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FABRICATING AN ALL-EPITAXIAL SILICON QUANTUM COMPUTER

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Scalable silicon quantum computers will require a material perfection that has never been attempted. Ground state wavefunctions for conduction electrons orbiting individual phosphorous donors must be polarized electronically and coupled to nearest neighbors with great precision. Elimination of all randomizing influences can be achieved only with a fully epitaxial structure; and we believe that output circuitry must also be integrated into the qubit arrays in order to achieve the uniformity needed for large-scale integration. A process that could potentially accomplish this will be outlined, based on scanning tunneling microscope (STM) removal of individual hydrogen atoms from the H-terminated silicon surface followed by phosphine dosing and ultra-low-temperature overgrowth. Self-ordering of PH_3 molecules onto extended areas of bare silicon should permit patterning of planar single-electron transistors along with P-donor qubits in the same lithographic step. Initial plans for an experiment to characterize exchange coupling under gate control will be described.

1 Introduction

Silicon-based quantum computers[1,2] are made possible by the large Bohr diameter for bound electron wavefunctions on individual P-atom donors, and the astonishing perfection of single-crystal silicon. Whether quantum logic of this type can be implemented in practice will be the focus of intense research over the next several years. Those efforts will also extend conventional silicon technology toward single electrons and individual spins, with many unforeseen possibilities in addition to a scalable quantum computer.

This larger framework is familiar to us, because much of our research over the past ten years has been devoted to developing scanning tunneling microscope (STM) patterning techniques for atom-scale electronic devices. Prior work had laid a good foundation by characterizing the properties of hydrogen-terminated silicon surfaces at atomic resolution[3], and by demonstrating desorption of hydrogen at nanometer dimensions using the STM's low-energy electron beam.[4] We and our colleagues saw an opportunity to employ this single-monolayer 'Hydrogen resist' for atom-resolved patterning on silicon, and set about developing the required techniques. Atomic resolution was first demonstrated by desorbing individual hydrogen atoms to expose bare silicon dimers on a Si(100)-2x1:H surface, as shown in Fig.1, using a tip voltage well below the ~4.5eV tungsten workfunction.[5] Systematic studies were then performed to characterize STM electron-stimulated desorption over the entire experimental range from ~1 to 12V, leading to a detailed theoretical interpretation of the desorption mechanisms in both tunneling and field emission regimes and the discovery of a large isotope effect for deuterium vs. hydrogen.[6] Atomic resolution on 'Hydrogen resist' can only be obtained in the tunneling regime below ~4V, where wavefunction coupling between particular tip and sample states limits the electron beam diameter. Voltage pulses can also be applied in tunneling mode to eliminate hydrogen atoms from an individual silicon dimer at any preselected location, creating two bare silicon dangling bonds and a reaction site small enough to accommodate only one adsorbate atom or molecule.

Our initial attempts at fabrication demonstrated selective oxidation of ~4nm-wide lines[7], and utilized these 'native oxide' patterns as masks in experiments on aluminum chemical vapor deposition (CVD).[8] Uniform CVD nucleation proved very difficult to realize at these dimensions, but we had some success in defining atom-scale metal patterns by direct evaporation of aluminum at ~0.1ML onto H-terminated surfaces containing ~2nm-wide STM-exposed lines of bare silicon at room temperature.[9] These experiments, and subsequent efforts to fabricate a 'single-atom wire'

using this technique[10], indicated a need for some type of self-ordering to eliminate gaps and clusters on the atomic scale; and it occurred to us that common dopant precursor molecules such as PH_3 might be ideal for this purpose. By coincidence, our proposal for fabricating electronic structures in silicon based on overlap of individual P-donor wavefunctions[11] was published simultaneously with Kane's proposal for a silicon-based quantum computer.

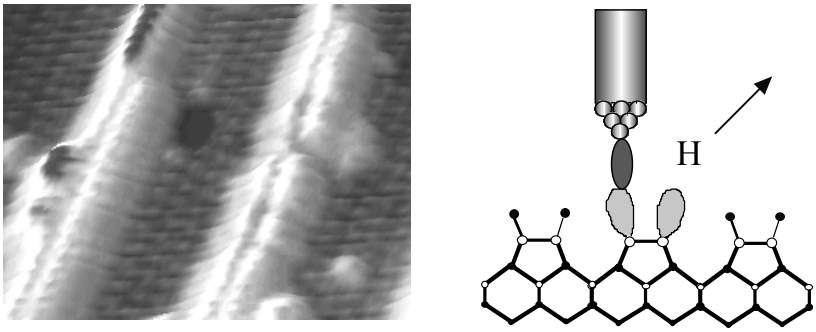

Figure 1. Lines of bare Si dangling bonds written 30Å apart along the dimer rows of a Si(100)-2x1 surface by STM-induced desorption of hydrogen. Sharp nodal lines of the bare Si-Si π-antibonding state are clearly seen, and hydrogen atoms are removed only from the left side of each dimer near the top of this image.

2 Patterning Atom-Scale Circuits

Atom-resolved studies of phosphine adsorption onto the bare Si(100)-2x1 surface[12] show very strong self-ordering of individual PH_3 molecules on alternating dimers within a single row at room temperature. The adsorption sites are staggered between adjacent rows to form a ~1/4ML c(4x2) structure (with ~5nm-size domains) at saturation coverage. On the other hand, phosphine does not adsorb onto H-terminated surfaces at room temperature; and substrates must be heated above ~500^{O}C to thermally evolve hydrogen and expose bare Si dangling bonds in order to sustain common CVD reactions involving PH_3, SiH_4, AsH_3, B_2H_6, and related molecular species. In a future industrial process, conventional e-beam sources might be employed *in situ* to selectively pattern the 'Hydrogen resist' and expose a 2D circuit pattern for selective deposition of self-ordered ~1/4ML P-donor arrays, with STM used only in those areas requiring atomic resolution or attachment of individual precursor molecules. Figure 2 illustrates one such pattern that might be employed in fabricating a planar single-electron transistor (SET).

The critical step in transforming these patterns into useful electronic devices will be to overgrow and activate all of the selectively deposited donor atoms inside the silicon crystal while limiting redistribution to the atomic scale. The planar density of a ~1/4ML c(4x2) donor sheet is ~$1.7x10^{14}cm^{-2}$, a factor of ~100 greater than in conventional δ-doped layers. Prospects for successful overgrowth appear excellent, however, in view of recent progress in low-temperature silicon molecular beam epitaxy (LT-SiMBE). Self-ordered 2x1 boron adlayers have been overgrown at temperatures as low as ~350K, and full activation is seen in Hall effect up to ~1/2ML coverage with only ~4Å spread in the growth direction.[13] More recent experiments with Sb donors[14] have yielded similar results. Surface hydrogen up to 1/2ML is found to have no discernible effect on LT-SiMBE[15], so it appears that these techniques can be successfully employed in overgrowing the patterned PH_3 precursor layers described here.

The overgrown ~1/4ML P-donor patterns are intended to function as 'metallic' electrodes in the planar SET structure sketched in Fig.2. Nearest-neighbor distances in a c(4x2) precursor adlayer are only 7.7Å, much smaller than the ~50Å average Bohr diameter for isolated donor bound states. Strong wavefunction overlap should thus yield high conductivity within the dopant plane. At low temperatures, the conduction electrons will be tightly confined within ~10Å in the vertical (growth) direction by the large electric fields of a ~1/4ML donor sheet. The resulting 2-dimensional electron gas (2DEG) is expected to populate only the lowest subbands for normal

effective masses $m_\perp$*=0.916m_O and m_t*=0.190m_O, respectively. However, the characteristic distance for lateral wavefunction spreading at the edges of these highly-conducting 2D patterns will still be set by the Bohr radius, so lateral tunnel junctions should correspond to ~10nm-wide gaps whose impedance levels can be accurately controlled. Through use of silicon-on insulator (SOI) device templates with pre-implanted contact regions, we hope to produce seamless atom-scale integrated circuits of overlapping donor wavefunctions with no barriers to the outside world.

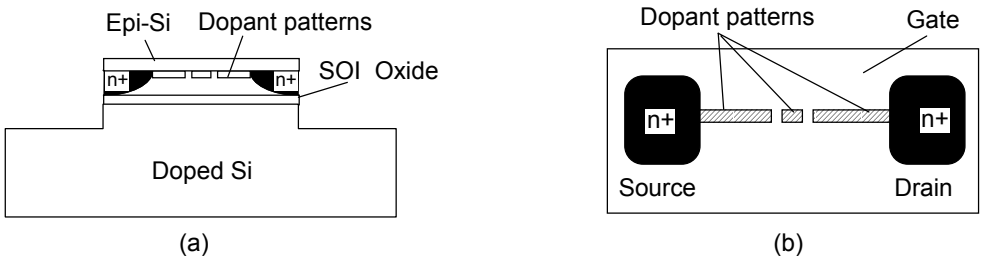

Figure 2. (a) Side and (b) top view schematic for a SET on SOI substrate utilizing the 2D dopant patterns fabricated *in situ* by STM. The mesa and source/drain regions are prefabricated *ex situ* by conventional processes. The heavily-doped Si substrate will be used together with a top-gate (not shown) to control wavefunction overlap across the lateral tunnel junctions.

Full activation of patterned 2D donor sheets offers a unique opportunity to eliminate the random offset charges that plague all single-electron devices today. The large 1/f noise of metal-oxide tunnel barriers should also be greatly reduced, yielding much greater sensitivity in detecting sub-electron charge displacements with SET electrometers. If realized, these extraordinary electrical properties could provide ideal output circuitry for a silicon-based quantum computer, imposing the smallest possible perturbation on individual donor qubits.

3 Controlling The Exchange Interaction

Perhaps the most critical step toward building a silicon quantum computer will be to demonstrate electronic control over the exchange interaction between isolated donor pairs, and characterize the quantum states of the resulting two-electron system. Figure 3 illustrates our conceptual approach to this problem. In addition to the SET circuit sketched in Fig. 2, STM pulses will also be used to create attachment sites for two individual PH_3 precursor molecules near the Coulomb island. A second set of planar electrodes will be patterned (contacts not shown) to apply a small ac electric field along the inter-nuclear axis, polarizing the spin singlet state of the coupled donor-pair. The magnitude of this in-plane electric field, E_x^{ac}~1kV/cm, will be limited by the relatively small binding energy of the 2D donor sheets, and we anticipate using an ac bias of ~20mV across a ~200nm-wide gap in order to polarize the coupled donor-pair.

The approximate separation between the donor 'qubits' shown here is R~300Å, much larger than the average Bohr radius, a_B~30Å, for individual 1s donor wavefunctions. The magnitude of exchange energy between the two 1s electron ground states will thus be very small at this distance. However, when a large dc electric field, E_z~100kV/cm, is applied normal to the dopant plane, the individual ground states will become highly polarized with a significant $2p_z$ component. For the sample configuration shown in Fig.2, this dc electric field would be established between the heavily doped SOI substrate and a common metal top-gate (not shown). Since the characteristic decay length for $2p_z$ states is $2a_B$, twice as large as for 1s states, it should be possible to establish gate control over wavefunction overlap and exchange energy in a convenient experimental range, with J~0.2meV for the parameters described here. This value of exchange energy corresponds to J/kT~40 at a measurement temperature T~50mK, and the singlet to triplet transition would be expected at an applied magnetic field B_z~2T.

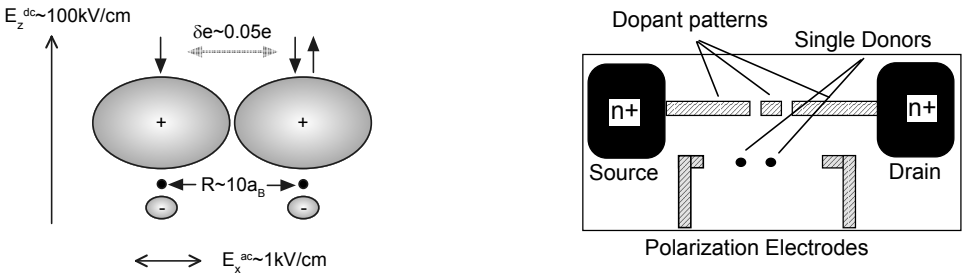

Figure 3. Top view schematic for an experiment to characterize the exchange energy of a pair of isolated donors with ground state electron wavefunctions polarized and coupled by a large dc electric field under gate control. A smaller in-plane ac electric field will also be applied to polarize the two-electron spin singlet state, resulting in charge oscillations that are detected as a modulation in SET current.

The basic output measurement, as outlined in Kane's proposal, is a determination of the two-electron quantum state for coupled donor-pairs via electronic polarization. For anti-parallel spins in the singlet state, a transverse electric field will push both electrons toward a doubly-occupied D^- configuration on one of the donor sites. Charge transfer will not occur in the triplet state, however, since double occupancy is statistically forbidden for electrons having the same spin. A nearby SET electrometer can potentially detect the presence or absence of this sub-electron charge transfer, through the polarization induced onto its Coulomb island.

According to a simplified Hubbard model, an ac electric field E_x^{ac}~1kV/cm can be expected to set up a charge oscillation δe~0.05e between the two donor sites for the experimental parameters described here. Because these two donors are placed asymmetrically with respect to the SET in Fig.3, a somewhat smaller polarization charge would be induced onto the Coulomb island, resulting in modulation of SET current at the applied frequency. Conventional SET electrometers have sensitivities in the range 10^{-3} to 10^{-5}e/√Hz, limited by large 1/f noise of Al-oxide tunnel junctions. Epitaxial SETs with silicon tunnel barriers are expected to have greatly reduced 1/f noise, so detecting charges of order 10^{-2}e should not be a problem. By employing lock-in and derivative techniques as the magnetic field is increased slowly, we expect to observe the narrow singlet-triplet transition of a single donor-pair in the presence of much larger background components of ac polarization. The value of magnetic field at the transition provides a direct measure of exchange energy; and the entire phase space for coupled donor-pairs could be mapped out as a function of gate voltage if this approach is successful.

4 Conclusion

Controlling the wavefunction coupling between individual P-atom donors in silicon may hold the key to large-scale quantum computation, but it is a very difficult undertaking. Our approach emphasizes the benefits of a fully integrated, all-epitaxial structure for several reasons. First, the SET output circuitry needed to detect the results of quantum logic can be incorporated along with donor qubits in the same STM patterning process. Major difficulties in registration can thereby be avoided. More importantly, growing the entire structure into single-crystal silicon can greatly reduce the density of defects and random polarization charges that might otherwise deform electron wavefunctions on the individual donor 'qubits', precluding high levels of integration. SiGe heterolayers can eventually be incorporated into the overgrowth for ESR tuning structures and epitaxial gate dielectrics. Given the already advanced state of silicon materials technology, there is room for serious optimism.

Acknowledgements

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