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Hierarchical simulation of transport in silicon nanowire transistors

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Abstract We propose a very fast hierarchical simulator to study the transport properties of silicon nanowire FETs. We obtain the transverse wave functions and the longitudinal effective masses and band-edges of the lowest conduction bands from a nearest-neighbor $sp^3d^5s^*$ tight-binding study of an infinite nanowire with null external potential. Then we plug these parameters into a self-consistent Poisson-Schrödinger solver, using an effective mass approach and considering the bands decoupled. We apply this method, which gives quantitatively correct results with notable time savings, for the simulation of transport in two different silicon nanowire FETs.

Keywords Silicon nanowires · Silicon nanowire FETs · Tight-binding method · NEGF

1 Introduction

Silicon Nanowire Transistors (SNWTs) are considered as valid substitutes for planar MOS devices because of their increased gate control over the channel and their perspective of high-speed operation [1].

It has been proved that an effective-mass approach based on the dispersion relations of bulk silicon gives good quantitative results only for not too thin nanowires: indeed, below ∼3 nm the influence of the band-structure on transport becomes relevant and therefore an atomistic study of the silicon nanowire is needed [2–5].

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On the other hand, a complete atomistic approach can be too demanding from the computational point of view [6, 7], so that it can be definitely prohibitive to perform an investigation of device performance over the whole design parameter space.

Here we propose a "quasi-atomistic" approach, in which effective masses, local density of states and 1D bands are computed by means of a semi-empirical tight-binding method, and then used to compute transport in SNWTs by means of the self-consistent solution of the three-dimensional Poisson and Schrödinger equations with open boundary conditions, within the NEGF formalism [8].

2 Atomistic study

To obtain the transverse local density of states and 1D electron bands of the nanowire constituting the channel of our FET (with transport direction along [001], in our simulations), we have made an atomistic study of the corresponding infinite silicon nanowire.

In detail, we have used an $sp^3d^5s^*$ tight-binding model (not including strain effects), in which only the interactions between nearest-neighbor silicon atoms have been considered. We have performed our simulations both including or neglecting the effect of spin-orbit coupling; we have therefore considered 20 atomic orbitals or 10 atomic orbitals, respectively, for each of the silicon atoms belonging to the nanowire unit cell (which for our transport direction includes 4 atomic layers). Using as a basis set the Bloch functions propagating along the nanowire axis and obtained from the atomic orbitals considered in the nanowire unit cell, we have computed the Hamiltonian matrix $H(k)$ for each considered longitudinal wave vector k. In particular,

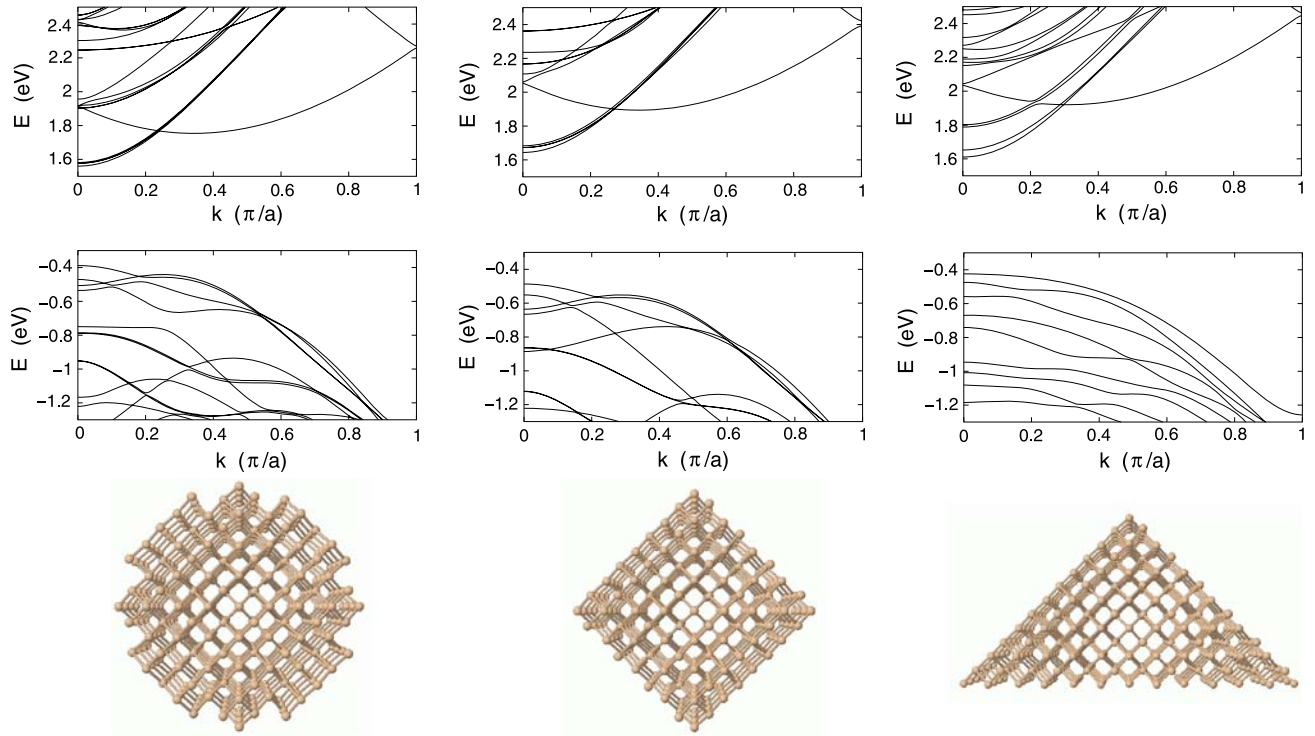

Fig. 1 Dispersion relations found for silicon nanowires with axes along [001] and with different cross-section shapes: circular with a 1.08 nm radius (*left panel*), square with sides along ⟨110⟩ directions and a 1.5274 nm edge (*central panel*), triangular with the hypotenuse of the right isosceles triangle located along [100] and 3.24 nm long. In each panel we show (from *top* to *bottom*): the lowest conduction bands, the highest valence bands and the atomic structure of the nanowire. These results have been obtained including the spin-orbit effect in the tight-binding calculations

the matrix elements between nearest-neighbor atomic orbitals have been obtained from the relations found by Slater and Koster [9] and by Podolskiy and Vogl [10], as well as the values proposed for the tight-binding parameters of bulk silicon by Boykin et al. [11].

To remove the effect of surface states, we have followed the method proposed by Lee et al. [12], increasing, along the surface of the nanowire, the on-site energy of the outward oriented hybridized sp^3 orbitals.

The eigenvalues of the Hamiltonian matrix $H(k)$ give the dispersion relations $E(k)$ of the nanowire and in particular the edges of the considered bands and the corresponding longitudinal effective masses. The eigenvectors of such a matrix give instead the coefficients with which we have to combine the basis Bloch functions to obtain the electron wavefunctions (and therefore their square moduli). In particular, exploiting the orthonormality of the Löwdin atomic orbitals used in the tight-binding method [9] and the fact that each orbital has non negligible values only near the corresponding atom, the electron density around each atom is proportional to the sum of the square moduli of the coefficients found for the Bloch functions involving the atomic orbitals centered on the atom. Such an electron density is assumed to be all localized at the coordinates of the atom.

In Fig. 1 we show the dispersion relations for three nanowires with different cross-sections (circular, square and triangular), including the effect of spin-orbit interaction.

3 Transport analysis

For the study of transport, we have neglected the effect of spin-orbit interaction, since we have noticed that it has a very small influence on the band structure. Moreover we have limited our calculations to the four lowest conduction bands. In particular, we have computed the electron wavefunction only for $k = 0$ (where these bands have a minimum) and we have evaluated the dispersion relations for $k = 0$ and for two small positive wavevectors. Exploiting the symmetry around $k = 0$, these values are sufficient for the application of the five-point discretization formula for the second derivative, that we need for the evaluation of the longitudinal effective mass.

In our computations the transverse local density of states (LDOS) is considered to be the same for all the 2D slices perpendicular to the transport direction, since we have verified that, for the nanowire sizes we have considered, the transverse eigenfunctions are almost independent of the po-

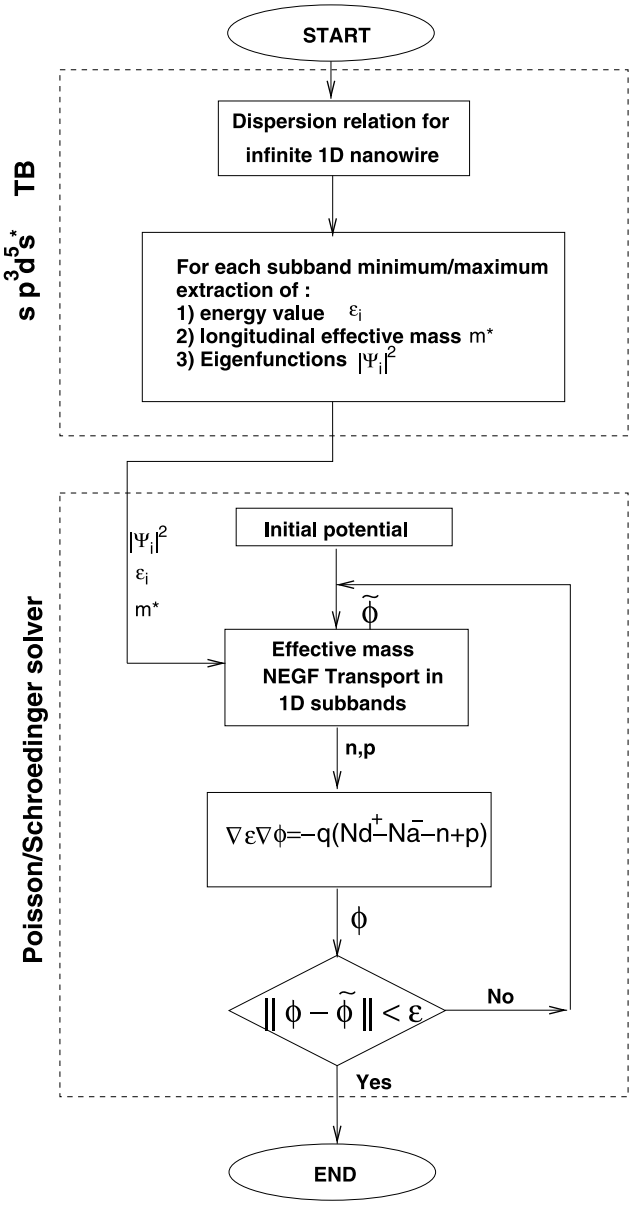

Fig. 2 Flow chart of the hierarchical approach that we have followed to study the transport properties of silicon nanowire FETs

tential due to the gate bias. Therefore the atomistic calculation is reduced to an initial solution of the Hamiltonian of an infinite nanowire with no external potential, and in the transport analysis we use the approximation of decoupled bands.

The flow chart of the followed hierarchical approach is shown in Fig. 2.

The band edges ε_i, the effective masses m_i^* for each energy band and the local densities of states $|\Psi_i|^2$ obtained from the solution of the secular equation containing the tight-binding atomistic Hamiltonian are passed to an iterative scheme, where the Poisson and the Schrödinger equations with open boundary conditions are solved self-consistently, within the Non-Equilibrium Green's function formalism (NEGF).

In particular the transmission coefficient and the longitudinal linear electron density on each band (n_{1D_i}) are obtained from the transport parameters computed with the NEGF formalism on uncoupled subbands for a given potential $\tilde{\phi}$. As far as the longitudinal approximate 1D bands are concerned, we shift the band edges by the mean value of the potential computed on each transverse slice and we use the previously obtained effective mass values.

The obtained electron and hole concentrations are then fed into the right-hand term of the 3D Poisson equation. In detail, the three-dimensional electron density n to be inserted into the right hand term of the Poisson equation reads

$$n(x, y, z) = \sum_{i}^{M} |\Psi_i(x, y)|^2 n_{1D_i}(z),$$

where the sum runs over the M considered modes, and $|\Psi_i(x, y)|^2$ is the transverse local density of states. This last quantity is obtained projecting the approximate value of the square modulus described in the previous paragraph (which corresponds to a point charge approximation) over the transverse section of the nanowire. Atomic eigenfunctions are also interpolated on finer or on coarser grids, in order to achieve better resolution, in the case of small cross-section, or to reduce the number of grid points, when the considered device has large transverse dimensions.

If the 2-norm of the difference between the potentials obtained at the end and at the beginning of the iterative cycle (ϕ and $\tilde{\phi}$, respectively) is smaller than a predetermined value (ε), the cycle ends, otherwise the new potential ϕ is used to compute again transport.

In order to test the possibilities of our approach, we have considered a double-gate silicon nanowire transistor, where the (undoped) silicon nanowire has a 1.5274 nm × 1.5274 nm square cross-section (with edges oriented along ⟨110⟩ directions). The source and drain reservoirs are 10 nm long, doped with a donor concentration equal to 10^{20} cm^{-3}. The channel length is equal to 10 nm, while the oxide thickness is 1 nm, as shown in the inset of Fig. 3, where the transfer characteristics in a linear and in a logarithmic scale are also reported for a drain-to-source voltage equal to 0.5 V. The sub-threshold slope is about 60 mV/dec, while the threshold voltage is quite large (about 1.65 V); it can however be reduced by means of gate work function tuning.

We have then studied the triple-gate SNWT analyzed by M. Luisier et al. in [6]. In this case the cross-section of the (undoped) silicon nanowire is a 2.1 × 2.1 nm^2 square (with ⟨100⟩ edges), the oxide thickness is 1 nm, the channel length is 13 nm and the source and drain reservoirs are 10 nm long doped with a donor concentration equal to 10^{20} cm^{-3}.

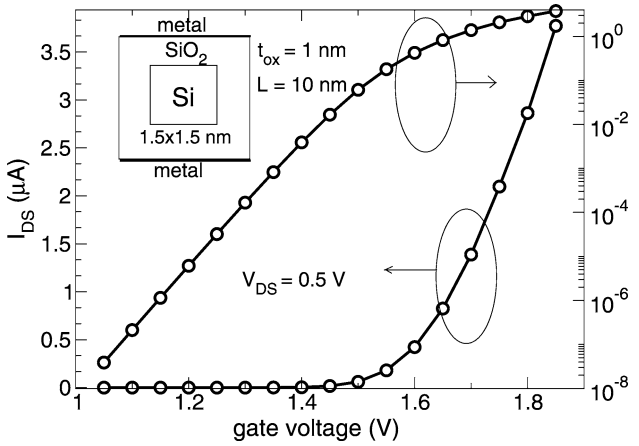

Fig. 3 Transfer characteristics obtained for $V_{DS} = 0.5$ V for the silicon nanowire transistor with the cross-section sketched in the *inset*, represented for a linear (*lower curve*) or logarithmic (*upper curve*) scale for the current

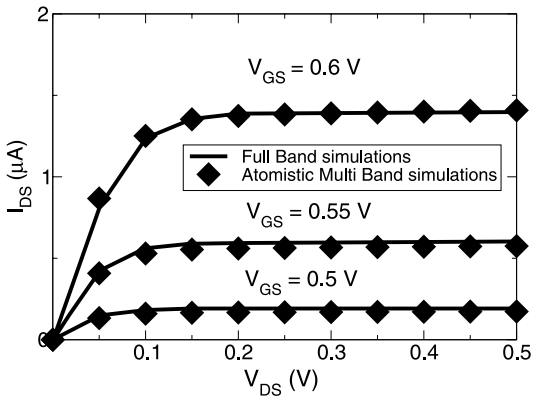

Fig. 4 Output characteristics for a triple-gate SNWT with a 2.1×2.1 nm^2 square cross-section computed in [6] (*solid lines*) and with our method (*diamonds*)

In Fig. 4 the output characteristics of the simulated device computed by means of our method are shown (diamonds), and compared with those obtained with an atomistic full band approach (FB) [6] (solid lines). In particular, the gate work function has been adjusted to fit the current value obtained by Luisier for a gate voltage equal to 0.6 V and a drain-to-source voltage (V_{DS}) of 0.5 V. Due to this adjustment, the choice of the position of the chemical potential with respect to the band edges is actually not relevant; in our simulations it has been assumed to be at the middle of the energy gap for an infinite undoped structure.

As can be seen, our results are in very good agreement with FB simulations, while requiring very limited computational resources. In particular, simulations performed on a 3.4 GHz Xeon workstation have taken 9 minutes per bias point, which is almost 30 times faster than FB simulations (Luisier: private communications).

4 Conclusions

Using a hierarchical approach based on the use of an $sp^3d^5s^*$ tight-binding atomistic model to find the input parameters for a self-consistent Poisson-Schrödinger solver, we have studied the transport properties of a silicon nanowire transistor. This multi-scale approach, together with the assumption of small dependence of the transverse local density of states on the actual external potential, has allowed us to obtain a very fast solution of the transport problem, with quantitatively correct results. In cases in which non-idealities in the nanowire introduce a significant variation of the transverse wave function in different nanowire sections, and thus a non negligible mode-mixing, this algorithm can however be generalized recomputing the transverse local density of states on each section.

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