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The future belongs to machines built at molecular scales—if we develop tools to engineer them.

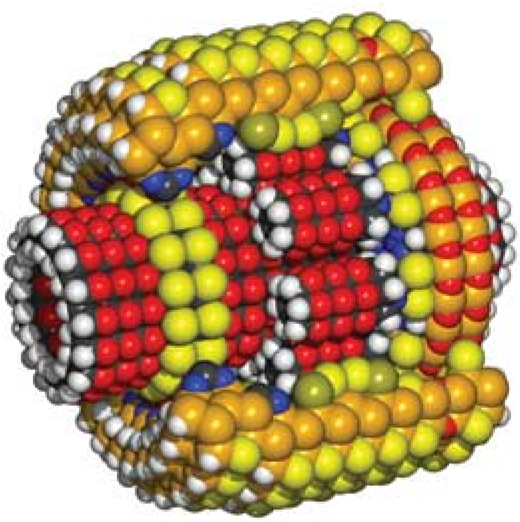
by Don W. Dareing and Thomas Thundat

We live in a world of machines. And the technical foundation for these machines lies in the steam engine developed during the 1780s by James Watt. The concept of deriving useful mechanical work from raw fuel such as wood, coal, oil, and now uranium was revolutionary. Watt also developed the slider-crank mechanism to convert reciprocating motion to rotary motion.

To improve on this first, basic engine, the people who followed Watt created the science of thermodynamics and perfected power transmission through gears, cams, shafts, bearings, and mechanical seals. A new vocabulary involving heat, energy, power, and torque was born with the steam engine.

Just as the steam engine sparked the industrial revolution of the 19th century, nanotechnology will likely ignite a new industrial revolution during the 21st century. Nanotechnology has the potential to impact all industries; the health care and computer industries are already capitalizing on it. New materials are being created that will affect everything from aerospace and energy to recreation and entertainment.

Even more important may be nanoscale machines, devices that function at molecular or even atomic scales. Some pioneers in the field envision the day when nanoscopic robotic submarines will kill off cancers one cell at a time, and foresee nano- scale factories in which tiny arms piece together products molecule by molecule.



Physicists have designed machine parts that could work at nanometer scales. This planetary gear, made up of a few thousand atoms, would perform much the same as some of its larger ancestors.

And yet, even when discussing such far-out developments, the notion of using an energy source to drive linkages is still a helpful concept in visualizing nanoscale devices. Sure, the sources of energy and the shapes of linkages are still being developed and are open to the designer's imagination. But the design problems associated with nanoscale devices in many instances are little different from those being tackled by engineers working on microelectromechanical systems. In other cases, however, the solutions to problems that arise at the nanoscale have better analogues in biochemistry or physics than in familiar mechanical engineering.

Right now, we need to figure out which is which.

Thanks to physics research conducted with atomic force microscopes and scanning tunneling microscopes, (which image surfaces down to the atomic scale and measure other surface properties such as friction), we know that Newtonian mechanics applies down to the level of just a few atoms. Other forces, such as van der Waals, electrostatic, and capillary, become important at the nanoscale. While these forces are not a factor in the design of MEMS or larger devices, they can be significant forces on nanoscale objects.

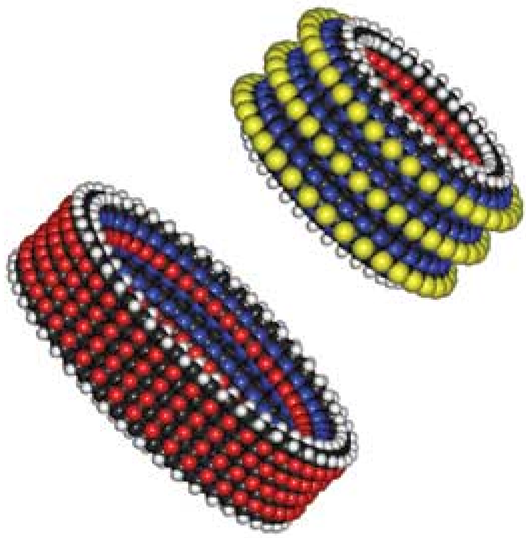
For instance, one consideration that makes design at the micro- and nanoscales unique relates to chemical and biological induced loads to machine structures. At present, those kinds of loads are not clearly understood nor are they formulated in a way that lets engineering design predictions be made. This is a major hindrance to the design and commercialization of micro- and nanodevices.

One marketable product that works on that scale which has achieved a level of success is the microcantilever sensor. That platform technology is capable of detecting the presence of certain biological and chemical agents, including explosives, with unprecedented sensitivity. The sensor works by bending when a molecule is adsorbed on one side of the cantilever, and by necessity, the dimensions of these cantilevers are quite small by macro standards—about 200 by 25 micrometers and 1 micrometer thick. This is a different type of beam loading from traditional external forces in macrostructures, and the key to controlling selectivity and sensitivity in design is the fundamental understanding of how biological and chemical agents cause the beams to bend.

In order to design for those types of forces, they first must be formulated in engineering terms or mathematically modeled for computer predictions. The interaction between an adsorbed molecular layer and a silicon surface can be modeled through the use of the Lennard-Jones potential. Total potential energy, including L-J and elastic strain energy in beams, are related to beam curvature. The equilibrium curvature is determined by minimizing total potential energy.

This works for simple situations, but when molecules become longer and more complex, the interactive forces become much more difficult to model. Experiment measurements that can provide the precise relation of potential energies (between specific molecules and surface atoms) to beam curvature are needed. Such data would allow microcantilever sensors to be designed to a given specified level of selectivity, sensitivity, and robustness.

Cantilevers are also being studied for use as microviscometers, which have tremendous applications in fields such as medicine, environmental control, surveillance, automobiles, and petroleum processing. To succeed at this, however, we need an accurate simulation of fluid flow on the surface of vibrating microcantilevers with rectangular cross-sections.



This bearing, shown here in an exploded view, may someday form part of a molecule-size motor. But machines based on biological forms may be more practical in the near term.

Already, research has shown that the flow around microscale devices is usually laminar and inertial forces are small in comparison with viscous forces. Except for hydrodynamic lubrication, such a situation rarely occurs in macrodevices. These flow characteristics greatly simplify the Navier-Stokes equations. But local and near-surface viscosities may not be the same as bulk viscosity and will probably have to be considered in design.

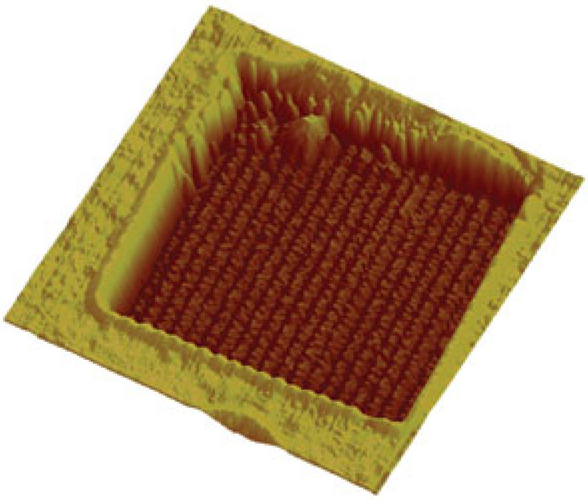
Designers also must pay attention to friction in nanoscale machines. A recent experiment used corrugated surfaces fabricated on a silicon surface to show that the friction measured by atomic force microscopes is quite sensitive to such factors as peak-to-peak distance. Even relatively smooth surfaces are subject to stick-slip mechanisms at the nanoscale. The magnitude of friction in both cases can be large enough to potentially damage or disable devices. An empirically based model of friction at this scale must be developed—and soon—in order to predict what level of force various nanodevices can be expected to face.

Beyond modeling, another challenge in designing micro- and nanodevices is the fabrication and testing of prototypes. The performance of macro prototypes normally is measured with proven sensors and instruments, and special diagnostic tools, such as fluorescence microscopy, may be needed to evaluate nanodevice performance. Computer simulation prototyping, based on molecular dynamics, may also be useful here. Either way, engineers must find a way to show that their designs are meeting performance specifications—no mean task when dealing with machines that can be as small as molecules.

Engineers may also have to rethink how they construct complex machines at the nanoscale. At human scales and with MEMS, parts or even whole devices are manufactured by larger ones: A stamping machine turns out metal parts, and computer chips are etched by photolithographic fabricators. It's not clear, however, if this model can be carried to the nanoscale, as the materials and forces involved may well elude top-down control.

Instead, we may find that nanomachines are better assembled from the bottom up. The bottom-up approach offers unlimited possibilities to the design engineer to use the basic building blocks of matter directly.

Eric K. Drexler, one of the founders of nanotechnology as a field of interest, envisioned in the 1980s that it could be possible to assemble certain atoms and molecules, which resemble components commonly used in macro machine design. One could build things from molecule-size bearings, gears, cams, clutches, and so on. This wouldn't be a complete analogue to present-day machine shops—material properties would be softer than in macro materials, for instance, and gear teeth may not satisfy the fundamental gear tooth law—but motion and energy could be transmitted by systems resembling macrodevices. This concept opens up a unique area for machine design at the atomic level.



Experiments that dragged the tip of an atomic force microscope across the furrowed surface indicate that friction can fluctuate across very small distances.

Until one could build fabricators that rival the size of the parts, however, the challenge would be to design molecules that would assemble themselves automatically into such components. Indeed, in spite of the ability of scanning probe microscopes to position individual atoms and molecules on a surface, it might be advantageous to find a method of building an entire device this way. The design imperative to minimize the number of machine components for low cost and high reliability may be especially important in the design of nanodevices.

The best place to look for inspiration for molecular-scale machines may not be in the world of turbines and linkages familiar to mechanical engineers. Instead, we may have to look inward. There are untold nanoscale mechanisms at work in the human body performing functions critical to life, from digesting food and circulating oxygen to creating and repairing cells. Each molecular device within the body is built to perform a specific task.

They may not look like traditional mechanical engineered devices nor do their components resemble machine elements, but each of these natural mechanisms provides a baseline for a future nanoscale engineering innovation. They are machines, each with its own energy source, kinematic linkage, and useful function to perform.

There are biological analogues of motors. Myosin and kinesin molecules are examples of linear motors. The end of the myosin molecule moves about 10 nanometers during the power stroke of its cycle, which is caused by the release of phosphate. The kinesin molecule works its way taking almost humanlike steps along structures called microtubules inside cells.

Rotary engines are also found in biosystems. The rotation of the ATP molecule inside an ADP molecule is controlled by the release of phosphorous at each stopping point. Engineers may be able to adapt or adopt such arrangements to produce useful motion within artificial nanoscale machines.

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Science is uncovering new technology almost daily, which will have a great impact on many aspects of society. These technologies are at various stages of development, but in the end, each spin-off product must withstand the test in the marketplace. The evaluation of each product will still be based on the same set of metrics as other products: performance, cost, risk or reliability, and availability. To satisfy these metrics, engineers will need analytical tools to make performance predictions, establish production costs and lifecycle economics, quantify the risk associated with new technologies, and satisfy a dynamic market.

These analytical tools are currently missing. Laboratory findings are outrunning the development of the needed analytical tools for reliable designs.

New design methodologies may be needed for molecular devices, especially those involving biological mechanisms. Methodologies involving trial and error and multiple testing, which are inefficient and often uneconomical in macro design, may be appropriate. Design methodologies based on benchmarking against biological nanoscale mechanisms may be useful. In the future, computer hardware, based on nanoscale transistors, may accommodate voluminous performance calculations of nanodevices routinely. Mathematical design tools and simulation models, which are currently not available, will be required.

It has been said that science owes more to the steam engine than the steam engine owes to science. The impetus for better, more efficient steam engines drove basic science for more than a century. Given the need for a better understanding of the forces and interactions at play at the smallest of levels, perhaps the same will be said some day about natural nano-biomedical mechanisms and the way they drove science in the next few decades.

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