Electronic Properties of Silicon Nanowires

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We investigate the electronic structure of Si nanowires demonstrating the effect of wire thickness on the bangap, conduction valley splitting, hole band splitting, effective masses, and transmission.

SiNWs are a direct bandgap material with a Brillouin zone 1/2 the length of that of bulk Si along the Δ line. In the conduction band, valley splitting reduces the averaged mobility mass along the axis of the wire, but quantum confinement increases the transverse mass of the conduction band edge. For the wire thickness range that we have considered (up to 2.7 nm), the effective mass at the conduction band edge is at least 35 percent heavier than that of transverse mass of bulk Si. Quantum confinement has the largest effect on the effective masses in the valence band. The effective mass at the valence band edge is at least 6 times heavier than that of the bulk in the [100] direction. The effective mass of the next highest band is even heavier.

Small energy splitting also occurs at the conduction band minimum. For wires greater than 1.54 nm thick, the 4 bulk valleys which compose the conduction band minimum are split into 3 energies. The center energy is twofold degenerate roughly evenly split between the lowest and highest energy so that the conduction band minimum becomes non-degenerate except for spin.

The wire-substrate interface acts as a heterojunction with a band offset between the bulk and the wire resulting in reflection in the transmission.

The single band model performs reasonably well at calculating the effective band edges for the 1.54 nm wire. Howerver, the accuracy of the single band calculation quickly becomes non-existent as one moves away from the band edges.

We use two different models, a three-dimensional (3D) discretization of the single-band effective mass equation, and a nearest neighbor $sp^3d^5s^*$ model, where the Hamiltonian matrix elements, are optimized with a genetic algorithm. Transmission coefficients are calculated using the non-equilibrium Green function (NEGF) formalism with a recursive Green function algorithm.

A full journal publication of this work will be published in the Journal of Computational Electronics.

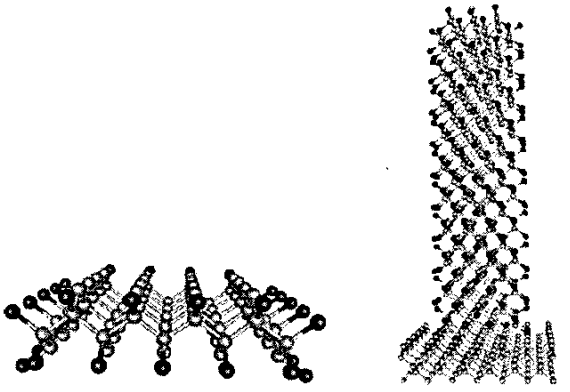

Fig. 1. (left) The unit cell of the 1.54 nm square Si wire passivated with H. (right) H passivated Si wire on a substrate.

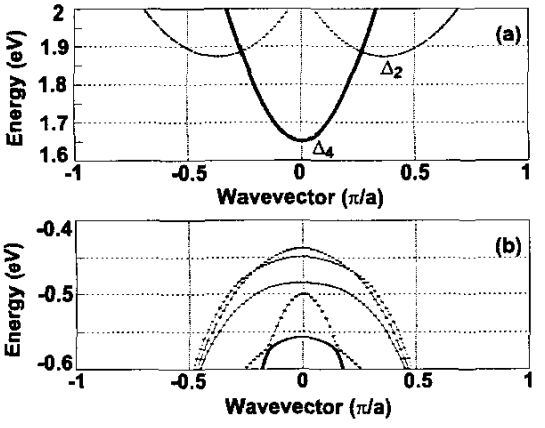

Fig. 2. The (a) conduction and (b) valence E-k relation for a 1.54 nm x 1.54 nm wire. The lattice constant a = 5.4 Å.

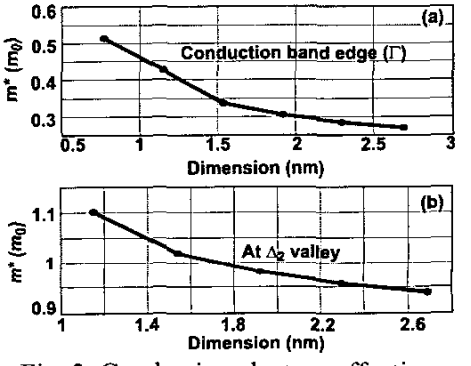

Fig. 3. Conduction electron effective masses vs. wire thickness at (a) the conduction band minimum and at (b) the Δ_2 valley.