Year 2000 and Beyond Talk

Text of Presentation

Molecular Manufacturing and Materials Engineering

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I want to change the way that you think about the future. Whether you are thinking about the future of materials processes or about the future of manufacturing of any kind, I want you to think in terms of low cost, massively parallel molecular manufacturing systems. In the brief time that I have, I'd like to:

{Slide 1: Outline}

- Give you a brief overview of this exciting new technology
- Show you that sufficient theoretical work has been performed to provide lower bounds to component and systems performance
- Show you that the potential gains in materials properties alone are extraordinary enough for this technology to be worthy of our attention (and, by the way, I don't know of any other existing or proposed materials process that has the ghost of chance of achieving materials with comparable properties)
- Explain why I think this technology is coming sooner than we think—within 15 years
- Share my thoughts on how materials policy and materials education can and should contribute to progress along these lines

{Slide 2: Definition}

To put us on common ground then, the definition of molecular manufacturing that I am using is: "the construction of objects to complex, atomic specifications using sequences of chemical reactions directed by nonbiological molecular machinery."

{Slide 3: Slide of ribosome building polypeptide chain}

In biological molecular machinery, ribosomes grab transfer RNA molecules which give up a bound amino acid onto a growing chain of polypeptides. The type and order of the peptide sequence is governed by a transcription of the DNA's genetic code. It's a very mechanical process but it is performed by—and results in—structures that do not look much at all like the mechanical devices we're familiar with.

{Slide 4. Sleeve bearing—Nanosystems, p. 298}

Molecular manufacturing systems, by contrast, will also build structures to atomic precision but use mechanical devices more familiar in appearance. Here is a molecular bearing designed by Eric Drexler, consisting of about 258 atoms. The dark atoms are carbon, the gray ones are nitrogen and the white ones are hydrogen, which serve to terminate the surfaces. It has a relatively small rotational energy barrier (<0.001 maJ—which means it is virtually frictionless) and calculations on the bond lengths show that the bearing could be assembled intact by popping the shaft into the sleeve. Larger bearings with higher axial stiffnesses are also possible.

{Slide 5. Sleeve bearing—Nanosystems, p. 296}

The large light gray atoms are sulfur, the next darker shade are nitrogens, and these are oxygens, carbons, and hydrogens. The atomic positions were computed by molecular mechanics techniques and the mechanical forces in the system were analyzed using a commercial program called Polygraf.

Similarly, gears are possible

{Slide 6. Figure 10.24, p. 305}

and an analysis

{Slide 7. Figure 10.26, p. 306}

shows that energy barriers to corotation are small—generally less than 0.01 maJ for large numbers of teeth even with substantial torsional loads. [comment]

These gears are highly efficient at transmitting power. For a gear system operating at a shear force of 1nN, phonon scattering and thermoelastic drag losses account for only three thousandths of a percent of the transmitted power. Gears can even be integrated with bearings

{Slide 8. Figure 10.28, p. 307}

by proper choice of surface atoms to tune the interfaces to either catch (for the gear teeth) or slide (for the bearing surface). Roller bearings

{Slide 9. Figure 10.29, p. 308}

can be used to allow low friction movement between two race surfaces. Planetary gears

{Slide 10. Figure 10.31, p. 311}

can be used to convert shaft power from one angular frequency to another. This particular gear system

{Slide 11. Figure 10.32, p. 312}

was designed to atomic detail by Drexler and Merkle again using Polygraf.

Moving up from these basic parts, subsystems of intermediate complexities can also be developed. These include

- Mechanical measurement devices
- Stiff, high gear ratio mechanisms such as harmonic drives {Slide 12. Figure 11.2, p. 323} and toroidal worm drives {Slide 13. Fig. 11.4}
- Seals and pumps for fluid transport
- Vacuum systems to remove contaminants {Slide 14. Fig. 11.7, p. 330}
- Cooling systems with fractal plumbing {Slide 15. Fig. 11.8, p. 332}
- Electromechanical switches and actuators {Slide 16. Fig. 11.10, p. 335}
- Electrostatic nanomotors {Slide 17. Fig. 11.11, p. 337}

Building from these subsystems, we can envision the following sort of materials processing operation to make structures to atomic precision.

{Slide 18. Fig. 13.1, p. 374}

Impurities could be separated from feedstock molecules using a sorting rotor as shown here. The binding site is constructed so that the desired molecules selectively stick there. As the rotor moves about the cam, follower rods push the molecules out into the reservoir. Here you see an error, where the wrong molecule has gotten through.

{Slide 19. Fig. 13.2, p. 378}

To reduce errors, an auxiliary rotor can bind the other side of the molecule which then passes through in a totally enclosed state.

The purified molecules can be transported away from the sorter system using the molecular equivalent of a conveyor belt.

{Slide 20. Fig. 13.6, p. 385}

To illustrate how a molecule can stick to the belt, here's an example of an ethyne molecule in a receptor site.

{Slide 21. Fig. 13.7, p. 387}

Once on a conveyor belt, the molecules can be transported to other belts, changing speed or frequency if necessary. The belt speed is 0.5 cm/s and the transition time from

belt to belt is less than 0.2 μs. A system for transforming a stream of small feedstock molecules into a stream of reagent moieties would be between one million and three million atoms in size. It could deliver the equivalent of its own mass in about 3 seconds. The error rate is estimated to be 1 in 10^{15} operations, at 10^6 operations per second this gives a mean time to failure of about 3000 years.

{Slide 22. Fig. 13.11, p. 401}

The reagent moieties can be transported up through the center of a hollow manipulator arm to a working tip for positional synthesis. The manipulator arm was designed to be highly stiff (25N/m) to keep the error rate below 10^{15}. Applying 1 nN of force would deflect the arm only 0.04 nm.

{Slide 23. Molecular mill from Foresight Update 17}

Parts could be made more rapidly with molecular mills. Here we see one such system adding a single hydrogen atom to a cylindrical workpiece. Mill-based manufacturing is well suited to making standard components at high rates. Mills of this type could be employed to make blocks of systems up to 1μm. A 1 kg structure would contain about 10^{15} blocks made from about 10^6 separate systems.

{Slide 24. Fig. 14.4, p. 418}

Convergent assembly is a technique used in automotive manufacturing, where many smaller parts are assembled to form fewer larger parts. In this diagram we see how a volume could be filled with assembler systems using convergent assembly to build macroscopic objects. The branching pattern could be extended through more than 30 generations, enabling the assembly of objects from more than 10^{27} pieces.

{Slide 25. Figure 14.8, p. 428}

The resulting exemplar system outlined by Drexler, would use inexpensive hydrocarbon fuel (about 10¢/kg), weigh 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.

Coming Soon

Well, that's a necessarily cursory view of the conclusions of some theoretical design work that has been performed to date, mostly by the Institute for Molecular Manufacturing. This may sound to you like a technology that is centuries ahead of where we are today. But it really isn't. Here's why I think so:

{Slides 26-35. Why MM is coming soon}

- No single path to development,

    - advances in scanning probe microscopy (esp. molecular manipulation)
    - supramolecular engineering and other types of synthetic chemistry
    - protein engineering

  all contribute
- No new science; chemical bonding is well-understood, to the best of my knowledge, all technical objections have been addressed; and we can import design principles and new advances from existing manufacturing technologies
- The pace of advances is increasing in computer hardware, software design tools, synthetic chemistry, protein engineering, the application of scanning probe microscopes to molecular manipulation, and for that matter the design cycle in general
- Designs for more and more complex assembler systems can proceed in parallel
- Incentives for development
    - High performance materials
    - High performance computational systems
    - Reduced energy consumption
    - Reduced environmental pollution
    - Military applications
- 1991: Japan's Ministry of International Trade and Industry announced a 185 million dollar program to develop related technologies [comment on Burgess Laird's assessment]
- The Institute for Molecular Manufacturing has been performing key design work to advance the technology since 1991
- Rice University announced program in 1993
- Quantitative measures of progress point to development between the years 2010 and 2020 (show graphs)

{Slide 36. Figure 4 from Keyes paper}

If we plot the number of atoms used to store one bit of information vs. time, we see that we will reach the molecular mechanical device regime between the years 2010 and 2020.

{Slide 37. Figure 6 from Keyes paper}

If we plot the amount of energy dissipated per logic operation, we see that we will reach the values calculated for molecular mechanical computers between the years 2010 and 2020.

{Slide 38. Figure 1 from Taniguchi paper}

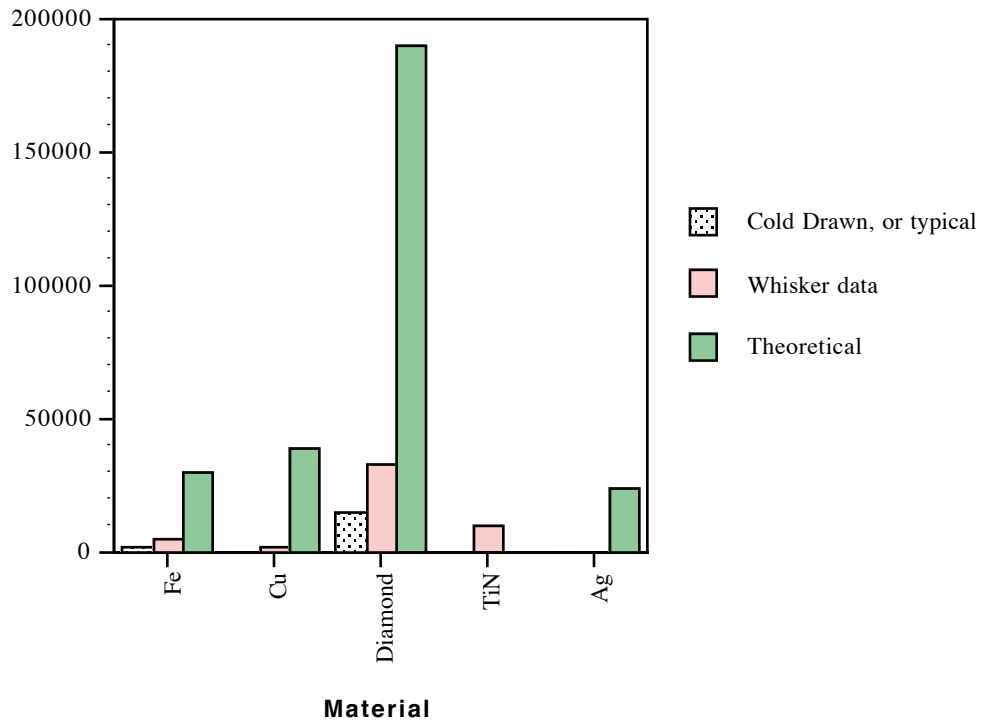
If we plot the rate of advance in of our ability to machine objects, once again we see that we will reach single atom precision between the years 2010 and 2020. So based on these qualitative observations and quantitative trends, 15 years is the best available estimate.

Implications for Materials Science and Engineering

Now I want to discuss a few implications of this technology as they relate to materials science and engineering.

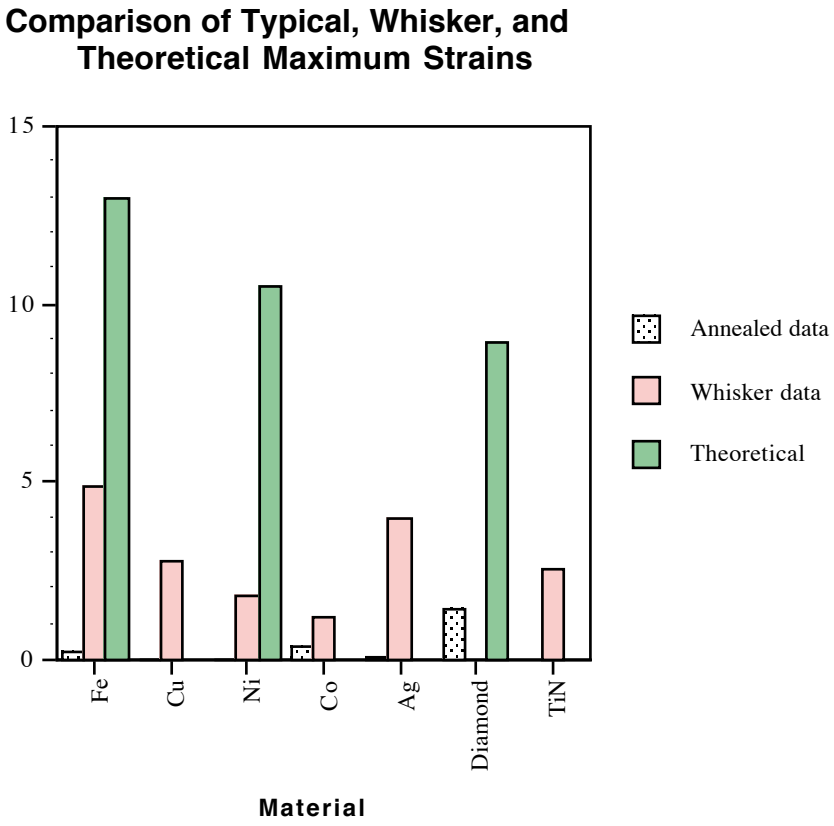
If you could make engineering structures to atomic perfection, you would find that they exhibit incredible properties.

{Slide 39. Tensile strength of metals}



If we compare the tensile strengths of cold drawn metals and some other materials with their whisker and theoretical strengths, we see that in all cases the theoretical strengths are about two orders of magnitude greater than today's typical values.

{Slide 40. Maximum elastic strain of metals}



If we compare the maximum elastic strain of annealed metals and other materials with whisker data and theoretical limits, once again we see a difference of about two orders of magnitude. You may notice that the theoretical elastic strains approach the plastic strain limits of conventional materials. It is clear that while we now value materials performance improvements that are on the order of 10 or 20 percent, this isn't even close—by two orders of magnitude—to the potential of the materials.

Other properties may benefit as well. For example, there are reports of exceptional corrosion resistance when iron is purified to less than 50ppm of impurities; that material is also ductile down to 4.2K. 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 presence of embrittling impurities, defect structures, and grain boundaries. Today we talk about smart materials with some small number of sensors imbedded in them. With molecular manufacturing, tomorrow's materials could be made entirely of electromechanical devices and computers and be made programmable in both geometry and properties.

Molecular manufacturing offers the prospect of producing these materials because the production environment will be what we call eutactic, or well-ordered—free of

impurities. And—as you have seen—because all the atoms in the process have controlled trajectories, we can put atoms exactly where we want them. By posing sufficient activation energy and kinetic barriers to defect formation, and then using error detection and correction, we can bring defect frequencies down to those generated by background ionizing radiation.

Clearly, molecular manufacturing will present new challenges in design for materials engineers, and new opportunities for materials scientists to study the physics of solids.

But I must tell you that there are reasons to be concerned about this technology and although in this last section of my talk I advocate increased involvement by the materials community, I 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.

I am equally concerned about the lack of activity on the part of the materials community regarding this technology, considering that these ideas have been in the open literature since 1981 and in TMS and ASM publications since early 1990. Most of the progress is being made by chemists, mechanical engineers, and computer scientists. I believe that we, too, should participate. First, we need to put molecular manufacturing on the materials policy agendas of our technical societies.

{Slide 41. Materials policy agenda}

- Evaluate the relative value of molecular manufacturing research along with other initiatives and recommend priorities to our governments

I believe that molecular manufacturing would be a likely target for government funding and for research at both national laboratories and academic institutions due to its 10-15 year time horizon. The promise of effective solutions to environmental and energy problems makes this doubly attractive.

- Better define the role of materials engineers and scientists in developing MM
- With other technical societies, promote collaborations to develop guidelines for safe systems (e.g., consensus standards)
- Work with other technical societies to encourage interdisciplinary collaboratives
- Collaborate and maybe participate with IMM and FI in their biannual technical meetings

Finally, the last item—and I feel that this is extremely important:

- Outline materials science and engineering curricula to prepare students for an eventual transition to molecular manufacturing
    - For those of you who don't yet see this as inevitable, I don't think this sort of training is necessarily inconsistent with what we should be teaching

anyway as it would stress fundamentals like materials design, 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

Having given you an outline of what needs to be done I'd like to conclude with this thought from Richard Smalley at Rice University: ". . . nanotechnology is where the action will be. We must have that reflected in the undergraduate curriculum. . . .Why should we be teaching students to become scientists and engineers in the old technology? They should be part of the future."

Thank you.

Special Acknowledgement

I'd like to thank the people at Molecular Simulations Inc. for the use of their Polygraf molecular mechanics software.