Open-Boundary-Condition Ballistic Quantum Transport using Empirical Pseudopotentials

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INTRODUCTION

Moore's law aggressively pushes CMOS technology into the nanometer scale. Finite size and quantum confinement change the band structure, which deviates significantly from the bulk. Meanwhile, the study of electronic transport requires a quantum mechanical approach. Based our previous work on quantum transport using the Pauli Master Equation with effective mass [1], we developed an atomistic full band quantum transport model using empirical pseudopotentials to provide improved physical insight into novel nanodevices.

METHOD

The Schrödinger equation with lattice potential $V^{lat}(r)$ and external potential $V^{ext}(r)$ can be written as

$$\big[-\frac{\hbar^2\nabla^2}{2m}+V^{lat}(r)+V^{ext}(r)\big]\psi(r)=E\psi(r), \quad (1)$$

where the wave function $\psi(r)$, in order to account for the effect of the spatially varying external potential, can be approximated by the envelop function $\phi^k_G(r)$,

$$\psi_k(r)=\sum_G \phi^k_G(r)e^{iGr}. \quad (2)$$

Substituting Eq. (2) into Eq. (1), we have

$$\sum_{G'}\Big\{\big[-\frac{\hbar^2\nabla^2}{2m}-\frac{i\hbar^2G'\nabla}{m}+\frac{\hbar^2G'^2}{2m}+V^{ext}(r)\big]\delta_{GG'} +V_{GG'}\Big\}\phi^k_{G'}(r)=E(k)\phi^k_{G'}(r). \quad (3)$$

Equation (3) can be solved accounting for the open boundary conditions with a nontrivial extension of the Quantum Transmitting Boundary Method (QTBM) [2].

SIMULATION RESULTS

We simulate Si nanowires using local empirical pseudopotential parameters from Zunger [3]. These devices have a cross section of 1x1 cells (0.384 nm x 0.384 nm). Each unit cell, containing 9 Si atoms and 12 H atoms terminating the surface, is isolated by one cell of vacuum in the x-y plane. Figure 1 shows the band structure and the density of states. Injected and reflected states are chosen according to the complex band structure shown in Fig. 2. In order to reduce computational cost, in Fig. 3 we compare results obtained using different restricted subsets of reflected states, considering that states with a large imaginary component of their wavevector result in a small contribution to the charge. Keeping the cross section fixed, we have considered nanowires with length of 1, 3, 6, and 9 cells. As an illustration, we show in Fig. 4 a particular wavefunction in nanowire 3-cell long. For these devices, source, channel and drain each shares 1/3 of the total length. The charge density is set to 10^6cm^{-1} in the S/D region and 10^0cm^{-1} in the channel. In Fig. 5 we show the self-consistent potential for a 9-cell long device and in Fig. 6 we compare the characteristics for devices of different length.

CONCLUSION

We have presented a nontrivial extension of QTBM to account for the full band structure and improved the computational efficiency by ignoring a subset of evanescent waves. For the application, we have shown simulation results of Si nanowires.

REFERENCES

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[3] S.B. Zhang, C. Yeh, and A. Zunger, Phys. Rev. B **48**, 11204 (1993).

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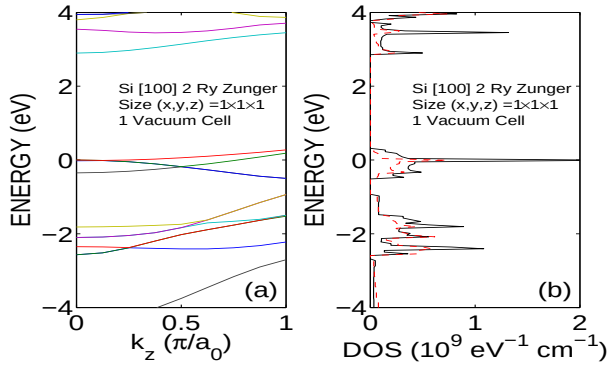

Fig. 1. Empirical pseudopotential band-structure (a) and density of states (b) for a [100] Si nanowire.

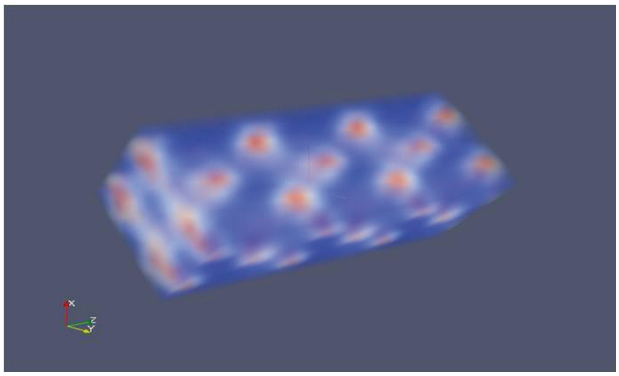

Fig. 4. Squared amplitude of a propagating wavefunction in a 3-cell long Si nanowire calculated using empirical pseudopotentials.

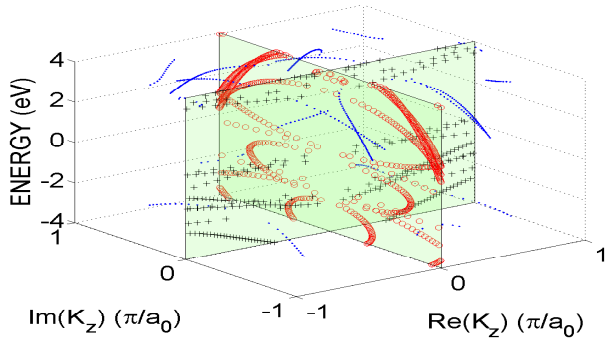

Fig. 2. Complex band structure of a Si [100] nanowire. Black crosses and red circles denote real and imaginary wavevectors, respectively, while the blue symbols denote fully complex wavevctors. The green planes show the projections of the dispersion onto the real and imaginare kz-planes.

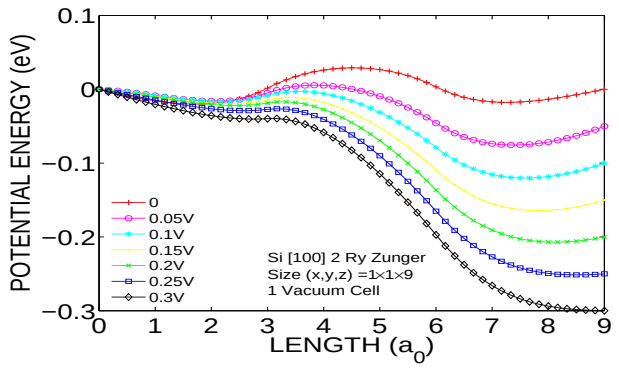

Fig. 5. Self-consistent potential energy for a 9-cell Si nanowire as a function of the applied bias.

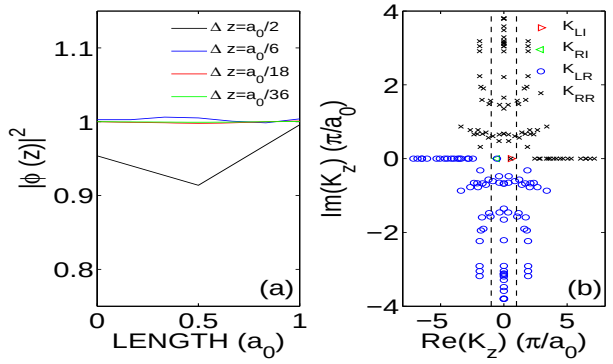

Fig. 3. Evolvement of propagating waves (a) under different choices of real space discretization Δz and reflected states k_z (b) at an incoming energy E=-1.5V.

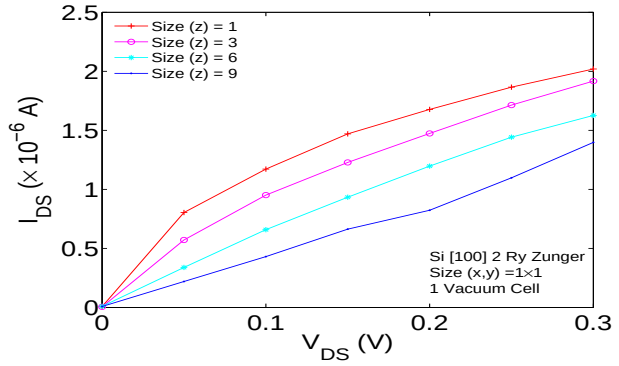

Fig. 6. I-V characteristics of 1, 3, 6 and 9-cell Si nanowires.