The quantum in your materials world

New ideas lead to new technologies, and new technologies demand new materials. Quantized matter – atoms – underpinned the 19th century chemical industry and quantized charge – the electron – is the basis of microelectronics.

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Atoms and electrons were once as exotic as the word 'quantum' is today, and just as hard to relate to the very real world of materials. Yet silicon technology spawned a whole series of materials innovations. There were the functional materials: ultrapure Si, strained Si/SiO_2, low *k* materials, Cu and Al for interconnects, etc. There were passive device materials, such as heat sinks, packaging, and diffusion barriers. New materials were needed for fabrication: lithography optics, photoresists, and metalorganics. New fabrication methods, such as ion implantation, transformed dopant control. The public saw the fruits of this research: solid-state lasers for compact disc players, colorful casings and straps for watches, light-emitting diode and liquid crystal displays, etc. Quantum information processing (QIP) computing will offer a new list of materials.

Two major forces drive quantum information technology. One comes from pressures within Si technology and the rapid changes described by Moore's law. Challenges include fabrication and operation for ultra-small features, handling the operating heat generation, managing power losses from electron tunneling, and funding the enormous costs of new fabrication plants. The second challenge involves the nanoscale. Even today's devices use gate dielectrics a few nanometers thick. But the nanoscale is different, and demands quantum ideas. The number of electrons needed to switch a transistor is predicted to fall to just one by 2020, and that must not be the end. Understanding the quantum is an opportunity that could transform the 21st century, just as understanding the atom and the electron transformed the last. The *International Technology Roadmap for Semiconductors* shows what might be expected from imaginative but incremental development. But could we seek a radical technology, a wholly novel quantum route, operating *alongside* existing Si and photonic technologies? Almost any large-scale use of QIP must be *Si compatible*. Key devices should be manufacturable in a near-future generation fabrication plant. Ideally, key operations and control systems should work at room temperature. Quantum ideas may be radical, but their impact depends on whether they are usable. Materials science provides some of the limits.

Novel techniques for quantum systems can prove equally useful for classical devices. Electron or nuclear spin manipulation goes beyond simply moving charges. Photon polarization and single-photon techniques go beyond color and intensity measurements. At the smallest scales, quantum behavior is unavoidable: this raises issues such as tunneling, but also offers opportunities for fabricating resonant nanocavities and control of nanoscale fields.

Quantum ideas are not yet intuitive. Could you convince your bank manager that quantum physics could improve the bank's security? Perhaps three questions identify the issues. First, how do you describe the state of a system? The usual descriptors, wave functions and density matrices, underly wave-like interference and

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entanglement. Entanglement describes the correlations between *local* measurements on two particles, which I call 'quantum dance.' It is the resource that could make quantum computing worthwhile. The enemy of entanglement is *decoherence*, just as friction is the enemy of mechanical computers. Secondly, how does this quantum state change if it is not observed? It evolves deterministically, as in the Schrödinger equation. The probabilistic results of measurements emerge when one asks the third question: how do you describe observations and their effects? Measurement destroys entanglement, as it singles out a specific state. This is why you can tell if an eavesdropper intercepted your message.

Classical computers use bits to encode numbers. By using bits with values of either 0 or 1, numbers can be represented physically: dipoles up or down, charged vs. uncharged, left- or right-handed polarizations. Such bits are manipulated by classical gates, and complex networks of a few types of such gates make today's impressive computers possible. Proposed quantum computers have qubits manipulated by a few types of quantum gates, again in a complex network. But the parallels are not complete[1]. Each classical bit has a definite value; it can only be 0 or 1; it can be copied without changing its value; it can be read without changing its value; and, when left alone, its value will not change significantly. Reading one classical bit does not affect other (unread) bits. You must run the computer to compute the result of a computation. Every one of those statements is *false* for qubits, even that last statement! There is a further difference. For a classical computer, the process is *Load* → *Run* → *Read*, whereas for a quantum computer, the steps are *Prepare* → *Evolve* → *Measure*[1].

It is never obvious whether a proposed quantum computing scheme is viable or not, quite apart from challenges of implementation[2–4]. The DiVincenzo[5] checklist asks key questions for an initial assessment. First, there must be well-defined quantum states to use as qubits, perhaps electron spins. Secondly, one must initialize the quantum system, somehow preparing suitable pure quantum states. Thirdly, the quantum system must be persuaded to evolve in the right way, with *decoherence* avoided for long enough for the computation to take place, until the results can be read via some measurement. These guidelines are challenging, raising seriously demanding issues of materials and system integration. Moreover, even if a usefully big quantum computer could be made to function, the algorithms will probably have to be written for it, whereas it is normal to build a classical computer to suit its function.

It is commonly (but wrongly) suggested that quantum behavior only matters at low temperatures. Quantum behavior is evident in two main ways. In quantum statistics, whether Bose–Einstein or Fermi–Dirac, Planck's constant $\hbar$, the key to quantum behavior, appears in the combination $\hbar\omega/kT$, implying that high temperatures will obscure quantum effects. But statistics relate primarily to behavior near equilibrium. In quantum dynamics, $\hbar$ appears without T. Quantum effects may open new channels, as in quantum diffusion[6]. There is no *intrinsic* problem with high temperatures. Successful quantum manipulations in diamond verify this[7–11]. QIP relies on dynamics, and on systems remaining far from equilibrium. Practical issues are another matter, since higher temperatures usually speed approaches to equilibrium.

Why should *materials* scientists be interested in quantum computing? Quantum devices are nearly always nanoscale devices. Whatever their nature, their fabrication usually exploits the enormous nanoscale know-how of silicon technology. This capability strongly favors Si-compatible technology[12–14], thereby integrating classical control with quantum devices. Moreover, Si-compatible technologies include nanophotonics and optical fibers, diamond, and perhaps III–V semiconductors. The promise of solid-state QIP lies in its potential *scalability*, the opportunity to link the large numbers of qubits and quantum gates needed for almost any serious application. But there are problems. Decoherence is often fast. Slow decoherence may not be as advantageous as it sounds since fast operating speeds go with fast decoherence, because fast processing needs strong interactions, and the fluctuation–dissipation theorem implies these strong interactions also enable decoherence[15]. This raises the question of whether large quantum computers can ever work; happily, this seems likely[16].

Proposals for solid-state quantum computers are many and varied. No current implementation dominates the search for scalable practical quantum devices. Any device that achieved, say, 20 successfully gated qubits would be a breakthrough, one that would encourage even competing designs. The issues become clear when discussing particular systems. I shall describe one of many, chosen partly to illustrate some desirable *materials* features. It needs existing (if advanced) techniques for both fabrication and operation: standard lithography; standard optics and photonics; random doping of Si. It should work above cryogenic temperatures, and perhaps at room temperature. It might well prove a robust device, built in a near-future fabrication plant. System integration will surely be a problem, as it was for early classical semiconductor devices – radios, televisions, computers, lasers, were all *very* bulky at first.

The issues are best understood for a specific system, so I now discuss ideas for an optically controlled spintronics system[14] that might also have value as a classical device (Fig. 1). The approach specifically exploits the properties of impurities in Si, and indeed most of its processing and operating steps have been demonstrated, though not put together. Quantum information is embodied in the electron spins of disordered deep donors. The typical separation of these qubits is such that their mutual interactions are small. Imagine these qubits in a thin Si layer, say 10–20 nm thick, atop a silica substrate. The qubits store quantum information, and are manipulated (qugate operation) by optically induced electronic excitation of distinct control spins, also deep donors. In the control's electronic excited state, entangling interactions between qubits occur. Only in these excited states is the entanglement – the quantum dance – of pairs of qubits manipulated.

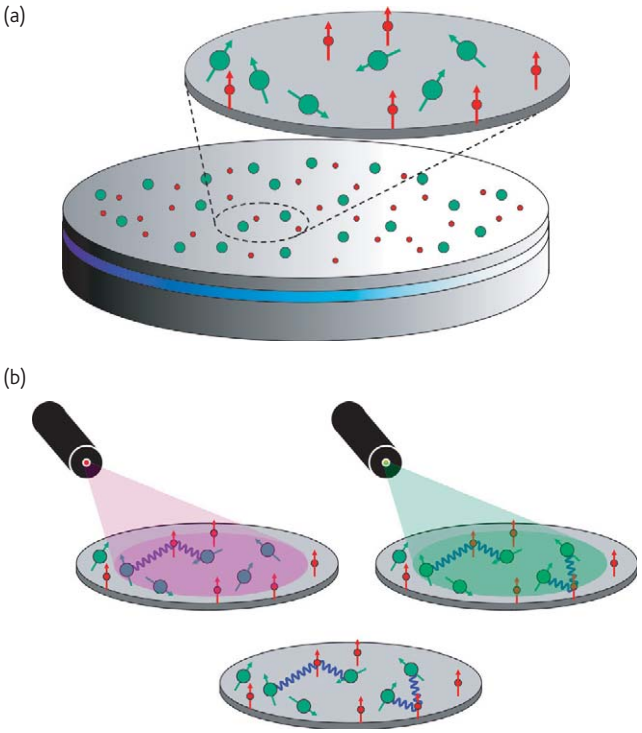

Fig. 1 (a) Architecture for the SFG quantum information processor[14]. The active region is a thin (1–2 nm) Si layer on a silica substrate. This thin film is randomly doped with qubit donors (red circles) and control donors (green circles). The entanglement of the qubit electron spins is controlled by the optical excitation of the control donors. Spectral selectivity will be combined with spatial selectivity to generate a sequence of controlled entanglements in a 'patch' a few optical wavelengths across. Each patch might contain perhaps 20 gates. (b) We can only focus light down to 1000–2000 nm. However, the dopant wavefunctions fix the scale of the separations over which entanglement is effective to a mere 10–20 nm, and we can exploit variations in excitation energies from one place to another: randomness and even surface steps help. Light of different wavelengths (shown schematically as red and green) will operate different 2-qubit gates; the entangling links are shown as wavy blue lines.

Such quantum gates do not rely on small energy scales for operation, so they might function near room temperature. Effective operation relies on knowing the natures of the excited states, and on defect engineering to optimize these states. Simulations indicate that this scheme can produce the gates necessary to construct a universal quantum computer[17].

For electron spins in semiconductors such as Si, effective entanglement of control and qubit spins needs overlap, meaning spacings of a few tens of nanometers or less, depending sensitively on the specific system (Fig. 2). For optical control, the natural length scale is the wavelength, say 1 μm for communications wavelengths. Yet even near-field optics can only focus down to about 100 times the 10 nm scale of control and qubit spacings. It is here that use can be made of the natural randomness of doping. Microelectronic devices are respectably precise, but standard fabrication plants certainly do not place dopants at preselected sites accurate to the nearest nanometer.

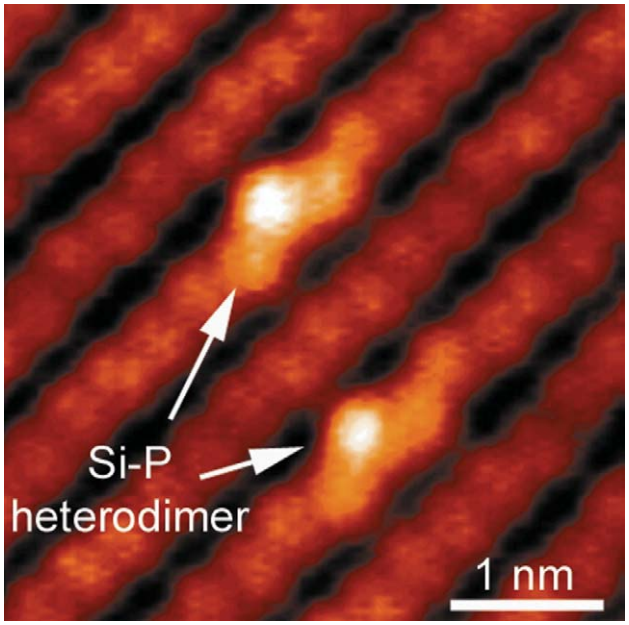

Fig. 2. Scanning tunneling microscope image of P in Si[18]. (Reproduced with permission from[18]. © 2004 American Physical Society.)

Conventional doping is inevitably random, whether by diffusion, implantation, transmutation, or using metalorganics. The Stoneham–Fisher–Greenland (SFG)[14] ideas *exploit* the randomness for systems reasons, benefiting from what is already available. In a disordered system, especially if there are the usual surface steps on the thin Si film, excitation energies for specific control/qubit gates will vary from one site to the next. Even the natural disorder and uneven surfaces of randomly doped semiconductors is good news. The individual gates can be addressed by exploiting both spatial and *spectroscopic* selectivity.

What might be good systems for Si? Common donors (P, As, Bi), though useful for demonstrating the principles, have small ionization energies, and would ionize at room temperature. These low energies can lead to rapid decoherence from fast spin lattice relaxation, and convenient lasers are not available. Double donors (Se^+, Mg^+) are much more promising[19,20]. In diamond (which is arguably Si compatible), substitutional N has a spin relaxation time of ~1 ms at room temperature, and would be an excellent qubit. The negatively charged N vacancy (NV^-) centre is excellent for initialization and readout. However, it is harder to identify a control species with extended excited states to manipulate qubit entanglements; the P donor might be a possibility.

Once the randomly doped thin film is made, special characterization must be done, though only once, in a process analogous to configuring a hard disk. Configuring the device will use a combination of scanning tunneling microscopy, optical excitation, and detailed modeling to determine which wavelength operates which gate, and to establish the connectivities, the topology of the system. There are materials limits on the system itself. How many gates (or qubits) could we have

within an area singled out optically, say 2 μm across? For Si, with its relatively narrow gap, and for reasonable qubit–control interactions, there might be 20 or so gates with distinguishable excitation energies within a smaller 'patch' perhaps 100 nm across. A 20-gate solid-state computer would be useful, but even better if some 'flying qubit' could link patches[21] (Fig. 3).

Just as friction defeated the largest mechanical computers, so decoherence – loss of entanglement – is the enemy of quantum computing. Anything that ensures fast switching may cause fast decoherence. For optically controlled spintronics, spontaneous emission could be the killer. For any spin-based approach, spin relaxation is destructive, whether spin–lattice relaxation (less important in systems with low spin–orbit coupling, such as diamond and perhaps Si) or spin–spin relaxation (so isotopic purity may be needed[23]). There can be decoherence from inadvertent state changes, such as two-photon ionization. A subtle problem for the SFG model is that the control spins may take quantum information from the qubits. This can be avoided by a proper choice of control pulses[24].

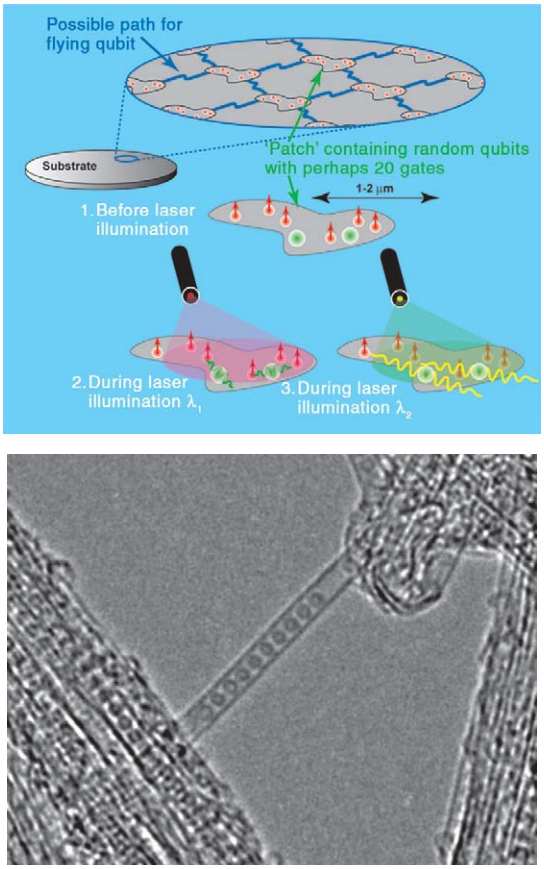

Fig. 3 Flying and static qubits. (a) The patches might be linked by flying qubits to form some larger processor, in this case a two-dimensional array, perhaps exploiting electrons in image states above a negative electron affinity layer. (b) Endohedral La in C_{82} buckeyballs in a buckeytube, where the rare earth spins would be static qubits, and the flying qubits spins moving (one-dimensionally) along the buckeytube. (Unpublished work, courtesy of Jamie Warner and G. A. D. Briggs; see also[22] for related material.)

In operation, the system must be initialized to a defined starting quantum state, and readout of the results of a calculation will require some measures of the final quantum state. Routes to initializing spins are usually *optical*, including microwave and radiofrequency methods, or *spintronic*, exploiting a flux of spin-polarized electrons or excitons. Thus the energy levels of NV^- complex in diamond (triplet ground state plus singlet state below the lowest triplet excited state) enable specific spin states to be prepared[7,9,] (Fig. 4) (see also Fig. 4 in Greentree *et al.*[10]). Readout strategies may invoke extra (non-active) qubits, or use virtual transitions that do not change spin state. There is a plethora of ways to read single spins, though most are slow, or hard to integrate with a substantial system.

Even if all the methods needed to fabricate and run these devices have already been done somewhere in the world, they are certainly not routinely available. Putting all the components together – system integration – may prove the ultimate challenge. One must think through *all* of the system. Challenges are also opportunities, and – at least as regards materials – any challenge that is overcome will

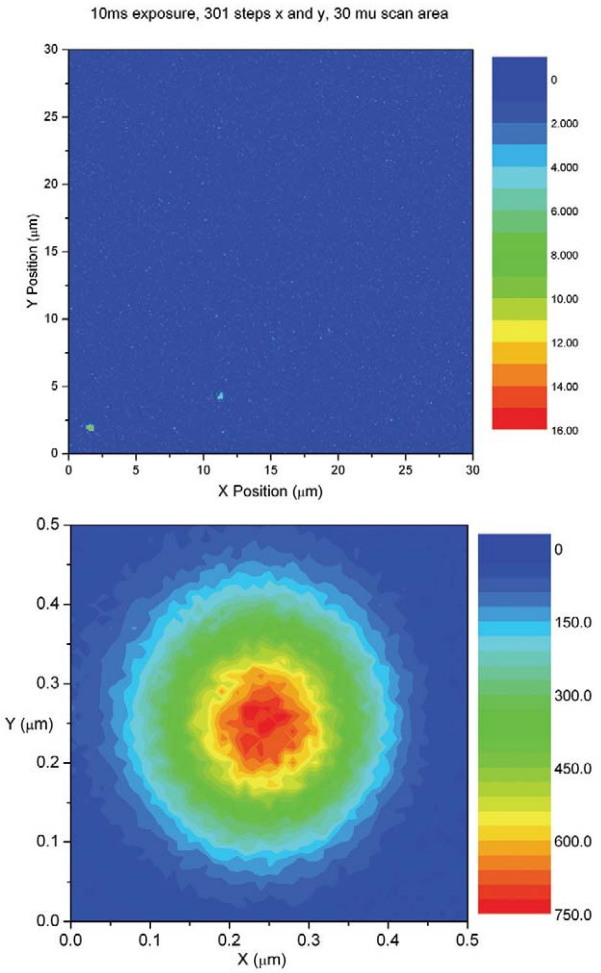

Fig. 4 Near-field optics image of NV^- centres in diamond; the lower figure shows an image of a single centre (Unpublished work, courtesy of Brian Patton and Jason Smith).

probably benefit classical nanoelectronics as well. The first challenge is *make your device*. Quantum devices will need at least the current state of the art at the nanoscale. New challenges may include isotopic purity, and probably very low thermal budgets with complex system integration. The devices will need nanoengineering of wavefunctions and spin states, ideally without exact placement of atoms. The second challenge is *characterizing your device*. All the best standard characterization techniques will be needed (thank you, Si technology). Standard defect elimination will be needed, but this may not prove too much of an obstacle, since the critical regions of a device should be very small indeed. The nanoscale is never precise. Our configuration step checks and quantifies what really was made during fabrication. Moreover, it is necessary to characterize a quantum state before and after each run. The third challenge is *integrating your device*. Standard (classical) Si technology dominates today, and will continue for many years[25]. QIP must work alongside standard systems, with standard Si technology to run them and ideally integrated with optical networks.

The big remaining questions are linked: will a quantum computer work? Probably *yes*, though there are reasons to be cautious[2]. Could a QIP device operate at room temperature? Probably *yes*, but there are formidable difficulties. Could a QIP device be as portable as a laptop? Possibly yes, but that is less clear. Since there is no major QIP industry, how useful might even an inexpensive room-temperature quantum processor be? This is uncertain[3]. Ideas mooted include the *probable* (i.e. demonstrated at a modest scale, like factorization or directory searches; the example of a router shown in Fig. 5 is unlikely to outperform classical versions, but gives a focus for an early QIP device), the *possible* (proven potential, e.g. designing a better quantum computer), or the *conceivable* (hard computational problems such as turbulence, to appeal to chemical engineers and aero engine designers). But the likely first use will be the *frivolous* (quantum games), just as new materials are found in golf clubs long before advanced-technology applications. Nor should one forget ideas not yet conceived. After all,

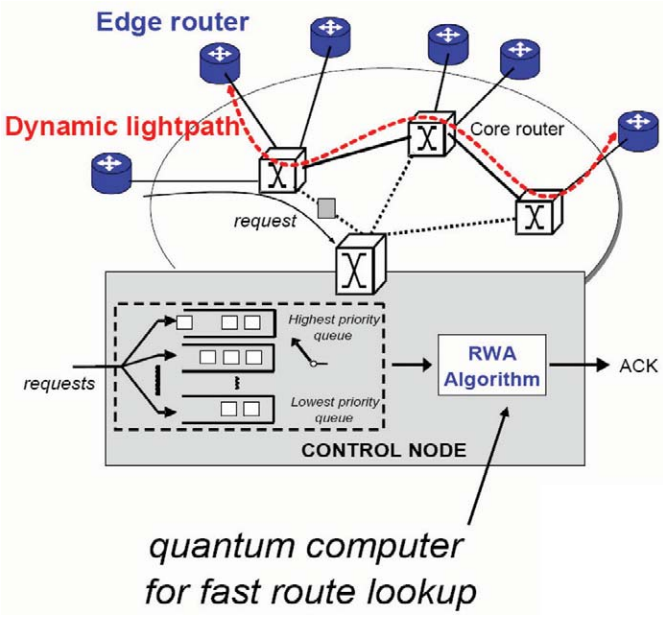

Fig. 5 How might you exploit a device? The router shown would probably not be competitive with conventional technologies, but shows how a potential QIP device must be integrated with other microelectronic and photonic devices (Unpublished work, courtesy of Polina Bayvel, Andrea del Duce, and Michael Dueser).

the solid-state laser was a solution without a problem for two decades prior to the compact disc. And will a quantum computer avoid those problems of standard computers that drive us paranoid? That must be science fiction: just think about rebooting a quantum computer. mt

Acknowledgments

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