Phenomena in silicon nanostructure devices

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Abstract. In nanostructures, whenever the electron mean-free-path exceeds the appropriate dimensions of the device structure, quantum natures may dictate the physical properties of devices. Among many important issues, some are selected in this work, whereas others, such as the reduction of dielectric constant, the increased binding energy of dopants, etc., are discussed briefly with references for further considerations. In the past several years, resonant tunneling via nanoscale silicon particles imbedded in an oxide matrix has shown striking similarity to the so-called soft breakdown (SBD), an important current subject in devices with ultrathin oxide gates. The relevance in applying results discussed here to SBD is discussed. A Si/O superlattice, a particular form of a new type of superlattice, semiconductor-atomic superlattice (SAS), is fully discussed. This Si/O superlattice can be used in silicon quantum and light-emitting devices. A diode structure with green electroluminescence has been life-tested for more than one year without degradation. High-resolution TEM shows defect density below 10^9/cm^2. Preliminary calculation shows that the Si/O complexes result in a barrier height of 0.9 eV for silicon, sufficient for an epitaxially grown SOI, which is potentially far better than the SOI using buried oxide implantation followed by high temperature anneal.

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As device size shrinks for higher speed and lower power, certain properties cannot be scaled due to the wave nature of electrons. The use of heterojunctions for the confinement of carriers initiated the man-made quantum devices [1, 2]. Basically, whenever the electron mean-free-path exceeds the appropriate device dimension, the wave nature dominates. An excellent review by Cahay and Bandyopadhyay discussed in detail the implications and consequences of electrons and holes dictated by the wave nature, the granularity of charges and the polarization of spins [3]. Several issues, such as the capacitance, the binding energy of dopants, and tunneling time, are reviewed briefly in this article for easy reference of the reader.

The use of nanoscale silicon particles imbedded in an oxide matrix was introduced [4, 5] for possible silicon quantum devices operated at room temperature. A diode structure with annealing and oxidation of a thin amorphous silicon layer sandwiched between oxide layers, followed by a proper electrical forming process [6] was chosen for studies. It is noted that electrical forming, presumably as means to remove inter-grain tissues, is essential for the minimization of possible breakdown with high electric field [7]. It may even serve to remove very small crystalline silicon particles to improve uniformity of size [8]. The evidences of resonant tunneling via nanoscale silicon imbedded in an oxide matrix are reviewed. Recently, there are increased efforts to incorporate ultra-thin oxide gates for MOSFET devices leading to the issues of soft breakdown (SBD) and hard breakdown (HBD) [9, 10]. The physics involved in the tunneling of nanoscale silicon particles embedded in an oxide matrix is quite similar to that of SBD. A comparison is made in this work showing the differences and similarities.

In the last section, recent results in building a barrier consisting of alternate monolayers of oxygen sandwiched between adjacent thin silicon layers [11, 12] are summarized. A multilayer Si/O superlattice shows electroluminescence in the visible, life-tested for over one year without degradation [13, 14]. A barrier consisting of several periods of Si/O shows excellent isolation. Silicon growth beyond the barrier region is epitaxial and free of stacking fault defects. This represents a step in the right direction for the fabrication of quantum silicon devices as well as for the replacement of SOI [15], in high-speed and low-power silicon MOSFET devices of the future.

1 Some issues important to nanoscale quantum devices

Quantum devices, at room temperatures, have a length scale of 2–20 nm, although at low temperatures, dimensions in the range more than double this length scale frequently apply. Transport properties are governed by tunneling. Quantum confinement effects, related to the wave nature of electrons lead to new definitions of capacitance, tunneling time, damp-
ing and binding energy in doping. Although these considerations were in the literature, for the sake of convenience and logical understanding of this work, some of the properties are repeated here [8].

1.1 Tunneling time in a quantum well

There appears to be some inconsistency in the description of the tunneling time. Cahay et al. show a pronounced dip in the tunneling time at the resonant state [16], whereas, the phase-delay time defined by

\[ \tau = \frac{d\phi}{d\omega}, \]

where \( \phi = kd + \theta \) is the total phase shift, with \( \theta \) being the phase of the transmission coefficient, and \( d \), the length of the DB structure, is a maximum at this energy [17]. Several approaches [18] were used: (a) solving the time-dependent Schrödinger equation with prescribed initial conditions, and (b), specifying a wavepacket and calculating the time it takes to traverse the double-barrier structure [19]. Results show that the tunneling time of a Gaussian packet from the time-dependent solution is very close to the phase-delay time. The delay time peaks at resonances.

These results are quite easy to understand. Resonances are produced by a wave bouncing back and forth for a number of cycles determined by the quality factor of the resonant system. This time is the standard delay time. The tunneling time given by the time for a wavepacket traversing the structure using the solution of the time-dependent Schrödinger equation gives essentially the same result [8]. Since the thesis [19] is not readily available, several salient features of this work are highlighted here. First, the Green’s function for the one-dimensional equation for the double-barrier (DB) structure is obtained. Excitation functions are chosen for various cases: specifying a spatial distribution at \( t = 0 \), or specifying a time function (usually a pulse at a given energy between \( t = 0 \) to \( T \)) at a given location such as \( x = 0 \), or \( x = \) center of the well, etc. Laplace transform is then used. The inverse transforms give the desired results. If one wants to calculate the charge inside the well at any given time for a particular distribution, it would be necessary to multiply \( Q(t) \) for the charge by \( n(\omega) - n'(\omega) \) and integrate over all \( \omega \), the energy, with \( n \) and \( n' \) given by the distribution functions on the inside and transmitted side of the DB, respectively. \( Q(t) \) confined within the system is obtained as a function of time by integrating \( |\psi(t)|^2 \) over both the well and the barrier regions. The decay time \( \tau \) is defined by \( Q(T + \tau) = Q(T)/e \), and the build-up time by \( Q(\tau) = (1 - e^{-1})Q_0 \) where \( Q_0 \) is the steady-state charge in the well. This definition is not unique particularly at energies away from the resonance, because the charge oscillates through the same value several times except near resonance. Uniformly growing or decaying behavior of the charge only takes place near resonance! Instead of specifying the initial condition at the left side of the DB structure, we have also studied the build-up time and decay time for an excitation exp \((-i\omega t)\) at a point within the well and calculate the steady-state wavepacket. To our surprise, as the point of excitation moves towards the center of the well from the edge of the barrier, the resonance behavior gradually disappears. The details of those cases are not quite the same, presumably precise results do depend on the form of the excitation. Although all these cases are similar, tunneling does slow down near resonance.

The delay time calculated from (1) is almost identical to the tunneling time for a Gaussian packet. Although tunneling time slows down near resonance, at the first resonance, it is still less than 0.25 ps, and 25 fs near the second resonance. Therefore, an ideal resonant tunneling device itself is very fast. As long as one is not asking for the detail, tunneling time is nothing but the delay time for a Gaussian packet near resonance.

1.2 Capacitance of a nanoscale sphere

A classical capacitor stores charges, and the electrostatic energy is the only energy stored. However, electrons have kinetic energy even as standing waves confined inside a quantum well or quantum dot. We have calculated the quantum-mechanical capacitance of a small sphere from the definition

\[ E_2 - E_1 = \frac{e^2}{2C_{\text{eff}}}, \]

where \( E_1 \) and \( E_2 \) are the one- and two-electron ground state energies of silicon sphere embedded in an amorphous silicon dioxide matrix [20]. Our results are useful for an understanding of transport measurements, such as resonant tunneling, because the voltages required to bring in additional electrons to the silicon particle are determined by the ground states, and the Coulomb energy involving the capacitance, known as Coulomb blockade [21, 22]. For optical response, excited states must also be included. Since we found \( C_{\text{eff}} \) at 12 nm approaches the classical value, approximately \( 10^{-18} \) F, we found that at 6 nm and 3 nm, \( C_{\text{eff}} \) is only one-half and one-third as large as the classical values, respectively. Likharev used a constant value for the capacitance in his Hamiltonian because the size of the quantum dot is quite large in his case [23]. In brief, quantum mechanically an electron has energy in addition to the electrostatic energy even confined in a well. The energy of an electron is inversely proportional to the square of the dimension of confinement, therefore grows faster than the Coulomb energies. Consequently, \( C_{\text{eff}} \) decreases when the ground-state energies dominate over the electrostatic energies. Appreciable decrease shows up only for particle size under 10 nm. In principle, it should be possible to synthesize a capacitor in a nano-composite, using this size effect.

1.3 Dielectric constant of nanoscale silicon particle

Reduction of the static dielectric constant becomes significant as the size of the quantum-confined systems, such as quantum dots and wires, approaches the nanometric range. A reduced static dielectric constant increases Coulomb interaction energy between electrons, holes, and ionized shallow impurities in quantum-confined structures. The increase of the exciton binding energy significantly modifies the optical properties, and the increase of the shallow impurity binding energy may profoundly alter the transport, i.e., resulting in an intrinsic conduction even extrinsically doped. The size-dependent dielectric constant \( \varepsilon(a) \) was first derived using a modified Penn model taking into account the eigenstates of a sphere instead of the usual free electron energy–momentum relation [24,