Productive nanosystems: the physics of molecular fabrication

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Abstract

Fabrication techniques are the foundation of physical technology, and are thus of fundamental interest. Physical principles indicate that nanoscale systems will be able to fabricate a wide range of structures, operating with high productivity and precise molecular control. Advanced systems of this kind will require intermediate generations of system development, but their components can be designed and modelled today.

Productive nanosystems are nanoscale systems that make things, working with atomic precision. This technological objective was first articulated by Richard Feynman in his famous 1959 talk to the American Physical Society, 'There's Plenty of Room at the Bottom'. Nature exhibits prototypes of simple productive nanosystems, but physical analysis indicates that artificial systems can go far beyond the biological model. The aim of this paper is to describe the nature of productive nanosystems—their organization and fundamental principles, and their relationship to other technologies and research objectives. (A more extensive technical analysis of the applied physics of productive nanosystems can be found in Drexler (1992).)

The basic idea is simple: to assemble precise, intricate structures by bringing molecules together using direct, mechanical control—that is, to make things by putting their elementary parts where they should be. Advanced productive nanosystems can exert tight control over molecular motions and bonding transformations. They can exclude unwanted molecular encounters while ensuring that desired encounters occur with a positional accuracy of ~0.1 nm. Although based on the same molecular physics as solution-synthesis (in which molecular motion is uncontrolled), this approach offers far more control and reliability. Organic synthesis can make small structures with atomic precision, but it can rarely extend this precise control beyond hundreds of atoms. Design and analysis indicate that advanced productive nanosystems will be able to extend precise control by orders of magnitude, even to macroscopic scales. Putting parts where they should be can be useful, even in the molecular world.

Progress in productive nanosystems will have broad implications. Fabrication plays a special, strategic role in physical technology. Most systems cannot make things—they merely compute, or display images, or transport things (and so on). Because they cannot make things, they cannot make anything that is new and better. Fabrication systems, in contrast, make all other products, including new and better fabrication systems. Only fabrication systems can directly, physically advance other technologies. From this perspective, fabrication forms the trunk of the evolutionary tree on which all other technologies are branches.

Biology and beyond

Nature demonstrates productive nanosystems of a sort. For example, ribosomes, found in every

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cell, work as digitally controlled machine tools. They read genetic information (six bits per codon) and use it to direct the assembly of sequences of amino acids. The resulting polymers, linked by bonds like those in nylon, fold to make nanometre scale objects with precise arrangements of atoms (figure 1). These objects are as strong and stiff as common polymeric engineering materials, such as epoxy, polystyrene and wood. Together with nucleic acids (made by other programmable machines) these molecular objects form the working parts of a wide range of molecular machines, including ribosomes themselves.

This example immediately indicates the immense productive potential of nanosystems: working as parts of larger systems of molecular machinery, ribosomes make billions of tonnes per year of atomically precise products, and they do so cleanly and inexpensively, using common raw materials. As shown by the contrast between birds and aircraft, artificial systems can go far beyond their biological models in important ways. How far beyond the biological model can this technology go? This question can be addressed in a cursory way by examining scaling laws, and in depth through design and detailed physical analysis.

Early and advanced productive nanosystems

Biological systems provide not only examples, but also tools to use and models to emulate. The attention given to advanced systems must neither obscure how far we are from implementing them nor discourage investigation of early steps. Practical work must begin with what we can make today. Not surprisingly, many proposals for early development goals centre on exploiting natural productive nanosystems to build next-generation systems. Each generation could make a wider range of materials and structures, moving further and further beyond biological models. Recently developed capabilities in the design of novel protein and nucleic acid structures—including simple molecular machines—have opened the door to a path of progressive improvement. The discussion here, however, will focus on where this path can lead as it moves closer to fundamental physical limits.

Biology shows one way to organize productive nanosystems, but not the only way. As

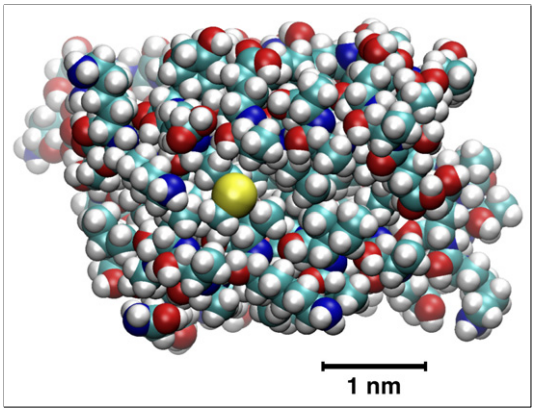

Figure 1. An engineered nanoscale object, the Top7 protein molecule. Protein engineering is based on computational design and modelling techniques and enables the fabrication of components like those in the molecular machinery of cells. These molecules can fit like puzzle pieces and assemble spontaneously, driven by Brownian motion.

with macroscopic machinery, the availability of stronger, stiffer materials will enable better performance. Operation in fluid media causes unnecessary drag; removing both liquids and gases provides a superior operating environment for advanced molecular machinery. Free of the structural limitations of biomolecules (large monomers, low bond density, low stiffness), advanced devices can be stronger, more fine-grained and more regular. Therefore, they can more closely resemble conventional machines (figure 2).

But *should* they resemble conventional machines? Perhaps not, but the fundamental tasks of powering and guiding motion are similar, regardless of length scale. Manufacturing systems shape and assemble parts, and they require powered, guided motions to put those parts in place. To do this, they use machines. It is natural to use machines for these same tasks on the nanoscale. It is likewise natural to consider organizing them in a way that resembles, at least roughly, a modern automated factory.

Looking toward advanced milestones in a long, multi-stage development program, a picture emerges of a desktop scale factory that converts inexpensive compounds into macroscopic products—for example, billion-CPU laptop computers, or sheets of high-efficiency photovoltaic cells. The factory builds macroscopic products layer by layer from diverse, multifunctional,

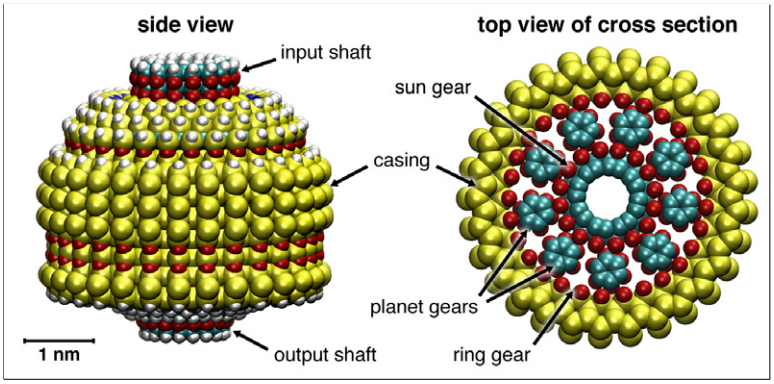

Figure 2. A molecular planetary gear. In mechanical systems, planetary gears convert shaft rotation from high speed and low torque to low speed and high torque. This highly symmetrical design employs stiff covalent structures that cannot be fabricated today, but can easily be modelled using standard molecular mechanics methods. Dynamical simulations show that this device can operate with a shaft angular speed of 10^9 Hz and a power density is in excess of 10^{15} W m^{-3} (see scaling laws in table 1).

micron-scale building blocks (a cubic micron can hold a CPU). It places these blocks using programmable positioning mechanisms similar in function to the pick-and-place mechanisms found in modern factories. The blocks, in turn, are assembled from smaller blocks. The smallest blocks can be made using fast, simple, efficient mechanisms that do only repetitive operations (figure 3). The nanoscale mechanisms at the heart of this 'nanofactory' form macroscopic arrays containing many trillions of elements, all integrated into a framework that provides power, cooling, materials and digital control.

The devices necessary to implement this advanced class of productive nanosystems have received considerable study. Macroscale, factory-like systems of this sort can be organized in many different ways, but all have a fundamental similarity. If there is a better, *fundamentally* different way to orchestrate the assembly of molecular fragments into large, intricate systems, it has yet to be proposed.

Some researchers might argue that so-called self-assembly of molecules in solution is that better, fundamentally different way. If one considers only near-term results, self-assembly is indeed better, because self-assembly can be made to work today. For this reason, self-assembly is the leading candidate method for implementing early-generation productive nanosystems.

In self-assembly, however, molecular building blocks must be designed to fit together in only one way—the building blocks themselves must encode the structure of the ultimate product. Matching surfaces must adhere to each other strongly, yet other pairs of surfaces must bind so weakly to one another (and so strongly to solvent molecules) that they do not adhere. If these conditions are met, Brownian motion can assemble intricate machines. Brownian motion, of course, is available without further development.

Biological systems exploit self-assembly, but they use programmable machines to make the required building blocks. There is good reason to think that early-generation productive nanosystems will do likewise, and hence that assembly by Brownian motion will be an essential technique at some time to come. As alternatives are developed, however, the practical costs of self-assembly will eventually outweigh the benefits. Direct, mechanical assembly can build a new design by combining standard parts in a new pattern. With unaided self-assembly, in contrast, interfaces among the parts must be redesigned. These intricate interfaces, buried during assembly of a product, typically serve no role in its ultimate function. Both the interfaces and the blocks themselves are typically soft and weak. Brownian self-assembly has a decisive advantage today—it is available—but mechanical assembly has decisive advantages in the long run.

Designing machines organized on the factory model requires attention to system-level concerns such as material flow, parts handling, power supply, waste heat management and so forth. At a finer level of detail, ordinary kinds of devices

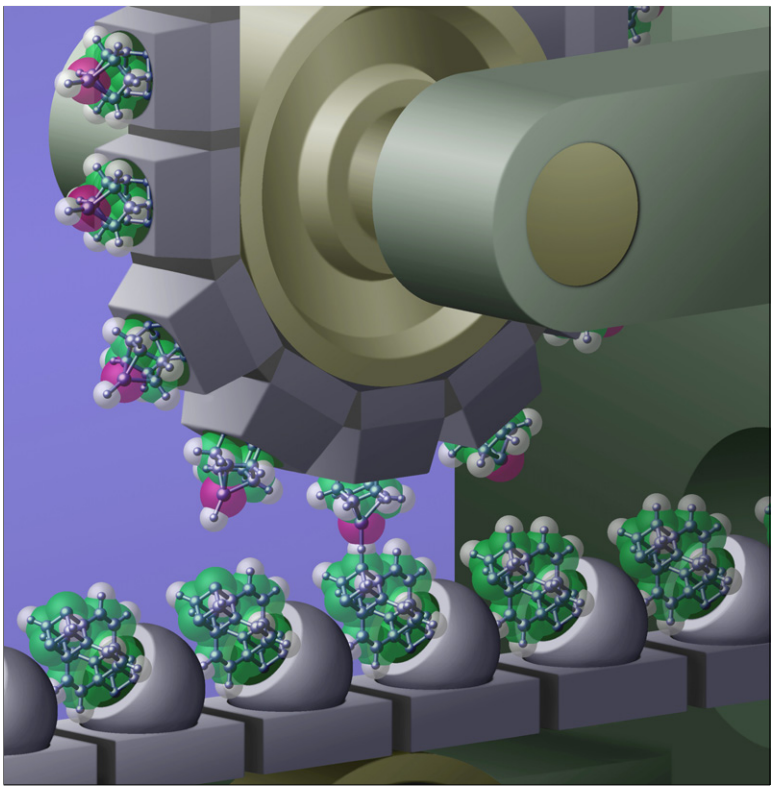

Figure 3. A molecular mill mechanism. Nanoscale machinery in a nanofactory can build products with atomic precision by guiding molecular reactions. Here, a moving belt applies molecular tools to products, depositing a single hydrogen atom on each. Systems of molecular mills and larger, programmable machines will be able to build macroscopic products quickly and inexpensively. This illustration is schematic, showing mechanical components without atomic features and somewhat undersized. Figure 2 shows a more intricate machine that has been designed and modelled in full atomic detail.

such as motors, bearings, gears, conveyor belts and digital computers become important, but in nanoscale forms that are subject to phenomena such as thermal motion. All these devices and systems have been examined in enough depth to provide estimates of volume, efficiency, throughput and other fundamental performance parameters. The following sections, however, will address physical principles common to a wide range of nanomechanical systems and fabrication processes.

Quantum and classical phenomena

We live in a quantum mechanical world: the properties of matter on all scales are consequences of quantum mechanics. Nonetheless, many macroscopic systems can be described with good accuracy by classical models, which are often more intuitive and tractable. Nanoscale systems operate in the borderland of the classical domain, where the applicability of classical models depends as much on the nature of the phenomena as it does on the scale of the device.

Many nanoscale electronic phenomena are inescapably quantum mechanical. Tunnelling, quantized energy levels and quantum interference can play large roles. The bound states responsible for atomic structure and molecular bonds are beyond classical analysis, yet determine such fundamental properties as the size and shape of structures.

In contrast, many nanoscale mechanical phenomena can be described well by classical models. Tunnelling, quantized energy levels and quantum interference typically play lesser roles owing to the large masses of nuclei and molecular structures, and at room temperature these quantum effects are usually blurred or overwhelmed by thermal fluctuations. Further, thermal fluctuations

and quantum effects can be qualitatively similar. Classically, thermal fluctuations make positions uncertain and enable systems to cross energy barriers. Here, quantum corrections to classical models mimic reductions in restoring forces and barrier heights—a quantitative not qualitative effect. In electronics, quantum effects are obvious and inescapable, but in mechanics, their observation is a challenge typically pursued at cryogenic temperatures.

Quantum nanoelectronic systems will doubtless be important products of productive nanosystems and may play an important role in their implementation. It is, however, possible to design and analyse systems in which all the important degrees of freedom are mechanical and are subject to classical analysis with quantum corrections. The resulting designs will surely be superseded by others that exploit a wider range of phenomena. However, if these simpler designs include all the phenomena relevant *to those selected structures*, and if the analysis is careful and conservative, then future systems will be different because greater knowledge and ingenuity has made them better.

Classical continuum scaling laws

Models of macroscopic machines ignore not only quantum mechanics but also atoms. This level of analysis is surprisingly useful at the nanometre scale, though only as a rough guide to expectations rather than as a basis for detailed investigation. In particular, continuum models yield scaling laws that suggest that nanoscale machinery can have remarkable performance.

Table 1 presents some classical continuum scaling laws that remain approximately correct down to lengths of a few nanometres or so. It also lists characteristic magnitudes for these properties, taking the characteristic length L to be 10 nm. The values assumed for stresses, field strengths, electrical conductivity and the like correspond to reasonable values for high-performance materials.

Because of adverse scaling laws, nanoscale versions of some macroscopic systems will not work. For example, the force between parallel segments of wire that are L (m) long, d (m) apart, and carry currents of i (A) is

$$F = 2 \times 10^{-7}\, i^2 L/d \text{ (N)}.$$

The scaling effects of L and d cancel, and i (at constant current density) scales with area, hence the force scales as L^{-4}. Because this force falls much faster than forces exerted by material stress, it becomes insignificant in nanoscale mechanisms. In compensation, low voltages across small distances produce strong electric fields (limited by electron emission at the negative electrode), making electrostatic motors attractive.

The sole non-integral exponent in table 1 describes the scaling of the amplitude of thermal vibrations constrained by an elastic component, $L^{-1/2}$. This scaling arises because the Hooke's Law dependence of spring displacement on stiffness, k_s (N m^{-1}), and energy, E (J), is

$$\Delta x = (2E/k_s)^{1/2} \text{ (m)}$$

while k_s scales as L^{-1}. Numerically, the root-mean-square amplitude of the thermal displacement of an elastic component at a temperature T (K) is

$$\sigma = (k_B T/k_s)^{1/2} \text{ (m)}$$

in which $k_B \simeq 1.38 \times 10^{-23}$ J K^{-1} is the Boltzmann constant. The statistical distribution is Gaussian.

From a manufacturing point of view, a few scaling relationships are key. The first is the scale-independence of speed of motion: following a motion path of a given shape and holding dynamical material stresses constant, speed is an invariant. Accordingly, operating frequencies scale as L^{-1}. A measure of productivity is the frequency with which a mechanism can process its own mass. If the mechanism handles parts that scale as L^1, the number of motions per cycle will be constant, and productivity will scale with the motion frequency: L^{-1}. Scaling a machine from 1 m to 100 nm thus increases productivity by 10^7.

If a machine handles parts of fixed size, the same measure of productivity varies as L^{-4}. With parts of atomic size, a change from 1 cm to 100 nm increases the productivity from (for example) $\sim 10^{-21}$ s^{-1} (absurdly low—the reciprocal exceeds the age of the universe) to a very attractive $\sim 10^{-1}$ s^{-1}. System-level calculations, however, must take account of raw material preparation and multilevel assembly. These calculations indicate system-level productivity of the order of 10^{-3} s^{-1} (the productivity of growing bacteria is also of the order of 10^{-3} s^{-1}). This far exceeds the productivity of an ordinary factory. Elementary physical principles thus *suggest* that productive nanosystems can combine the ultimate in precise control of material structure with extraordinary productivity. This has motivated a deeper analysis.

Table 1. Classical continuum scaling laws, with characteristic magnitudes for $L = 10^{-8}$ m. These relationships break down at smaller scales, where atomic structure and (in some instances) quantum effects become important, and volumes become too small to hold all the components of a productive nanosystem. Note that mechanical power densities can be reduced to values that are more reasonable by reducing forces and speeds.

Quantity	Scaling	Magnitude	
Magnetic force	L^4	10^{-19}	N
Volume	L^3	10^{-24}	m^3
Mass	L^3	10^{-21}	kg
Electrostatic energy	L^3	10^{-19}	J
Torque	L^3	10^{-15}	m N
Gravitational force (weight)	L^3	10^{-20}	N
Area	L^2	10^{-16}	m^2
Force (at working stress)	L^2	10^{-7}	N
Mechanical power	L^2	10^{-7}	W
Electrostatic force (constant field)	L^2	10^{-11}	N
Electric current	L^2	10^{-6}	A
Length	L^1	10^{-8}	m
Deformation (constant stress)	L^1	10^{-11}	m
Motion time	L^1	10^{-8}	s
Stiffness	L^1	10^{4}	$N\,m^{-1}$
Voltage (constant field)	L^1	10^{0}	V
Gravitational stress	L^1	10^{-5}	$N\,m^{-2}$
Mechanical working stress	L^0	10^{9}	$N\,m^{-2}$
Modulus of elasticity	L^0	10^{12}	$N\,m^{-2}$
Electrostatic stress (constant field)	L^0	10^{5}	$N\,m^{-2}$
Adhesive strength (dispersion forces)	L^0	10^{9}	$N\,m^{-2}$
Strain	L^0	10^{-3}	—
Density	L^0	10^{3}	$kg\,m^{-3}$
Speed	L^0	10^{0}	$m\,s^{-1}$
Current density	L^0	10^{10}	$A\,m^{-2}$
Electric field	L^0	10^{8}	$V\,m^{-1}$
Amplitude of thermal vibrations	$L^{-1/2}$	10^{-12}	m
Acceleration	L^{-1}	10^{8}	$m\,s^{-2}$
Spring stiffness	L^{-1}	10^{4}	$N\,m^{-1}$
Deformation (constant force)	L^{-1}	10^{-11}	m
Mechanical power density	L^{-1}	10^{17}	$W\,m^{-3}$
Electrical resistance	L^{-1}	10^{0}	Ω
Motion frequency	L^{-1}	10^{8}	s^{-1}
Relative productivity (scaled parts)	L^{-1}	10^{5}	s^{-1}
Relative productivity (atomic parts)	L^{-4}	10^{3}	s^{-1}

Classical atomistic models

Although classical continuum models offer only a rough guide, atomistic classical models have a well-established role in analysing nanoscale systems. These models have their roots in the Born–Oppenheimer approximation, which treats electronic degrees of freedom as responding instantaneously to changes in nuclear positions. The result is a potential function that determines the dynamics of nuclear motion, which then is often treated classically. Approximate solutions of the electronic Schrödinger equation (the basis of 'quantum chemistry') provide relatively accurate potentials for small structures (tens of atoms or less). In another approach, analytical approximations to the potential function that governs nuclear motion can be fitted to experimental or quantum-chemical results. This is the basis of 'molecular mechanics' methods, which enable computational experi-

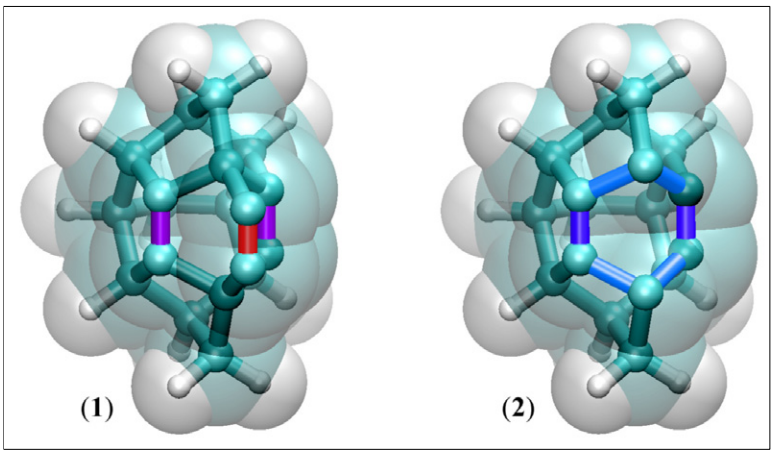

Figure 4. A tool for mechanically guided synthesis. In state (1), the tool binds a pair of carbon atoms linked by a triple bond. In state (2), the carbon atoms have been transferred to a product structure. No broken bonds (radicals) are left on the tool, because an electronic rearrangement creates a six-member ring of carbon atoms analogous to benzene. A quantum-chemical analysis using density functional theory shows that the stability and binding energy of this tool enable extremely reliable molecular assembly at room temperature, with failure rates $\ll 10^{-15}$.

ments involving the dynamics of thousands to millions of atoms. The widespread use of molecular mechanics in the molecular sciences attests to the utility of classical atomistic models.

Molecular mechanics methods can describe only a limited range of structures and geometries, but they are at their best in describing the structures of greatest interest in advanced molecular machinery: strong covalent solids. For these structures, molecular mechanics can be used to investigate elastic deformation and contact interactions such as adhesion, binding and friction. Most work on molecular machinery has used these models. Results include designs for bearing interfaces that have effectively zero static friction (barriers $\ll k_B T$ at room temperature). These interfaces exhibit dynamic friction through phonon interactions. Like viscous drag, these forces are proportional to sliding speed.

At the heart of productive nanosystems are processes that transform bonding, building larger structures from reactive molecular fragments. These processes are modelled using quantum-chemical techniques, which enable a designer to identify molecular tools (such as the one shown in figure 4) that transfer fragments reliably despite thermal fluctuations. Fabrication can resemble a reliable digital process: at each step, an operation either completely succeeds or completely fails, because in the structures of interest, different bonded states are stable and distinct. No small errors accumulate, hence the result of an immensely long sequence of operations can be exact with some non-zero probability. The challenge is to make that probability large.

The challenge of thermal fluctuations

At room temperature, thermal fluctuations present the chief difficulty in achieving reliable fabrication. (Radiation damage is an important secondary constraint, mitigated by the small target size of nanoscale devices.) A standard approximation in the analysis of thermal fluctuations, based on the Boltzmann distribution, relates the probability P_i that a system will be moving through a particular region i of configuration space to both the temperature T and the energy ΔE_i required to displace the structure to that region:

$$P_i = K \exp(-\Delta E_i / k_B T)$$

where K is a constant determined by the system and the region. The product of P_i and a characteristic fluctuation frequency (typically of the order of 10^{13} s^{-1}) provides an estimate of the transition rate for crossing a barrier of height ΔE_i. The condition for reliability is that $\Delta E_i / k_B T$ exceed a suitably chosen threshold for every state i that corresponds to a failure condition (or a transition to a failure condition), and that $\Delta E_i / k_B T$ be low (or zero) for every transition to a desired state. Some states and transitions

are effectively excluded by molecular energy barriers: for example, the energy required to break a single carbon–carbon bond is about 150 times the room-temperature value of $k_B T$, hence $\exp(-\Delta E_i / k_B T) < 10^{-65}$.

Molecular machines can fail because their structures fragment or rearrange. With careful design, the barriers to this sort of failure can be made comparable to bond energies, and the room-temperature failure rates can be correspondingly low.

Molecular machines can also fail because of transient displacements. The most important case in productive nanosystems is the displacement of a molecular tool during an operation intended to transfer a molecular fragment to a workpiece: this can cause an unwanted bonding transformation. Displacement energies are usually well described by Hooke's law, $\Delta E_i = K_i \Delta x_i / 2$. The threshold value for Δx_i is $\sim$0.1 nm (about a bond length). For the failure probability P_i to be $< 10^{-18}$ at room temperature, it suffices to have $K_i \gtrsim 15\ \mathrm{N\,m^{-1}}$. Careful design using stiff materials can meet this criterion for molecular tools positioned by 100 nm scale devices.

Thermal fluctuations also raise the energy cost of reliable assembly operations. Although they do not directly impose a cost on accurate positioning, they can make bonding transformations fail by enabling the system to exit with a molecular fragment in the higher of two potential wells—that is, still attached to the tool. The simplest way to reduce errors of this kind is to expend energy, allowing a transformation to 'drop' the system into to a deep enough potential well. This dissipates energy into distributed vibrational modes, which quickly thermalize. A drop of of $40\,k_B T$ suffices to make the probability of a failed transformation $< 10^{-18}$. If the steps required to process each atom require a total of ten times this energy, the energy consumed per kilogram of product will be less than half the energy cost of smelting a kilogram of aluminum.

Conclusion

Design and analysis at several levels of physical modelling supports the expectation that advanced productive nanosystems will be able to build atomically precise structures on a large scale, and that they can do so with high productivity and reasonable energy efficiency. This suggests that productive nanosystems can have large-scale impact on a broad spectrum of physical technologies and their applications.

One would naturally expect that artificial molecular machine systems will have broad medical applications, since living systems are built and maintained by natural molecular machine systems. One would expect that atomically precise control of fabrication would result in superior materials, energy conversion devices, scientific instruments and weapon systems. Accordingly, one would expect a large-scale impact on medical, economic, environmental and military affairs.

Questions about the physical limits of fabrication are of inherent interest, and the study of productive nanosystems seems a good area in which to seek answers. Because they operate in the borderland between what can be considered classical and what must be considered quantum mechanical, they lend themselves to framing problems of educational value. Physicists will play a key role in the development of productive nanosystems because a physics background provides the knowledge necessary to understand and solve the key problems. For all these reasons and more, productive nanosystems provide a worthy focus for both physical analysis and physics education.

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