire.com

Proposed desktop-scale molecular manufacturing appliance. Tiny machines join molecules, then larger and larger parts, in a convergent assembly process that makes products such as computers with a billion processors. (Parts shown as white cubes.)

The third set shows a schematic of a stiff robotic arm composed of about four million atoms (left), and an illustration of the concept of convergent assembly (right). Simple hydrocarbon molecules are fed to the tip of the arm through an internal conveyor system; atoms are transferred from those molecules to the workpiece at processing speeds approaching 500,000 atoms/second—about the rate that a fast enzyme processes molecules in biological manufacturing systems. The diagram to the right of the arm illustrates convergent assembly: small assembly stations feed products into successively larger sub-assemblies. The fourth illustration shows a rendition of a desktop molecular manufacturing system. Simple hydrocarbon molecules are fed into the system from the tanks at the left, sorted and purified, attached to conveyors, positioned, and then reacted to build up atomically exact structures.

State of the Art

In the twelve years since the last ATAC white paper was written on this topic [7] there have been significant theoretical and experimental advances in molecular technologies that are enabling the development of the molecular manufacturing concepts shown above. Here, we focus on key experimental advances, which are summarized in Tables 1-3.

Table 1. Molecular Construction

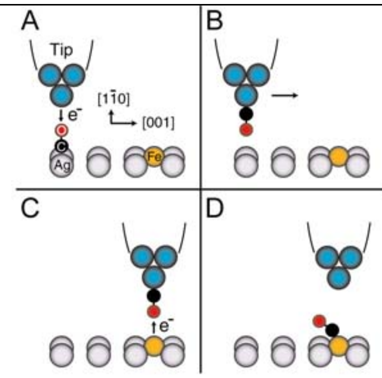
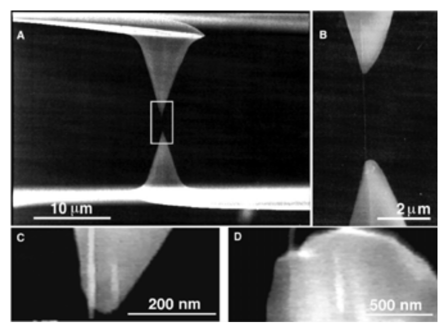
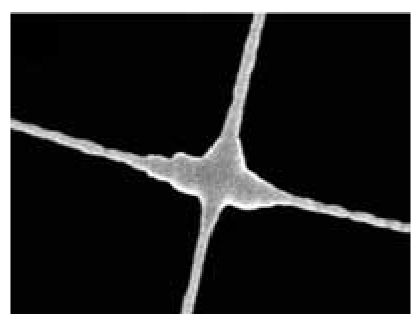
1999	**Positioning and assembly**. Ho and Lee (Cornell U.) used a scanning tunneling microscope to pick up a single carbon monoxide molecule and chemically bind it to a single iron atom by applying a voltage [8] (see picture, right). This proved the concept of positional assembly using a non-biological robotic system.	
1999	**Parts from DNA**. Seeman (NYU) developed a nanomechanical switch that built upon earlier work with DNA as both a functional and structural material.	
2000	**Mechanical testing**. Ruoff's group (Northwestern U.) used an electron beam to attach individual nanotubes to cantilevers, then measured their tensile strength (up to 63 GPa) [9].	
2001	**Welding**. Banhart's group (U. of Ulm, Germany) used an electron beam to attach individual nanotubes to each other [10].	

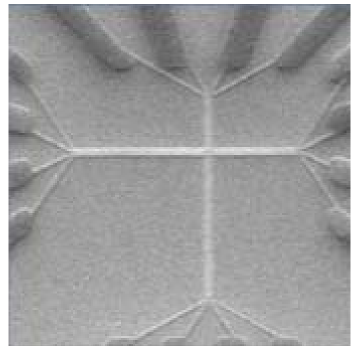
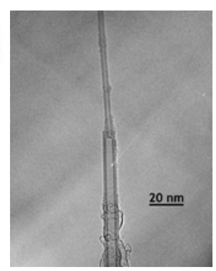
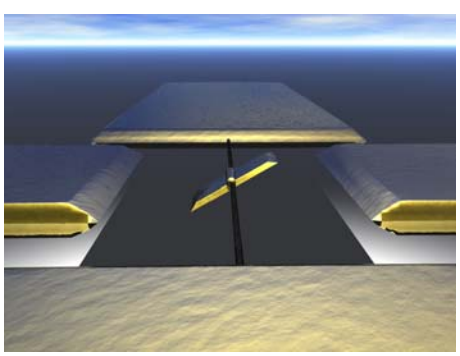
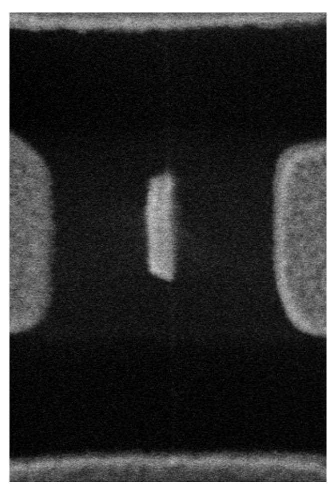
Table 2. Molecular Computers		
1996	The first conductivity measurements of single molecules using an STM [11].	
1997	• The first measurement of electronic conduction in a single molecular wire [12]. • The electrical conductivity of carbon nanotubes was demonstrated. • The first molecular diodes were synthesized [13, 14].	
1998	Carbon nanotube transistors were made and characterized.	
1999	Reversible molecular switches were synthesized and tested (Hewlett Packard/UCLA, Yale/Rice)	
2001	Stan Williams' group at Hewlett Packard demonstrated a 64-bit molecular electronic memory [15].	
2004	Target year for completion of a DARPA-funded 16 kilobit molecular electronic memory (10^{11} bits/cm^2), now under development [16].	

Table 3. Molecular Machines		
1999	**Molecular biomotor**. Carlo Montemagno and George Bachand (Cornell) created the first organic/inorganic integrated molecular motor, using a molecule of the enzyme ATPase coupled to a metallic substrate with a genetically engineered handle. [17]	
2001	**Molecular bearing and telescoping arm**. Alex Zettl's group at Lawrence Berkeley Laboratories developed a nearly frictionless cylindrical molecular bearing (that can also serve as a telescoping arm) based on nested carbon nanotubes [18].	 
2003	**Molecular electrostatic motor**. Alex Zettl's group at UC Berkeley developed an electrostatic motor using electron beam lithography to pattern a 100-300 nm gold rotor suspended with a carbon nanotube bearing [19]. 	

Research Initiatives. In 1993 Rice University announced the first laboratory in the U.S. dedicated to nanotechnology research, and since then several dozen institutions worldwide have established their own dedicated centers. In 1996 Jim Von Ehr formed Zyvex, the first molecular nanotechnology company. Their goal is to develop the technology and build self-replicating molecular assemblers. Other nanotechnology companies have since been established (or divisions created within larger companies), many focused on (1) molecular electronic devices for computer applications, (2) the synthesis of carbon nanotubes and other fullerenes, and (3) the synthesis of inorganic nanoparticles. In 2000, President Clinton announced the National Nanotechnology Initiative (NNI) with a doubling of funding on nanotechnology research to about $500 million annually. This move cemented the already growing interest in nanotechnology in the United States, and stimulated new initiatives in Europe, Japan, and China. The NNI FY2005 funding level is about $1 billion.

When will this happen?

As shown in the *State of the Art* section, groups are building molecular machines *now*, and the technology is projected to mature within ten years. In its market analysis Deutsche Bank AG identified molecular manufacturing as one of only three areas of high growth development in nanotechnology [20]. Molecular manufacturing R&D, and indeed *all* technological progress, is proceeding at an accelerating pace. This has been quantified by Ray Kurzweil, who has shown that the rate of progress doubles every decade [21]. In the next ten years we will perform the equivalent of twenty years worth of research at today's rate of progress, and the next century will see the equivalent of 20,000 years of progress (measured against today's rate). Double exponential growth curves are not intuitive, rendering even the best timeframe guesses by leading experts wrong by orders of magnitude. We can avoid these guesswork errors to some extent by focusing on trendlines for several technologies related to molecular manufacturing. Trendlines for rates of advance in the distinct fields of precision machining and microlithography point to the mass production of atomically exact mechanical structures and computer chips around the year 2015 [22, 23]; Kurzweil's trendline for the decreasing size of mechanical devices (Figure 2, below) includes the advent of molecular mechanical devices a few years ago. Given (a) trendlines for electronic and mechanical devices, (b) the current state of the art, including the fact that the first robotically-controlled positional molecular assembly was demonstrated in 1999, and (c) these more general increasing rates of advance, a molecular manufacturing system will likely be developed by about the year 2015.

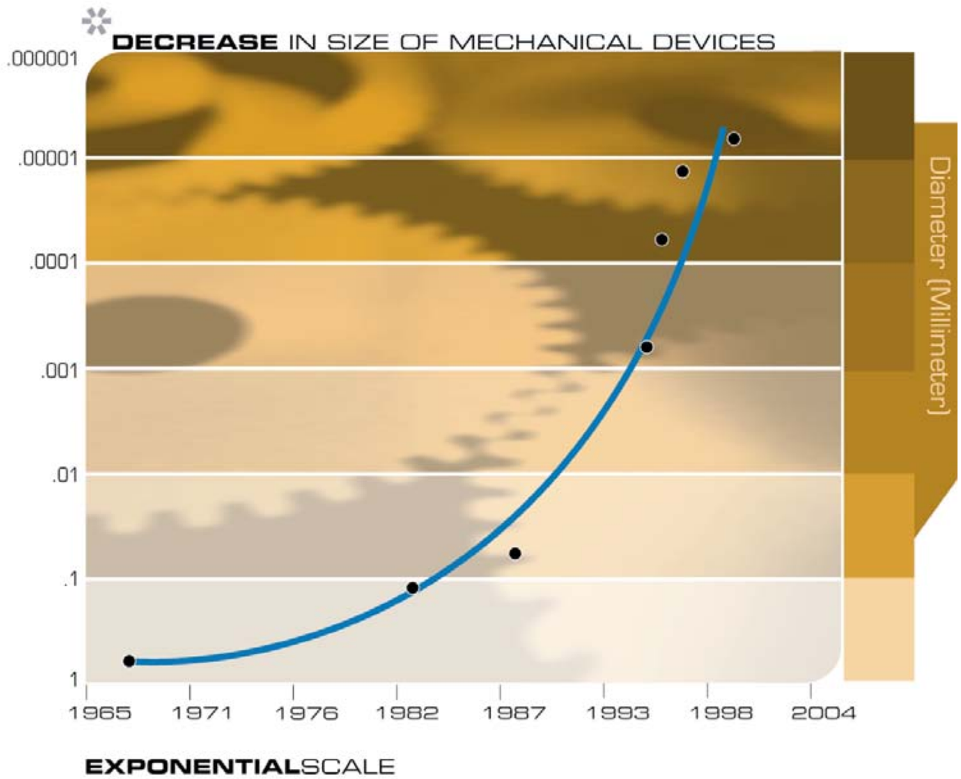


Figure 2. The double exponential decrease in the size of mechanical devices over time (scale is in millimeters). The advent of molecular mechanical devices occurred roughly where the curves intersects 10^{-5}mm (or 10nm--the diameter of a nested carbon nanotube). *Illustration courtesy Ray Kurzweil, KurzweilAI.net.*

Barriers to Progress

Despite ongoing successes in developing the molecular robotic components described above, and the passing of 13 years since the publication of the first theoretical treatment on molecular manufacturing systems, there is no coordinated movement within the technical or industrial community to develop molecular assemblers. Zyvex remains the lone U.S. company openly committed to building a molecular assembler, and only a few academics are building molecular machines (Zettl and Montemagno) or developing relevant molecular assembly processes (Seeman, Merkle, and Schafmeister). Molecular manufacturing is also not yet a stated goal within the National Nanotechnology Initiative. Part of the reason for this sparseness of effort has been an ongoing debate about the feasibility of molecular assembly [24, 25], in which critics claim that the technology is either not possible or will not mature for many decades or centuries. Politics is an important factor: there is a belief that potential risks posed by molecular manufacturing may create a public backlash and jeopardize funding for all nanotechnology-related activities.

There are two principal concerns about the imbalanced focus toward nanoscale science and away from manufacturing systems:

1. *Lack of safeguards*. If current trends continue, safeguard systems will not be developed at the same pace as the enabling technologies. Development of individual

molecular machines will continue with or without an integrated approach to develop molecular assembly systems. But needed safeguards may be omitted, without proper systems engineering in conjunction with the development of individual components, because the prospect for molecular manufacturing has been widely discounted.

2. *Development by adversaries*. Critical research on molecular manufacturing has been slowed in the United States by the feasibility debate, but not in other countries, thus providing an opportunity for countries unfriendly to the US and its allies to catch up technologically. The technology trends described by Kurzweil are blind to the politics of debate; if the assembler systems can be built, they will be—with or without the United States and its allies. The potential for molecular manufacturing to be the dominant manufacturing technology of the future is a critical reason to accelerate development in the United States and maintain a domestic manufacturing knowledge base.

Implications for Materials Technology

A new paradigm, or a very old one? For materials technologists who serially process metal, plastic, and ceramic products, materials processing based on massively parallel molecular machinery may seem like a radical concept. For those who work with natural textiles and wood products, this may seem like an extension of ordinary biological system technology, with an important difference: instead of biological assembler systems producing wood and cotton (that conventional machines then cut into lumber or spin into thread and yarn), non-biological assembler systems would create complex finished products directly from simple chemicals in one continuous manufacturing operation.

Strength. The ability to make materials to atomic specification implies that a new class of metastable alloys and compounds is possible: materials that are virtually defect free and can therefore perform near their theoretical property limits. For most metals and ceramics this translates to a strength improvement of about 100X; for plastics it's a factor of 1000 or more. As Prof. Rodney Ruoff has pointed out, these tremendous improvements in strength are achieved because perfect crystals can tolerate huge elastic strains—10% or more—so using them near their property limits will require rethinking how to deploy them in our structural designs. Given that this sort of redesign is possible, in combination with substitution of diamondoid[3] composite materials for denser materials where appropriate, many commonplace items could be reduced in weight by one or two orders of magnitude.

Reliability. Virtually all mechanical properties would be improved with molecular manufacturing, and with these improvements comes greater reliability. Greater improvements can be expected with the elimination of defects as localized 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 detrimental effects of embrittling impurities, defect structures, and grain boundaries. Failure will occur at higher stresses and dynamic loading rates as initiation sites are reduced to subatomic dimensions on atomically smooth surfaces, and crack

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[3] Diamondoid: Structures that resemble diamond in a broad sense: strong, stiff structures containing dense, three-dimensional networks of covalent bonds, formed chiefly from first and second row atoms with a valence of three or more [5].

propagation will also be inhibited without the presence of inclusions or dislocations; the dispersion of naturally occurring point defects could also be controlled more precisely.

Active materials. A rich integration of sensors, computers, and actuators within structural materials will blur the distinction between materials and machines, allowing the design and construction of objects that can be programmably reconfigured to sub-micron precision. These materials could monitor and report on their own state of "health." Figure 3 illustrates this concept with a latticework of machines linked by telescoping, interlocking arms. Both information and power would be transmitted through the arms to individually addressable motorized nodes.

In practical terms, this means that we will be able to make objects that change their shape quickly in order to adapt to changing needs. Airfoils could change shape to adapt to particular performance envelopes, for example, or a piece of clothing could resize itself to fit its wearer. The ability to do this should not come as a surprise: arrays of molecular actuators (the actin-myosin system—we call this muscle) operating in a massively parallel fashion allow animals to change their shape quickly, although with different degrees of freedom than in the design concept shown below.

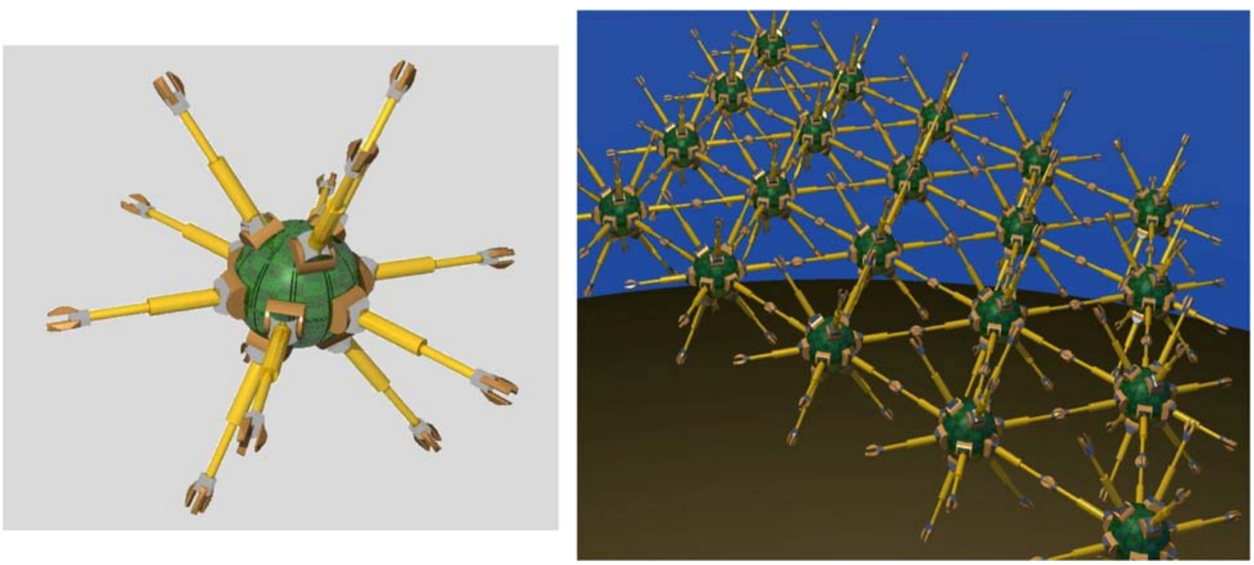

Figure 3. An individual "foglet" (left) and a 2D array of interlocked foglets (right). Materials made from these arrays could be instructed to change their shape in rapid fashion. The nodes could be as small as several hundred nanometers apart. *Illustration by J. Storrs Hall, Institute for Molecular Manufacturing.*

Relevance to ASM Members

At first blush, it would seem that robots moving atoms around would have little relevance to (for example) a shop floor metallurgist worried about the immediacies of this week's QC issue. For now this is true. But if the projections provided above are correct, and molecular manufacturing will emerge around the year 2015, the ensuing revolution in manufacturing will directly affect the materials careers of all of us who still expect to be in the workforce around that time. And it will certainly affect the careers and lives of our children.

The good news: the tools of molecular manufacturing will likely spur a revolution in materials development by factoring out the complicating effects of conventional materials synthesis and processing, and allowing us to focus on designing the right materials system for the job (down to atomic detail). Materials scientists will be able to cheaply and quickly synthesize any physically-allowable configuration of matter—considerably shortening the design cycle and greatly expanding the range of potential products. Indeed, it is conceptually staggering to envision materials design that takes into account all combinations and permutations of the stable elements in the periodic table, and on top of this to design multi-functional materials imbedded with molecular computers, energy harvesting systems, energy storage systems, sensors, passive mechanical components, and mechanically active and reactive modules. For the near term, there will be a significant need for innovative materials design and application engineering services. There will be a related demand for modeling and computer aided engineering tools to facilitate designing with these complex parameters, and for the associated manufacturing software. We have no experience with bulk materials with extremely low levels of defects; significant amounts of new research will be required to understand the physics, behavior, and properties of these materials.

The bad news: Organizations that do not position themselves to (a) participate directly in developing molecular manufacturing systems, or (b) take advantage of the capabilities afforded by molecular manufacturing will likely not survive this revolution. Large swaths of our centralized manufacturing infrastructure will likely become obsolete within a very short timeframe. For example, mining and primary metals industries will experience significant reductions in demand for raw materials, because of (a) the substitution of locally available materials for raw materials used in centralized manufacturing, and (b) multiple order-of-magnitude reductions in the *amount* of material needed for finished goods. There may be zero demand for semi-finished product forms.

Turbulent times ahead: Significant materials market segments will disappear, and others will emerge in their place. Portions of the commercial transportation industry (e.g., packaging and container firms, air freight, shipping, rail, and trucking) will become seriously endangered by the return to use of local materials, because there will be no need to move materials and finished goods from point to point. This represents a substantial market segment for both steel and aluminum. Alternatively, new applications may be created within the transportation industry, such as novel personal transportation vehicles (sea, land, air, and space), and enhancements to mass transit systems. Advanced materials derived from molecular manufacturing systems will play a key role in the development of these new applications.

It is difficult to predict molecular-manufacturing-era materials needs for large scale construction projects (e.g., factories, high rise business buildings, and shopping centers). New factory construction will be disrupted, if not eliminated, unless there is a compelling need to retain centralized manufacturing facilities.[4] High rise business buildings may become unnecessary if virtual working environments at home, coupled with high bandwidth communications, can effectively bring the office environment into the home. Shopping centers may no longer be needed for similar reasons, and because of restructuring of the distribution chain.

Biomaterials would theoretically be unecessary since damaged biological tissues and bone could be repaired to atomic precision, indistinguishable from the original. However, it is likely that there will be a new market employing atomically precise synthetic materials that allow people to enhance or augment the performance of native biological structures.

There may be a need for a new communication infrastructure based on atomically precise materials and devices (fiber to the home, finally), furthering materials development in this area. Similarly, development of molecular electronic materials and devices will continue for the foreseeable future, through the advent of molecular manufacturing, ultimately supplanting conventional electronic materials.

Life in the molecular manufacturing era will clearly not be "business as usual" for our materials society, and to say that adapting to the rapid and extreme changes will be a "challenge" would be a monumental understatement. ASM's Education Dept. can play a critical role in preparing our current and student members for the coming changes, and in developing new skill sets that will be required. This technology comes fraught with complex public policy issues, and the Federal Affairs Committee is charged with identifying these, and in pursuing studies and reports to assist in the formulation of public policy. The FAC is also charged with providing ". . . mechanisms for generating progressive relationships and joint activities among technical societies," and given the interdisciplinary nature of molecular nanotechnology it is essential that we cooperate with societies such as ASTM, ASME, SME, and life science organizations in our technical programming, policy formulation, and standards development for safe manufacturing systems.

Summary

During the past twelve years, since the first ATAC white paper on this subject, molecular manufacturing has progressed from theoretical studies to the construction of working molecular machine components. Positional molecular assembly has been demonstrated in the laboratory, and a potentially useful artificial molecular motor has been synthesized and tested. One company, Zyvex, has announced its intention to design and build a molecular assembler, and many companies are designing and building molecular computer components. Molecular transistors have been built and tested, and a working molecular electronic memory unit is targeted for completion in 2005. That said, much work remains before molecular robots begin assembling copies of themselves, ushering in the era of molecular manufacturing. The best projection for this breakthrough is approximately the year 2015.

Molecular manufacturing will stimulate a revolution in materials development, and many traditional industries will become obsolete while new ones emerge that take advantage of the new technological capabilities. The development of advanced materials will be essential to the success of new applications that capitalize on the capabilities of molecular manufacturing systems.

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[4] Temporarily retaining centralized manufacturing facilities that employ molecular nanotechnology has been proposed to facilitate the safe transition to global use of molecular manufacturing [26]

ASM can address the needs of its membership on the issue of molecular manufacturing by:

- informing and educating current and future members about ongoing developments
- providing high quality, timely, and relevant technical programming
- promoting inter-society collaborations on standards development for safe materials and devices, and safe manufacturing systems
- participating in public policy formulation

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