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Molecular Manufacturing: Perspectives on the Ultimate Limits of Fabrication

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Molecular manufacturing: perspectives on the ultimate limits of fabrication

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Molecular machine systems, common in biology, can become a basis for a new style of physical technology. Characteristic features of the proposed systems and their products include nanometre-scale structures, atomic precision, low defect densities, and high manufacturing productivity.

1. Introduction

Physical technology rests on our ability to fabricate physical objects, whether they be scientific instruments, consumer products, or tools used to fabricate other physical objects. To understand the ultimate limits in fields that use physical technologies, one must understand the limits of fabrication. Our understanding of the limits of fabrication has been constrained by the analytical intractability of current fabrication technologies, which are simultaneously complex and diverse, yet narrow in their capabilities. This difficulty has stunted our understanding of the limits of physical technology as a whole.

Conventional fabrication technologies resist overall analysis not only because of their diversity and complexity, but because of their sensitivity to features of molecular potential energy functions on the order of 10^{-21} J per molecule. These differences can determine, for example, the stability of solid phases in materials science and the yield of reactions in organic chemistry, yet they are hard to predict using available computational techniques. Anticipated molecular manufacturing technologies (Drexler 1981, 1992), in contrast, will exploit direct positional control to guide sequences of discrete, reliable molecular transformations in a manner that can be comparatively insensitive to small differences in potential energy functions. The relative simplicity and generality of this approach, together with its reduced sensitivity to molecular unknowns, combine to facilitate understanding of the limits of fabrication and therefore of the limits of technology.

Section 3 examines how the concept of ultimate limits can be applied to simple and complex domains, and to domains in which scientific knowledge is known to be incomplete. Section 4 surveys conventional fabrication processes and their limitations, and § 5 examines molecular manufacturing as a fundamental alternative with fundamental advantages. Taking molecular manufacturing processes as a basis, §§ 6 and 7 revisit the implications of physical principles for limitations on fabrication. Widespread (though perhaps unexamined) opinion in the scientific community, however, suggests that a fundamental preliminary point (§ 2) must be first discussed.

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2. Can physical law tell us anything about technological possibilities?

It is, of course, philosophically possible that we are all quite wrong about the nature of the world in general and therefore about the consequences of physical law for the behaviour of matter in particular. Nonetheless, it is both conventional and wise, in most contexts, to base discussions of technological possibilities on phenomena that are observed or that are predicted by standard approximations to the best available models of physical law (i.e. the current standard model of theoretical physics). Inasmuch as physical law as presently understood implies many constraints on the behaviour of physical systems, including technological systems, it is clear one should, with some degree of confidence, be able to sort technological proposals into three categories: (1) those that are physically feasible, (2) those that are physically infeasible, and (3) those for which physical feasibility has not (or cannot) be determined. This proposition seems non-controversial.

Nonetheless, it is sometimes suggested that studies of the future of technology must by their nature be fruitless. This view seems rooted in a confusion between efforts to distinguish the feasible from the infeasible on physical grounds, and efforts to predict the detailed course of technological development in the marketplace. Since the latter would entail predicting the detailed course of human events, it is presumably unachievable. This paper confines itself to the more modest, less useful, but more practicable goal of exploring a few aspects of what physical law can tell us about the shape of technological possibilities. Because these possibilities depend on physical law and not on human activity or history, they have nothing to do with time or prediction except in one quite limited sense: we are reasonably sure that the ultimate limits of technology have not been approximated in the past or present, and so these possibilities – if they achieve physical reality at all – can do so only in the future. To the extent that one is willing to speculate that past trends toward greater technological capabilities will continue, the prediction that recognized physical possibilities will be achieved or exceeded may perhaps have some plausibility.

3. What are 'ultimate limits' in technology?

To examine the ultimate limits in some domain of technology, one typically adopts a model of physical law and attempts to draw inferences regarding its implications. The model itself may be questioned, but this constitutes an inquiry of a different kind. The nature of the appropriate model and degree of abstraction depends on the domain: studies of quantum measurement adopt standard quantum formalisms as a basis for analysing measurement processes, but seldom concern themselves with the materials properties of components of actual instruments. Studies of the thermodynamics of computation adopt standard principles of thermodynamics and statistical mechanics as a basis, but again seldom consider the materials properties of components.

To study fabrication processes, however, requires an approach that takes account of the complexities of condensed-matter structures and their transformations. In pursuing these studies, one typically adopts a model that embraces only ordinary matter under accessible conditions, implicitly excluding hypothetical processes involving exotic matter, monopoles, or pressures and densities found inside neutron stars (it is convenient that almost any conclusion regarding matter applies equally to antimatter, save for practical difficulties involving raw materials and tools).

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In domains that build directly on fundamental physical principles, results regarding ultimate limits are often clear and simple: the product of the uncertainties in the simultaneously measured position and momentum of a particle must exceed $h/4\pi$, the speed of light cannot be exceeded; a cycle that writes and erases a bit must dissipate at least $\ln(2)kT$ of free energy (Landauer 1961, 1982), and so forth. In domains involving materials and fabrication, however, many results will have a different character – not stating a limit precisely, but instead identifying upper or lower bounds on the value of an imprecisely known ultimate limit. For example, the tensile strength of diamond sets a firm lower bound to the ultimate limit of tensile strength. A series of upper bounds to the ultimate limit of tensile strength can be derived from quantum mechanical principles, with the easiest-to-derive upper bounds being quite large compared to the actual physical limits. Finally, the most accurate available picture of the ultimate limits in a complex field may include qualitative uncertainties. The best available picture of a set of complex limits may consist of fragmentary survey of what sorts of capabilities seem likely and unlikely to be possible.

4. Conventional fabrication

Many limitations of conventional fabrication processes result from their inability to directly control the motions of atoms and molecules during the formation of product objects. A brief review of the nature of typical conventional processes illustrates this point.

(*a*) *Inexact structures*

Most macroscopic objects are made by shaping materials either by a subtractive process (such as machining), a near-net-shape process (such as moulding), or an additive process (such as stereolithography). These processes are imprecise on an atomic scale, providing only approximate control of the shape of the resulting object. Further, the materials themselves either are imprecise on an atomic scale (e.g. having amorphous or granular microstructures) or are single-crystal structures of extreme regularity and simplicity. Relative to the vast number of ways that atoms can be arranged to make a 1 kg object, the number of arrangements that can be produced by conventional fabrication processes is minuscule.

In macroscopic objects made by conventional fabrication, most nearest-neighbor atomic contacts (which, taken together, define the structure) result not from the operations used to shape the object, but from the operations used to prepare the materials from which the object is made. These processing operations typically control the time-history of macroscopic variables such as composition, temperature, stress, and the like. The trajectories and final locations of the constituent atoms result chiefly from thermal vibration and interatomic potentials in a disordered, diffusive system. The final configurations accordingly depend on the thermodynamics and kinetics of spontaneously formed local patterns of atoms.

Most microlithographic processes are similar to macroscopic processes in this regard. Although many patterning technologies can produce submicron structures, the variables controlled are usually macroscopic relative to the atomic size scale, and most processes involve either volumetric or surface diffusion. Even the atomically precise layered structures produced by molecular beam epitaxy result from control

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of fluxes distributed over a macroscopic area, and accordingly give no precise control of transverse dimensions.

(*b*) *Exact structures*

The chief technology for producing complex, atomically precise structures today is organic synthesis. By controlling macroscopic variables such as composition and temperature during a series of reactions and purification processes, chemists can build atomically precise structures containing hundreds to thousands of atoms. In doing so, they exploit a large body of knowledge regarding the thermodynamics and kinetics of spontaneously formed local patterns of atoms in diffusive, solution-phase systems. Organic synthesis has in recent decades been extended to supramolecular chemistry, in which covalent structures are synthesized that subsequently undergo non-covalent assembly to form larger structures.

Organic synthesis and supramolecular chemistry face several basic difficulties. Because they rely on diffusion through solution to bring substructures together, at least one component in each reaction must be soluble. Further, each substructure must be chosen (or designed) to exhibit strong reactivity with only a single partner and with a single result; tendencies for a substructure to combine with copies of itself, or with inappropriate parts of other substructures, usually reduce the yield of the desired product. In organic synthesis, a yield of 90% is ordinarily considered high, yet a series of 200 sequential steps with this yield would convert 10^3 kg of reagents into less than 0.001 g of product. One thousand sequential steps would quite reliably yield no product at all. These difficulties impose severe constraints on organic synthesis and significantly limit the kinds of structures that can be built by supramolecular assembly. Despite these limits, however, it appears that chemical techniques can produce structures that can assemble to form devices that can perform the operations necessary for molecular manufacturing (Drexler 1994).

(*c*) *Limitations of current fabrication processes*

The shortcomings of current fabrication processes, when considered from the perspective of ultimate limits, are dramatic. The number of distinct covalent, three-dimensional, highly polycyclic structures (here termed 'diamondoid') that can occupy a volume of one cubic nanometer has been estimated to be greater than 10^{148} (Drexler 1992). This volume can contain more than 100 atoms, each chosen from one of many elements, and even a pure-carbon structure with exactly 100 atoms could exist in many stable bonding patterns.

Most of these structures are irregular and asymmetrical, and hence cannot be made by techniques that produce crystals. Since 10^{148} is greater than the number of particles in the observable universe, random generation processes would be ineffective, to say nothing of inefficient. The technology most nearly suited for this task today is organic synthesis, yet no irregular, prespecified diamondoid structure approaching 100 atoms has ever been made by these means. Accordingly, the probability that modern technology can fabricate a particular randomly picked structure from the set defined above is effectively zero. Present synthetic techniques can make almost any specified structure, provided that it is stable and contains no more than a few atoms. Out of the total set of stable objects containing 100 or more atoms, however, present technology can make almost nothing.

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5. Molecular manufacturing

The term 'molecular manufacturing' has been coined to describe a set of anticipated fabrication capabilities based on mechanically guided chemical synthesis (mechanosynthesis). In his 1959 talk, 'There's plenty of room at the bottom' (Feynman 1960), Richard Feynman pointed in this direction, stating

> The principles of physics, as far as I can see, do not speak against the possibility of maneuvering things atom by atom. ... Ultimately, we can do chemical synthesis. A chemist comes to us and says, 'Look, I want a molecule that has the atoms arranged thus and so; make me that molecule.' ... [It] would be, in principle, possible (I think) for a physicist to synthesize any chemical substance that the chemist writes down. ... How? Put the atoms down where the chemist says, and so you make the substance.

The principles of physics do indeed permit chemically precise manoeuvring of atoms and molecules, although the processes that occur during mechanosynthetic encounters might better be described as chemical reactions than as putting down atoms. Current analyses of molecular manufacturing include considerable detail regarding these processes, and embrace systems able to produce chemically precise structures containing more than 10^{10} atoms, far beyond the descriptive abilities of even the most diligent chemist.

Practical molecular manufacturing processes must use machines with components of microscopic scale, preferably built with atomic precision. (Such machines are themselves natural candidates for production using molecular manufacturing.) Design and modeling exercises indicate that machines of substantial complexity (e.g. six-axis robotic positioning mechanisms) can be built on a 100 nm scale (Drexler 1992). The physical possibility of durable, nanoscale moving parts (despite intermolecular forces) is demonstrated by the durable mobility of solvent molecules in solution, by the low frictional forces between misaligned graphitic planes, and by the observed motions of molecular machines in biological systems (e.g. the bacterial flagellar motor).

In conventional manufacturing, a standard method for creating complex structures is to grasp parts and place them where the designer has directed. (Other techniques, such as machining and moulding, have a comparable directness in the relationship between tool geometries and product structure.) Molecular manufacturing will apply this elementary principle to the molecular domain, replacing diffusive molecular motions with mechanically guided motions. The spelling of 'IBM' using 35 xenon atoms positioned by the tip of a scanning tunnelling microscope (Eigler 1990) provided the first clear laboratory demonstration of this principle. Although the specific technique demonstrated in this work was unable to produce stable structures of practical interest, Feynman's vision of 'maneuvering things atom by atom' had clearly been realized.

In conventional manufacturing, no two products are identical. In molecular manufacturing, as in digital logic, processes can be precise: the products consist of a precise number of parts (atoms, bits) of distinct kinds (elements, logic states) in distinct arrangements (patterns of bonding, sequences in memory). Accordingly, two products can be identical, and the distinction between a correct structure and an incorrect structure can be unambiguous. The following section discusses the physical principles that determine the reliability of the potentially precise processes of molecular manufacturing, together with the broader issue of physical limits to fabrication processes.

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6. Physical limits to fabrication

In a pure but impractical sense, the fundamental physical limits on what can be fabricated appear to coincide with the physical limits on what can stably exist. In the approximation that physical law is time symmetric, any structure that can be converted into a thermodynamically equilibrated high-temperature vapour can with some non-zero (but usually negligible) probability be formed from such a vapour. (Given the observed charge–parity–time symmetry of physical law, a more precise statement would be that any structure can be formed from a vapour with some non-zero probability, provided that its antimatter equivalent could be vaporized, but this is an academic refinement of a rather academic point.) Condensation is, of course, seldom a practical fabrication technique for precise objects more complex than fullerenes.

A less well-defined but more significant set of limits circumscribes the set of objects that can be made with high reliability given a reasonable amount of time and material. These limits appear to be more constraining than mere physical stability. Although no formal proof has been given, it seems reasonable to assume that structures can be designed such that they would be stable in their final configuration, yet unstable on all trajectories through phase space leading to that final configuration. Certain structures with large internal stresses may be members of this class. More generally, structures of low stability (e.g. liquids, gels) do not lend themselves either to precise structural definition or to step-wise construction using reliable assembly operations. The upper bounds on fabrication capabilities in such areas resist clear definition.

(*a*) *Diamondoid structures*

Lower bounds on fabrication capabilities are more clear among objects selected from the relatively narrow set of highly stable covalent solids. These diamondoid structures are, fortunately, of special interest in technology. They include the extrema for strength, stiffness, and thermal conductivity among known and projected materials. They include excellent semiconductors, good insulators, and (if one includes locally polymeric and graphitic structures) excellent conductors. What is more, many of their mechanical properties can be well described by highly localized models based on two- three- and four-body potentials defined in terms of atomic coordinates (Burkert 1982; Clark 1985). The field of organic chemistry has gained extensive knowledge of the structure and properties of carbon-rich covalent objects of subnanometer size (i.e. typical organic molecules), and has found that this knowledge applies with little modification to objects of larger size (e.g. macromolecules and covalent solids with surfaces of low chemical reactivity). It will not do to say that nanoscale covalent objects constitute a domain in which we are fundamentally ignorant. Knowledge here is of course incomplete, yet it is both broad and deep.

Research in organic synthesis has developed techniques for making a wide range of small covalent structures. Most of these result from a series of molecular collisions, rearrangements, and fragmentation reactions that occur spontaneously in solution, driven by thermal energy and directed by intermolecular potentials. Molecular manufacturing will exploit these and other interactions, driven by both thermal and mechanical energy and guided by stiff positioning mechanisms. In light of the wide range of operations and products demonstrated by organic synthesis, the chief physical question to be answered regarding molecular manufacturing is whether

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nanomechanical positioning mechanisms can in fact guide these operations with high reliability, so as to enable the construction of objects with many distinct molecular features.

(*b*) *Thermal noise and quantum uncertainty*

Thermal noise and quantum uncertainty cause positional errors that degrade the reliability of molecular manufacturing processes. Provided that ionizing radiation levels are moderate and that the structures being manipulated have good thermal stability, these positional errors are the chief identified cause of defects in molecular manufacturing. A fully quantum mechanical treatment of positional uncertainty resulting from the joint effects of quantum uncertainty and thermal noise in a variety of structures is presented in (Drexler 1992). For nanometer scale objects at room temperature, this analysis indicates that the simpler results from classical statistical mechanics predict mean square displacements to within a few percent or better. For a displacement along a coordinate characterized by a restoring force of k_s N m^{-1}, the mean square displacement,

$$\sigma^2 = kT/k_s.$$

The probability density function along such a coordinate is Gaussian. The reaction rate between a positioned molecular species A and a potentially reactive structure B will be proportional to the probability density of A at the position of B, all else being equal. The error rate of a mechanosynthetic process will accordingly depend on the ratio of probability densities at the target reaction site and at the nearest sites that can undergo a misreaction. This, in turn will depend on the stiffness of the positioning mechanism k_s, the temperature T, and the distance between the target site and the potential error sites.

The separation of lattice sites on a diamond (111) surface, 0.25 nm, can be taken as a typical distance in the above calculation. At room temperature, 300 K, the probability of a reaction directed to one site instead occurring at an adjacent site will be less than 10^{-15} provided that the stiffness $k_s > 5$ N m^{-1}. Inasmuch as the shear stiffness of a cubic-nanometre block of diamond is about 500 N m^{-1} (and stiffness increases in proportion to size), while the bending stiffness of a single carbon–carbon bond with respect to an sp^3 site is about 30 N m^{-1}, it should not be surprising that positioning mechanisms with stiffnesses greater than 10 N m^{-1} are feasible (Drexler 1992). Error rates for molecular assembly of less than 10^{-15} permit the construction of nanoscale systems of substantial complexity.

7. Speed, efficiency, and productivity

The discussion in § 6 addresses the qualitative limits of fabrication, asking what kinds of objects can be made, and with what reliability. For the special but technologically important case of stable covalent solids, it appears that these limits are quite broad: such structures can be build incrementally with reliable control over the destination of each atom.

It might be thought that this physical possibility is of little practical interest because any process that handles matter in such small particles will of necessity be slow and expensive. Surprisingly, this expectation appears to be incorrect. As suggested by the scaling laws illustrated in figure 1, the high frequencies characteristic of small machines enable them to be extraordinarily productive, both in terms of

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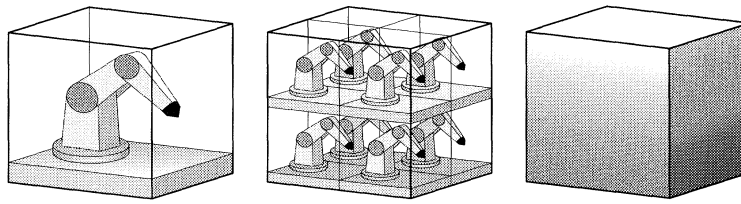

total mass/kg	100	=	=	=
arm length/m	1	$\frac{1}{2}$	10^{-7}	=
number of arms	1	8	10^{21}	=
frequency/s^{-1}	1	2	10^{7}	10^{4}
assembly rate/s^{-1}	1	16	10^{28}	10^{25}
throughput/(kg s^{-1})	1	2	10^{7}	10^{4}
friction losses/W	10	20	10^{8}	10^{2}

Figure 1. Physical scaling laws imply high productivity for small-scale manufacturing devices. The first column lists arbitrarily chosen parameters for a hypothetical metre-scale manufacturing assembly unit. The second and third columns present scaled parameters for geometrically similar devices of 0.5 m and 0.1 μm scales. The scaling of power dissipation corresponds to a viscous drag mechanism (such as interfacial phonon scattering), with forces proportional to shearing speed. The final column illustrates power savings resulting from slower motion. The illustrated arrays of assembly units do not correspond to complete, workable systems, which would require mechanisms for materials transport, power supply, cooling, control, and so forth.

parts handled per second per kilogram of mechanism and in terms of kilograms of product per second per kilogram of mechanism. Moreover, detailed studies of molecular manufacturing processes (Drexler 1992) have not identified a requirement for grossly wasteful energy dissipation at any stage. The free energy input required to organize matter into a precise solid structure, starting with raw materials in solution, is typically dominated by the change in the molecular potential energy of the system. The entropic cost of the transformation is comparable to that of solidifying a liquid to a crystalline solid. Accordingly, the present evidence suggests that molecular manufacturing processes can be precise, highly productive, and reasonably efficient.

8. Conclusions

Present knowledge of physical law, combined with present abilities in physical and computational experimentation, cannot tell us all we might like to know about technological possibilities. This body of knowledge and ability is, however, adequate to set both upper and lower bounds on technological possibilities in some areas with some degree of confidence. Fabrication capabilities are basic to technological capabilities in most fields, and hence the limits of fabrication are a central question in addressing the limits of technology.

It seems likely that some physically stable structures will prove impossible to make with any significant probability of success. Members of a broad class of diamondoid structures, however, are both stable and accessible through a series of stable intermediate structures. Mechanical devices can guide reactive molecules with atomic precision and high reliability, enabling the construction of covalent solids having complex, atomically specified structures. This capability will greatly expand the range of structures that can be made, and will greatly increase the performance of devices

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that are constrained by strength of materials, stiffness, defect densities, geometrical precision, or any of several other parameters. Because molecular manufacturing also promises to be productive and reasonably efficient, it appears that developments in this area could open a broad new domain of science and technology.

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