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The challenges of nanostructures for theory

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Abstract

It is tempting to believe that modelling in nanotechnology is much the same as that for conventional solid-state physics. However, important areas of nanotechnology address different systems. The mechanics of DNA (for instance) resembles spaghetti more than silicon, the statistical physics needed is often not carrier statistics, and the role of viscosity (the low Reynolds number limit) is not always the familiar one. The idea of equilibrium may be irrelevant, as the kinetics of nonequilibrium (perhaps quasi-steady state) can be crucial. Even when the issues are limited to nanoscale structures (rather than functions), there is a complex range of ideas. Some features, like elasticity and electrostatic energies, have clear macroscopic analogies, but different questions emerge, such as the accuracy of self-organisation. Others concepts like epitaxy and templating are usually micro- or mesostructural. Some of the ideas, which emerge in modelling for the nanoscale, suggest parallels between molecular motors and recombination enhanced diffusion in semiconductors.

Keywords: Materials modelling; Nanotechnology; Knowledge management; Validation

1. Introduction

Nanostructures present both generic challenges and temptations to the theorist. The first challenge is to identify the issues. What are the most important scientific ingredients? The temptation is to assume the significant questions are the familiar questions. The second challenge is to bring together appropriate theories to address the key issues, whether computer-based, analytical, or statistical. They may be bottom–up theories, reaching from electrons and atoms towards large objects. They may be top–down theories, starting from the macroscopic, hoping to avoid the problems of the atomic scale. The temptation is to believe that all the ingredients are available at the starting level. The third challenge is how to introduce microstructure specific to the mesoscale. Does one use an empirical structure from an electron micrograph, or is it preferable to use theory to mimic a mesostructure? The temptation is to believe that structures that look alike actually behave alike.

The fourth challenge may be the most important: process is more significant than structure. Structures are not validated by appearance alone, but by how they perform. Knowledge of ground-state energies for idealised systems, crystal structures, and surface reconstructions is only a start. Knowing genome structure is a start to understanding how defined molecular components generate a physiological output [1]. It is far more important to understand behaviour, even if prediction is incomplete.

Understanding is crucial in real-world applications. It may be hard to define an appropriate central problem in computable form. Many biomedical phenomena have still to be formulated in computable ways. How can protons passing through a membrane drive the complex motions of soft solids in ATP production? Yet, without understanding, it may be even harder to convince others, especially those with a real-world problem, that nanoscale models provide valid and useful solutions. Even in mature areas, the best methods with experienced users can still give poor results. This weakness matters less if understanding has been achieved in attempts to answer key questions. In evolving areas, we must seek to identify the right questions, not merely follow the easier option of using our favourite codes.

2. Seeking the nanoscale

Nanotechnology exploits smaller and smaller ensembles of atoms. There are typically 10^{16} atoms in a 0.1 mm dust particle, 10^{13} atoms in a typical 10 μm grain, 10^{8-9} atoms in typical bacterial DNA, 10^{6-8} atoms in a typical self-organised nanodot (one which shows the Coulomb blockade), 10^{3-4} atoms in a small single-wall buckeytube, and a mere

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10^{2-3} atoms in small nanodots showing electron confinement effects, or in certain neurotransmitters, like serotonin. As interest focuses on smaller and smaller units, so computer power is growing enormously with rapid, apparently exponential, growths of the number of devices on a chip, of global users of communications, and of fabrication plant costs. There is a correspondingly rapid fall in the numbers of atoms needed to store a bit of information and in the number of electrons to turn a transistor on or off [2]. It is common to see so-called first-principle calculations with 10^{2-3} atoms, or over 10^3 atoms handled with simpler self-consistent methods; as many as 10^{10-11} atoms have been treated with molecular dynamics.

Does this mean we could solve all the key problems by large calculations? Sadly no, although computer-based science makes potent contributions. Scientific computing has three interdependent strands: hardware, software, and links to real or imagined worlds. Research is more than writing or running code. Is there something significant to compute? Will new ideas emerge from large calculations, ideas not surmised in earlier work, such as major new ideas on dislocations not appreciated by Cottrell, Frank, and Mott? Even supposing that one can define a central problem in computable form and run appropriate software, will we be sure that the ideas are right, in the sense that model systems and real systems behave similarly? Last, but by no means least, convince others that the results are both valid and useful?

3. The uniqueness of the nanoscale

The prefix "nano-" is often used imprecisely. At one extreme, there are characteristic lengths that are clearly "micro-": grain diameters are often of order 10 μm; the wavelength of yellow light is of order 5 μm; conventional thin films are 1–2 μm thick. At the other extreme are atoms and small molecules. In between, one has Debye–Hückel screening lengths of perhaps 10 nm, neck displacements in the myosin motor of order 5–10 nm, globular proteins of 6 nm diameter, and II–VI quantum dots of 1–2 nm diameter; gate oxide films of a few nanometres, falling towards 1–2 nm. The use of both inorganic and organic systems opens new fields. The organic component can be biological, even if not, it could include chiral molecules and other more exotic forms. Two common views of the nanoscale are *top–down* (macroscopic written small) or *bottom–up* (molecular written large). Both are valuable, but both are seriously incomplete.

Nanotechnology spans the physical and the biological sciences. This immediately challenges some common views. Physicists commonly think in terms of internal energies and enthalpies. Some of the physics community believe the major questions are of bulk (infinite size) crystal structure, meaning the structure of lowest internal energy (hence graphite, not diamond, for carbon). Biologists, who deal with soft solids, may find that the entropy is more significant. Physicists often take homogeneity for granted, and regard the elasticity as the basic continuum model for condensed matter. Biologists have to deal with soft, non-crystalline, solids, interface phenomena including hydrophobicity and low Reynolds number systems [3]. When the issues are ones of structural control on the nanoscale, these differences matter. Computer modelling cannot concentrate on a single vision of what is important. Nor can it concentrate on equilibrium: the kinetics of nonequilibrium (maybe quasi steady state) systems can be crucial. This is especially important when energetic particle radiation is used [4]. Excitation provides an important opportunity. Thermal processing becomes an indiscriminate tool at the nanoscale. Processes, which are more selective in space and in species, are needed. Electronic excitation is one approach since it offers spectral and spatial selectivity: the electronic ground state is not always helpful.

What makes this smaller length scale special includes the so-called $(N+1)$ problem. If there is a nanoscale object of N atoms, then adding an atom can transform its behaviour. The $(N+1)$ atom system can differ from the N-atom system in several ways. Adding an ion to a II–VI dot will lead to a very large electric field, which will polarise electron-hole excitations and may suppress radiative recombination. A minor change in the topology of a buckeytube can give it quite different electronic properties. Surface energy terms gain importance, e.g., causing the Rayleigh instability in fine wires [5]. Electrostatic interactions are very important. Even for the larger quantum dots, the (static) Coulomb blockade restricts the charge, which can be localised on a small particle. Dynamically, the charge, which can be introduced into a small region by a photon, puts an upper limit on the energy of ions [6] ablated from MgO [7]. The image interaction at interfaces [8] between media of different polarisabilities can switch nonwetting to wetting. Magnetism is much weaker (1 μ_B gives a field of about 1 T at 1 Å); electromagnetism at the nanoscale can usually be ignored. The range of elastic interactions makes them important in self-organisation and in correlating motion of particles on surfaces [9,10]. Vibrational energies cannot be assumed continuous. For a 200-atom quantum dot of no special symmetry, with a maximum phonon energy of 35 meV and 600 modes, the typical spacings between vibrational mode is of order 1 cm^{-1} (10^{-4} eV). Structures as complex as proteins are enabled by molecules with hydrophobic terminations in aqueous solution (e.g., Ref. [11]). Whereas physicists assume that enthalpy dominates, entropy can prove important. For allosteric effects (in which adding a molecule X at one point in a structure affects the binding of molecule Y at a remote site (e.g., Ref. [12])), it is possible that vibrational entropy is the crucial factor [13]. In templating, a major factor can be configurational entropy.

Statistics and fluctuations are recurrent features of the nanoscale. The Casimir force can be significant, associated in part with zero-point energy. Thermal fluctuations matter. The root mean square volume fluctuation of a 200-atom quantum dot is about 1% at room temperature [14]. In every second, a typical 1 μm radius cell in water "experiences a thermal knock equal to its weight" [15]. There are continuing arguments about how cells make new parts, and whether there are static frameworks (templates), or whether intracellular structures form and disappear in a dynamic self-organised manner [16]. In some processes, it is the rare events, which are crucial, rather than fluctuations close to an average value. These sometimes lead to behaviour which is referred to as self-organised criticality, but is more often simply identified with extremal statistics [17,18].

Forces at the atomistic level are usually defined in terms of interatomic potentials. Forces due to the change of zero-point energy of light atoms may be included, yet generalisation to handle other vibrational or entropic terms is rare. In a macroscopic description, stress is the natural concept. For the nanoscale, for instance, in a molecular motor, different approaches are needed. First, the fluctuations may be comparable to the forces. Secondly, there is a temptation to be casual about where the force acts. Thirdly, the dissipative forces of viscosity and friction become much more important than inertia [3]. Stick/slip behaviour (stiction) can become crucial. Fourthly, the balance between forces may change. Scanning probe tips will crash because of instabilities associated with dispersion forces [19].

Molecular motors illustrate the complexities of fluctuation phenomena. Different "force" definitions [20] include a maximum driving force (defined by the free energy available and the step length), an Einstein force (related to Brownian-type motion), and a stalling force determined by the effects of an external force due to optical tweezers. These forces are formal, in the sense that no questions are asked about where the forces act. Yet, to link to either the atomic scale or the macroscopic scale, such questions matter. In the molecular motor, which creates ATP, protons moving through a membrane appear to cause a cylindrical structure to rotate, in that a molecule on the top of the cylinder rotates as ATP production proceeds [21]. But what is the means by which the available energy can cause a cylinder of material with the consistency of cooked spaghetti to rotate almost rigidly? Since viscosity will dominate inertia, this seems possible only if the rotation is driven by forces on the outside of the cylinder. It is hard to give these forces a physics-style description. An alternative, if heretical, speculation [22] is that there is no rotation, simply the rotational equivalent of peristalsis, driven by phased compression near the axis of the cylinder. The rotation of the added molecule would then resemble that of a well-known children's toy in which a propellor rotates at the end of a rubbed notched stick.

4. Modelling and its role in microtechnologies

The major aims of research include *understanding* and *insight*. Understanding allows one to interpret, to identify the important, and to recognise potential extreme situations. Insight allows one to generalise, to unravel ill-posed questions, and to create a *framework* for the next level of question. Theory (of which computing is one component) supports these aims at several levels. The simplest provides the framework. Even the most practical engineer uses theoretical ideas to shape empirical information. Theory's next stage is *scoping*. When faced with something new or complex, theory helps to decide which factors matter. For the complex, validated simple ideas can enable useful decisions, e.g., the image interaction picture of metal/oxide adhesion. Scoping is especially important for hierarchical situations, where there is a history dependence. In some cases, serious modelling offers the chance (dare one say it?) to beat experiment, especially for regimes where experiment is impractical: reaching for extremes, such as the femtosecond and million year scenarios; the light year and the nanometre. When is the computer essential, as opposed to merely aiding decorative graphics and tidy preprints? The very best computer experiments can be full of insight and surprises but only if they address the right questions, rather than concentrating on the calculations which are convenient.

Microelectronics materials modelling is a natural area for the computer. Band structure calculations were among the first *general-purpose* codes. Science and need together led to the phenomenal progress in the 1950s and 1960s. Will materials modelling have the same impact on 21st century nanotechnology? If not, is this because the problems are solved and technology is getting on with it, or because science and technology are ignoring each other?

With continuing miniaturisation, modelling is still needed. The Semiconductor Industry's Roadmap describes its best judgements of achievable trends, and indicates that at least four new materials will be needed at the 0.18 and 0.13 μm levels. Quantum computing, if viable, will need still more. The Semiconductor Industry's Roadmap identifies roadblocks, where there is no known solution to the technical problem. The gate dielectric is an example. Miniaturisation demands thinner silicon dioxide dielectrics. Below about 10 atomic layers of oxide, there are problems of tunnelling and of degradation and breakdown. A conceivable solution is to choose another oxide with higher dielectric constant, to obtain the same performance for a thickness sufficient to reduce tunnelling acceptably. The challenges are formidable. A credible alternative is wanted in 4 years; yet, silicon dioxide has the fruits of nearly 40 years of experience and development.

The gate dielectric issues are varied (e.g., Ref. [23]): the value of the dielectric constant, limits on charge traps, band offsets, reproducibility (including density, if amorphous, and stoichiometry, for instance), processability, and stability against degradation and breakdown. Other issues concern assessing the oxide quality without driving it to failure, and establishing diffusion processes. Silicon dioxide has a major advantage in that most diffusion is by neutral species, whereas it is ionic in many other oxides, so that solid-state electrolysis will occur. Defects (whether point defects, topological defects, or dislocations) can trap charge, and the relative energies of different charge states are needed. The dielectric need not be homogeneous, with possible qualitative differences near the interfaces. Some important aspects concern the nature of the excited states, and the energy localisation which can drive degradation [24]. These are areas where current materials modelling is weak: its emphasis on ground states and homogeneous crystal structure are of limited relevance.

How has theory and modelling contribute to the gate dielectric problem? At the simplest level, the reaction–diffusion (Deal–Grove) model provides the accepted framework. This model fails worse and worse as thinner oxide is needed [25]. Atomistic studies [26] lead to interpretations consistent with both the major and the subtler features of oxidation. These same results also suggest strategies based on applied electric fields, which might lead to improvement in oxide quality.

5. Computing for emerging technologies: nanotechnology and its challenges

We shall use the term *nanotechnology* to indicate that there are critical features with dimensions of a few nanometres. Such scale lengths are shorter than photon wavelengths and often less than electron mean free paths. Electron tunnelling may be significant; excitations, including plasmons, are substantially modified; interface boundary conditions need special care, and macroscopic averages may mislead. It includes the means to monitor, control, and carry out experiments on the nanoscale. The systems are not limited to semiconductors, micromachines, quantum dots, wires or layers, or to conductors whose dimensions are less than electron mean free paths. Soft matter is included. One seeks the capability to mimic natural phenomena, photosynthesis, protein folding, and molecular motors [27]. It should be possible to combine the organic and inorganic, and to replicate on a large scale. How can computing address the range of related scientific and technological themes encompassed in nanotechnology? The brute-force method is to *compute* the behaviour of large numbers of atoms. Another route is to use the computer to *understand* the characteristics of the driving forces. The aim is to identify those key useful ideas, which can be applied to really useful systems, even when those systems are far too complex for state-of-the-art basic science.

Nanotechnology rightly includes ways to build chosen spatial structures, and how to manipulate energy levels or densities of states. One hope for nanotechnology is the creation of replicated nanolaboratories so that many experiments (like drug testing) might be done in parallel. This relies on a nanoengineering capability to control structures at the smallest scale, and on the ability to analyse routes to exercise such control.

If we wish to model the mechanisms that enable control, what are the computing issues? The ideas being exploited might include epitaxy (and hence templates, ordered surface structures), elasticity (and so elastic strain as a part of self-organisation), electrostatics (including dipoles associated with water), hydrophobicity and hydrophyllicity, controlled instabilities and spatial features, which characterise the fastest-growing instabilities (as in spinodal decomposition), the use of selective excitation to define processes which are to be enhanced, and the direct manipulation of atoms and molecules with scanning probes.

These ideas are not handled on an equal footing in standard codes. Indeed, it is not clear that a single code should be used. What is clear is that any description should give a realistic estimate of the *accuracy* of control. Will self-organised dots be accurate enough for a chosen application? Tunnelling is very sensitive to barrier thicknesses, and needs far greater structural accuracy than electron confinement [28]. Can one use efficiently systems with properties that are variable from one nanoobject to another? Will a biological process be so well adapted that it only does what you would wish? I shall discuss some of the pervasive ideas (epitaxy, elasticity, electrostatics, templating, excited states, hierarchical behaviour) in the context of available computing capability.

The familiar idea of *epitaxy* comes from crystal structure: which interfaces will form when one tries to fit two crystals lattices together? Sometimes, one can draw on macroscopic analogies with surface tension, such as wetting. Geometric structure and mismatch are always important on the nanoscale. For ionic solids, there is a large energy cost in placing two ions of the same sign in proximity. This leads to the characteristically different structures for twist and tilt grain boundaries [29], which incidentally, were identified by thought and validated by computer. For ideal surfaces in contact, computer methods are well developed, and there is a substantial framework of understanding [30]. Ideas such as misfit dislocations, if tricky to include explicitly in atomistic codes, present no major problems.

However, the idea of a “perfect” interface is unreal. Cleaved MgO, for instance, usually has steps and sites where dislocations or grain boundaries intercept the surface. These are unpredictable, but important: they provide sites that readily absorb energy in laser ablation; they are sites where nucleation of adsorbed phases is relatively easy; they are usually electrostatically charged. The issues leading to an understanding of “real” surfaces are not addressed in current computer methods, yet they are important in many applications. Even for the simpler interfaces of simple oxides, like MgO, there is little cause for complacency.

Misfit dislocations are not the only consequence of nanoscale *elasticity*. A surface will be deformed by the particles on it, and the strain causes interactions between these particles. It is these strains that drive *self-organisation*, both in the bulk (the void lattice, shear planes) and at surfaces. For many purposes, continuum elasticity suffices, generalised somewhat to include interfacial energies. Finite difference methods are useful, if questionable for lengths below a few nanometres. A central problem in self-organisation, not addressed in discussions of average behaviour, is that self-organisation is not especially accurate for real systems. This is very clear for the void lattice [31], where the long-range order of tens of millions of voids is excellent, but the individual voids vary. It is not clear that self-organised quantum dots will be sufficiently reproducible for some of their planned applications. The accuracy needed, of course, depends greatly on the application. It remains to be established whether vertical-emitting cavity lasers based on self-organised dots will be accurate enough, or whether some combination of modulators and external sources would be preferable. For photonic devices, clever processes can achieve good quality [32,33]. For certain self-assembled organic FETs, the level of self-organisation does not have to be too great [34]. In biological systems, concepts such as pattern, complexity, emergence, positive and negative feedback, and the amplification of fluctuations are essential [35].

Both physical and biological processing exploit *templating*, in which a pattern is created on a surface, and that pattern is transferred to some object coming into contact with that surface. Templates often underlie ideas of nucleation, although the ideas can be simplistic, and sometimes ignore the substantial effects of thermal motion. The simplest pattern transfers involve plastic deformation, like stamping a coin. However, the nature of plastic deformation at the nanoscale may be unfamiliar in form, since dislocations will not have the same central role. Quite different is graphoepitaxy, where a film grows on a structured substrate. In this case, straightforward Monte Carlo methods may suffice. For example, there is the remarkable observation [36,37] of an epitaxial relation between substrate crystal C' and deposited crystal C'' when there is an intermediate amorphous layer A (i.e., a $C''/A/C'$ structure). The key assumption [38] is that the substrate C' has crystallographically determined surface features, like steps. The surface topography of the amorphous layer A maintains some memory of these steps, which guide the crystallographic orientation of C''. Monte Carlo calculations support this idea for nanoscale amorphous layers.

For templating by flexible polymer or biomolecule coils, the configuration is guided by specific sites on the substrate to which certain components of another molecule bind preferentially. There is a nontrivial problem in statistical physics [39], and an analytical treatment may be more useful than a computer approach. A fully computer-based explanation would need to combine the statistical ideas with local energetics, and including thermal fluctuations, which can have significant amplitude. Thermal fluctuations are so significant that, in living things, nature does not seem to attempt to achieve perfect fidelity using repair enzymes [40], a situation far removed from average solid-state modelling.

Specificity of interactions is a common idea, with applications ranging from gas sensors to transmitter/receptor interactions. Whereas templating can be achieved by “lock and key” mechanisms, it is necessary but by no means sufficient in other applications that critical parts of molecules must fit. “Lock and key” ideas are exploited in molecular modelling software and in computer-aided drug design. Far less attention is given to what happens when the fit is successful. There must be more than physical contact and shape matching; something must happen as a result. There may be electron transfer, or proton transfer, for instance. These processes are far harder to model, although a proton transfer mechanism for serotonin has been shown using self-consistent molecular dynamics [41].

How could templates be created? Lithography is a possibility, whether by photons or electrons. The writing, and subsequent processing before use, will usually involve electronic excited states. Alternatively, the templates might be written by a nanomachine, perhaps a scanning probe system. Or they might exploit reactions with a molecule of specific shape, dimensions, and with chosen properties, such as hydrophobicity or hydrophyllicity. Still, further methods could exploit geometrical features of a substrate, such as steps on low-angle surfaces. They might include ordering which minimises some energy, as in a domain structure, which results from the fastest-forming instability, as in spinodal decomposition. When only the most simple templating is needed (one might include texturing as an extreme limit), ion-beam methods or even mechanical combing can suffice.

Modified surface layers can be very significant for moving interfaces at the nanoscale. For micromechanical machines, the underlying atomic structure may be less critical than the thermal oxide on silicon, or adsorbed moisture on a surface exposed to the atmosphere, or a space-charge layer in an insulator. The importance of these layers stems partly from the increased significance of friction over inertia, and partly because contact charging and tribocharging can be important and, on the whole, not understood.

At the nanoscale, *electrostatics* and the quantisation of electric charge become important. Two carriers in a modest-sized quantum dot will interact with energies in excess of thermal energies or those from standard applied voltages (the Coulomb blockade). In a medium of dielectric constant 5, two electronic point charges closer than 10 nm interact with an energy greater than kT at room temperature. The screening of Coulomb interactions is crucial in understanding colloids and near-surface defect atmospheres. For still smaller dots, typically II–VI dots with a few hundred atoms, one key feature is their net dipole moment [42]. The dipole moment affects strongly the electronic states, with the large internal electric field affecting matrix elements for recombination after optical excitation. The dipole moment further affects the lattice vibrational modes and energy transfer to the dot’s environment, with distinctive local modes which can remain excited for significant times.

Electrostatics is a major factor in the interaction between ionic oxides and relatively unreactive metals. A key idea is the *image interaction* [8,43]. If a conductive material, like copper, is in contact with an ionic material, like sodium chloride, the ions cause charge to redistribute in the metal. State-of-the-art computer methods validate the idea of the image interaction, so that the simple ideas can be exploited for systems (like the interaction between spent nuclear fuel and its irradiated alloy clad), which are far too complex for state-of-the-art approaches. The same ideas can be carried over to the nanoscale, where image interactions influence AFM imaging. In principle, surface phenomena can be controlled by using scanning probes to manipulate charge on surfaces, although this can be slow.

As feature sizes of microelectronic devices fall, so standard thermal processing becomes problematic. Thermal budgets become small, and thermal diffusion must be limited. Thermal diffusion should only move the species that one wishes to move. But thermally induced diffusion is less discriminating; the activation energies allow only limited control. Certainly, focussed lasers or electron beams can supply heat to relatively small regions, but such sources are more effective for *electronic excitation*. Electronic excitation can give local control of diffusion, energy deposition, or atom emission [24]. Excitation, and especially the localisation and controlled local transfer of excitation energy, underlies such phenomena as nanolithography of inorganic and organic species. Even ultra-low energy electrons (a few electron volts) can have substantial effects on DNA [44] or on silicon oxidation. It is not simply one-electron excitations that matter: collective excitations like plasmons can also be used in nanoscale devices [45]. Current codes are not well equipped to study excitations.

In nanotechnology, methods to produce some chosen structure must satisfy certain conditions, such as *speed*, *performance*, and *precision*. Computer modelling has done more than finding a structure that minimises an internal energy. A likely trend is the use of computer modelling for control of nanoscale phenomena in real time. To achieve this, one must model not only the nanoscale phenomena, but also the experiment that monitors what is happening. Among the more challenging areas are the control of instabilities, the control of interfacial charges, and the control of processes induced by electronic excitation.

Parallels can be drawn between diffusion in semiconductors enhanced by electron-hole recombination (e.g., Ref. [24]) and the actin/myosin motor of muscle, driven by ATP hydrolysis. Experiments with myosin attached to an AFM tip [46] show the myosin motor to be strongly biased (a thermal ratchet), with jumps often correlated over perhaps five of the obvious jump lengths, and thermal motion of the myosin head amplitude of 13 nm (not bound to the AFM; 4.5 nm when bound), cf. typically 0.01 nm for the shorter, unbiased, semiconductor diffusion. For neither system is the mechanism clear by which energy is transformed into motion, and there are reasonable doubts about the more popular descriptions.

There seems little doubt that *quantum* ideas and quantum phenomena will be central to 21st century science and technology, as were the electron in the 20th century and the chemical atom in the 19th century. Quantum encryption is possible, indeed demonstrated. Quantum computing beyond the most modest level is conceivable. Such quantum computing will need universal gates, which if realised in a silicon-compatible form, will need skillful nanotechnology in their construction and linkage.

6. General issues

New hardware and software provide opportunities for future nanotechnology. But is the science that results driven by computational opportunism, or is there some deeper intellectual idea or application need that determines the broad trends? Can we make sense both of the real nanoworld and of the imagined world in our computers? Even in major research areas, whether the rapidly developing current areas of microelectronics, or the emerging nanotechnologies, one sees core issues to which most scientists have paid little attention. Some are technical gaps: how to carry out certain calculations effectively. Some are serious conceptual difficulties: what are the right questions to ask about protein folding?

Research and development have different computer needs. In development activities, key requirements include *reliability*, *realism*, and *compatibility*. Issues might also include avoidance of the side-effects of technology, designs for safety and ease of operation, or the optimising of processing and use of materials, so reducing use of natural resources and minimising waste and pollution. The problem is *social acceptance* and, again, *confidence in the answers*. Building a physical prototype of a car engine can be replaced by a computer model based on finite elements, finite differences, and computational fluid dynamics. These standard tools rely on classical mechanics, electromagnetism and thermodynamics, and on accepted empirical data. But they must operate so as to allow collaboration between engineers at different sites. The software must work on all the computers and operating systems likely to be encountered. It must be understood by engineers who hanker after the previous physically real “mock-ups”. Confidence in the answers has been achieved at the engineering level, where software credibility has been helped by a large user base. This trust remains elusive for much scientific atomic-scale modelling, where a major obstacle to take up of state-of-the-art (so-called a priori) electronic structure methods by industry is the significant fraction of cases for which the answers are either unsatisfactory or are disputed in the academic community [47]. If macroscopic science is mature and atomistic science maturing, where is nanotechnology?

7. Conclusions

Does computing *identify* or even *select* directions in leading-edge science (whether for good or bad), or *respond* to new ideas? Computer experiments should have the range and variety shape nanoscience, and there are signs of such experiments becoming seminal. Yet, there is a temptation to follow fashion, just as predictions for solid-state spectroscopy dwindled when local density methods arrived, since the new methods were primarily for ground states.

Even if one can identify the important issues in a new field, it may not be easy to link them to available computer methods or conventional wisdom. This is especially true when understanding a process matters more than optimising a structure. For instance, protein folding is clearly a major challenge of some sort. But what are the right questions? Having a model able to mimic some aspects of protein folding would be good, although limited. Modelling a specific protein folding accurately, with appropriate hydration and other possibly relevant features (such as zero-point motion) is beyond current computer capacity. Success might expose modelling to those moral questions that arise when key molecules of life are modified. If it is true that certain diseases result from protein misfolding catalysed by a prion, then it would be a major success if one could identify some way to prevent or reverse the misfolding. That is not trivial.

In the new science associated with the nanoscale, one must distinguish between the possible, the conceivable, the likely, and the desirable. Some of the ideas, of course, are conventional science, relabelled. But the mixture of the soft and the hard, the readjustments of the relative importance of different forces and energies, and the many subtleties offer a remarkable diversity of new concepts, challenges, and temptations.

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