Electrostatic Formation of Coupled Si/SiO₂ Quantum Dot Systems

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We present three-dimensional numerical modeling results for gated Si/SiO₂ quantum dot systems in the few-electron regime. In our simulations, the electrostatic confining potential results from the Poisson equation assuming a self-consistent Thomas-Fermi charge model. We find that a very thin SiO₂ top insulating layer allows an effective control with single-electron confinement in quantum dots with radius less than 10 nm and investigate the detailed potential and resulting charge densities. Our three-dimensional finite-element modeling tool allows future investigations of the charge coupling in gated few-electron quantum-dot cellular automata.

Keywords: 3D simulation and modeling, finite element method, silicon/silicon-dioxide quantum dots, quantum-dot cellular automata

We present numerical simulations for electrostatically confined few-electron quantum dot systems in the technologically important Si/SiO₂ material system. Our emphasis is modeling a possible so-called *Quantum-dot cellular automata* (QCA) structure [1] in which a bi-stable occupation by two excess electrons in a small and strongly charge-coupled quantum-dot system defines logic 0/1.

The *bottom panel* of Figure 1 shows a schematic of the Si/SiO₂ material system: a thin silicon-dioxide layer serves as excellent insulation of the bottom silicon slab from the set of top gates. Applying finite biases at these gates allows the formation of electrostatically confined quantum

dots just below the heterostructure interface (at $z = z_0$). Mesoscopic transport investigations in gate-induced quantum-dot arrays [2] documents the feasibility of fabricating few-electron quantum-dot systems in the Si/SiO₂ material system. This development has in turn resulted in a proposal for room-temperature single-electron Si/SiO₂ memory cells [3].

Previous (two-dimensional) modeling results [4, 5] of few-electron Si/SiO₂ quantum dot systems exploited an axial symmetry to investigate the electrostatic confinement within an individual dot. Encouraged by recent three-dimensional modeling of larger quantum-dot systems [6] we investigate

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FIGURE 1 Schematics of possible gate-confined Si/SiO₂ quantum-dot cellular automata (QCA). The *lower panel* shows material composition: thin (5 nm) SiO₂ insulating layers grown on a Si block with an unintentional $p = 10^{15} \text{ cm}^{-3}$ p -doping. Top gates define quantum dot system just below the hetero-interface at $z = z_0$. The *upper panel* illustrates potential QCA cell formation: group of four positive small attractor gates (shaded circles) from charge-coupled system of close quantum dots. The entire QCA cell is surrounded by negative depletion gate (also shaded) to enhance confinement.

here a possible realization of a Si/SiO₂ quantum-dot cellular automata.

The *upper panel* of Figure 1 shows schematics of the small but experimentally accessible top-gate geometry assumed for our model Si/SiO₂ QCA system. A negative depletion gates (shaded) surrounds a group of four positive attractor gates (shaded circles) with a $r = 10 \text{ nm}$ radius and mutual separation of 30 nm . The attractor gates are biased to about 1 V to ensure a single-electron equilibrium occupation in each of the four electrostatically confined quantum dots. For the top silicondioxide layer we assume a 5 nm thickness.

In our $T = 100 \text{ K}$ simulations, the confining potential is obtained from the Poisson equation within a self-consistent Thomas-Fermi charge model. The silicon is assumed to have a small unintended but fully ionized doping, $p = 10^{15} \text{ cm}^{-3}$ and to ensure convergence we investigate a 1.5 nm thick bottom slab with in-plane extension of approximately 300 nm by 300 nm . The top metal depletion and attractor gates are described by Dirichlet boundary conditions. For the exposed SiO₂ surface we assume for simplicity a potential fixed at the mid-gap SiO₂ value, that is, again a Dirichlet boundary condition.

Our finite-element calculation uses a 129 by 129 nonuniform grid to allow a 1 nm resolution from the surface and well below the Si/SiO₂ interface, that is, around the quantum dot system. The *top panel* of Figure 2 shows how most nodal layers (at constant z) are connected in a mesh with alternating tetrahedron orientation to eliminate a geometrical bias. The *bottom panel* of Figure 2 illustrates the repeated thinning of our finite-element mesh undertaken deep below the interfaces where a high in-plane resolution is no longer needed. However, our numerical simulation still involves 6×10^5 nodal points for which we determine the electrostatic potential within the self-consistent Thomas Fermi screening model. Using the Newton-Raphson procedure we solve in each iteration the resulting huge linear system using a quasi-minimal residual implementation [7].

Figure 3 shows our finite-element determination of the electron potential and charge distribution along the interface ($z = z_0$) for our possible QCA realization. The electron confinement potential (*top panel*) is calculated relative to the Fermi energy with negative values corresponding to a strongly enhanced electron concentration n_{el} (*bottom panel*). Note how the thin silicon-dioxide top layer allows a very well-defined set of quantum dots with a finite inter-dot potential barriers. The total equilibrium occupation is set to exactly four electrons and the strong Coulomb blockade effect will prevent multiple occupation of the individual quantum dots.

FIGURE 2 Three-dimensional finite-element modeling of gated Si/SiO₂ quantum-dot systems. The *upper panel* shows tetrahedron-based mesh with alternating cell orientation used in most in-plane layers (i.e., with constant z) to eliminate geometric bias. The *lower panel* illustrate repeated mesh thinning at layers deep below the interface ($z \ll z_0$) used to obtain a factor-of-two reduction in numerical complexity.

Figure 4 shows our modeling results for the simpler double-quantum-dot system in which we are preparing to investigate the *mutual* charge coupling between the quantum dots. We assume again $r=10$ nm attractor gates with a mutual separation of 30 nm and adjust the positive bias to achieve a single-electron equilibrium occupation of each of the quantum dots. The *upper panel* shows the variation of the confinement potential both along the axes (x) connecting the two quantum dots and in the growth direction (z). The heterostructure-cut panel illustrates the excellent top-gate control of the electrostatic potential into the Si/SiO₂ slab well below the heterostructure interface, $z=z_0$.

The *lower panel* of Figure 4 shows the corresponding equilibrium charge distribution, n_{el} .

FIGURE 3 Electron potential and charge distribution of possible QCA cell at the heterostructure interface ($z=z_0$). Potential is calculated for an experimentally accessible gate geometry: four attractor gate of radius $r=10$ nm with mutual 30 nm separation. The *upper panel* shows potential dips (measured relative to Fermi energy) with corresponding contour plot and illustrates the crisp gate control allowed by the thin SiO₂ top layer. The electron potential confines in equilibrium exactly four electrons with very well-defined charge distribution n_{el} (*lower panel*).

Note that this electron distribution, i.e., the equilibrium quantum dot, is confined within 1 nm of the interface and about 5 nm of the attractor-gate center. Future modeling will investigate the charge coupling of such quantum-dot disks in the presence of the attractor and depletion gates.

In summary, we have presented three-dimensional finite-element calculations for gate-confined few-electron Si/SiO₂ quantum-dot systems. We have documented the feasibility of crisp electrostatic gate control for also few-electron quantum-dot systems and have investigated the detailed charge distribution and confinement potentials. Our modeling tool allows future investigations of charge coupling in few-electron quantum-dot cellular automata structures.

FIGURE 4 Growth direction (z) variation of confinement potential (*upper panel*) and corresponding (equilibrium) charge distribution (*lower panel*) in simpler double-dot model system. This system is defined by two $r = 10$ nm attractor dots also with a mutual separation of 30 nm. All z -positions are given relative to the interface $z = z_0$. Note that the equilibrium electron distribution n_{el} is confined within 1 nm of the interface and about 5 nm of the attractor-gate center.

Acknowledgements

This work has been supported by the Advanced Research Projects Agency through the Office of Naval Research.

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