NIRT Highlight
Self-Aligned and Self-Limited Quantum Dot Nanoswitches"

This research project will demonstrate nanoscale computing by developing a process technology to fashion Si / SiGe quantum dots (Qdots) of a predictable size, shape, and placement suitable for mass production and simple electrical contact or sensing. The design-space to explore for such devices is huge necessitating the use of 3D quantum device modeling tools. Previous 3D simulators have focused on calculating the eigenergies and eigenstates of an isolated Qdot or a periodic array of dots. Our emphasis is on Qdots with contacts that allow current flow or charge transfer – a necessity for electronic devices. We have followed a 2 pronged approach for model development. (1) We have developed the theory and written the software for a full 3D quantum device simulator with open system boundaries at any or all points on the exterior. A single band simulator has been written and tested; wavefunction isosurfaces, are shown at right in Fig. 1. The code is written such that upgrading to a full-band sp^{3}s*d^5 model is straightforward. Our approach can explicitly model up to 2x10^6 atoms with an sp^{3}d^{5}s* basis. (2) For model verification, we have continued to enhance our full-band sp^{3}s*d^5 planar-orbital non-equilibrium Green function theory and code, since, at this time, only planar devices are experimentally well characterized enough to permit quantitative comparisons. With this full-band, full quantum approach, we include indirect, phonon-assisted, tunneling and bandgap states [1]. This code has been used to analyze the bandgap states of tunnel diodes as shown in Fig. 2. We have also determined design guidelines for Si / SiO_2 interface quality for proposed Si / SiO_2 tunnel devices [2]. These tools will streamline the quantum device development cycle by providing design criteria for the device material, epi-layer, and geometry configuration and providing analysis of experimental data.

One level above the physical device models are the compact (SPICE) models used for circuit design. We have enhanced the compact model of a resonant tunnel diode to include the quantum capacitance. The capacitance peaks precisely in the center of the negative differential resistance region which is the desired operating point for linear applications [3]. The compact model compares well with the predictions of the full quantum device model as shown in Fig. 3. Accurate, efficient compact models are a necessity for both conventional and quantum circuit design.

1. C. Rivas, R. Lake, W. R. Frensley, G. Klimeck, P. E. Thompson, K. D. Hobart, S. L. Rommel, and P. R. Berger, "The excess current in a delta-doped MBE grown Silicon tunnel diode," submitted.
2. T. Sandu, R. Lake, and W. P. Kirk, "Effect of interface roughness on a Si / SiO_2 resonant tunnel diode," *Superlatt. Microstruct.,* **30**, 201 (2001).
3. R. Lake, "Full quantum simulation, design, and analysis of Si tunnel devices, MOS leakage and capacitance, HEMTs and RTDs," *2001 IEDM Technical Digest* (IEEE, New York, 2001) p. 5.5.1.

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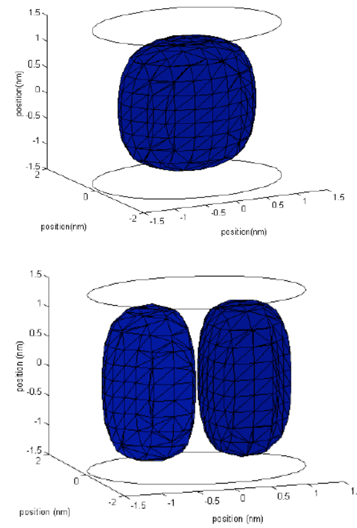

Fig. 1.Wavefunction isosurfaces of 1st and 2nd eigenstates.

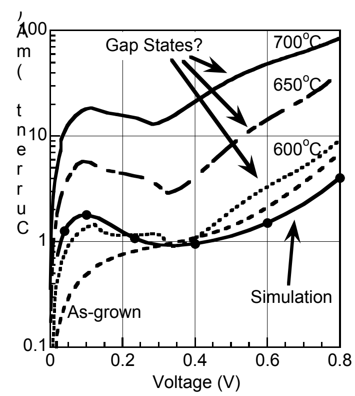

Fig. 2. Analysis of data. Full-band, full-quantum model with phonon-assisted, tunneling and bandgap states [1].

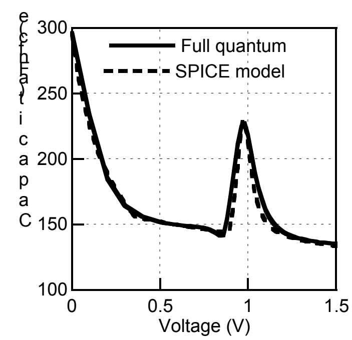

Fig. 3. Demonstration of SPICE model of quantum capacitance.