# Low-dimensional Quantum Transport Models in Atomistic Device Simulations

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*Abstract*—**The paper presents a method for atomistic quantum transport simulations in nanowire (NW) MOSFETs. The original tight-binding (TBM) Hamiltonian of the nanostructure is replaced with an approximate model which reproduces the transport properties at atomistic level. Small size of the equivalent model (EM) makes the atomistic transport simulation computationally cheap and allows the inelastic scattering effects to be incorporated easily. The method is applied to various p-SiNW and n-SiNW MOSFETs.**

## I. Introduction

Rapid progress in semiconductor device technologies has led to development of a variety of novel devices such as double-gate transistors [1], carbon nanotubes [2] and gate-all-around (GAA) metal-oxide-semiconductor field-effect-transistors (MOSFET) [3]–[5]. Experimental studies of Ge/Si nanowire heterostructures have shown excellent gate control, high drain current and reduced sensitivity to temperature [6], [7]. This technological progress has stimulated a growing interest to both experimental and theoretical studies of quasi-one-dimensional quantum transport in such devices. In nanoscale regime, a device can no longer be described as a continuous system and the theoretical modeling of quantum transport requires atomistic quantum models taking into account the lattice orientation and non-elastic scattering [8]. The nearest-neighbor tight-binding models with various levels of approximations are commonly used for this purpose [9]. The non-equilibrium Green's function technique with the tight-binding type of Hamiltonian provides a suitable technique to perform transport simulations with atomistic resolution including possible inelastic effects [9], [10]. However, compared to the effective mass models, large size of the tight-binding Hamiltonian makes the atomistic transport simulations is computationally very demanding.

In the present study, we develop a general scheme to substitute the original tight-binding Hamiltonian of the nanowire device by a low-dimensional quantum transport model with equivalent transport characteristics. We start with a one-particle quantum state in an ideal nanowire and construct a new atomistic basis which reproduces all the scattering states and the band structure in a narrow ($\sim 0.5\,\text{eV}$) energy window at the bottom of the allowed band of the wire. This basis transformation is further used to obtain a low-dimensional open device Hamiltonian in the basis representation. The com-

putational burden is greatly reduced and the atomistic transport simulations can be performed on ordinary PC computer. As a test, we construct the equivalent transport models for a number of p-SiNW and n-SiNW MOSFETs with different diameter and lattice orientation of the Si channel. The ballistic transport simulations show better than $1\,\%$ level of numerical accuracy in computed drain current. The utility of the present approached is further demonstrated by calculating electron-phonon scattering in p-Si [100] NW MOSFET in scope of non-equilibrium Green's function formalism (NEGF).

## II. Atomistic basis in quantum wires

The basis expansion method for quasi-one-dimensional transport is well known in the effective mass model: a current carrying state of the NW is represented by a small number of subband eigen-functions obtained from the two-dimensional quantization in the wire cross-section. Such a mode-space approach allows the actual three dimensional transport problem to be reduced to a much easy task of computing a few one-dimensional wave functions. The required number of channels depends of the energy scale and the band structure, i.e. the effective mass and diameter of the NW. The subbands representation can be also thought as an expansion in terms of scattering states of the corresponding ideal wire, since the dependence of these states on the energy and the transport coordinate in the effective mass model is trivial. In the present work we make an attempt to generalize this picture to atomistic NWs with realistic band structure.

We consider an infinite wire with one-particle tri-diagonal block Hamiltonian

$$H_{nn} = H_0 + V_n; \quad H_{n\,n+1} = H_{n+1\,n}^+ = W, \tag{1}$$

where $n$ numerates unit structures, $H_0$ is the Hamiltonian of isolated unit structure, $W$ is the transfer Hamiltonian between the nearest unit-structures, and $V_n$ represents the potential term. The definition of the unit structure in the reference ideal wire and the original size $N_{\text{TBM}}$ of the blocks (number of atomistic orbitals) depend on the lattice orientation and the tight-binding method. The elements $n = 1, 2, \ldots, N$ are taken as the device coupled to two leads $V_{n<1} = V_1$ and $V_{n>N} = V_N$. We consider a non-equilibrium one-electron state as a result of scattering effects between quantum states in the ideal NW. Under normal conditions, the transport characteristics are

dominated by mobile carries near the band gap of the NW. The scattering solutions are calculated as the Bloch eigen-states [11]

$$\left[W^+ Z_\nu^{-1} + H_0 + W Z_\nu - \varepsilon\right]\chi_\nu = 0 \qquad (2)$$

in open channels with $|Z_\nu| = 1$. These states occur in $M_{op}$ pairs of complex conjugated functions, where $M_{op}$ is the number of subbands at the reference energy $\varepsilon$. Thus, we can construct $2M_{op}$ real basis functions which exactly reproduce the quantum transport though the ideal wire at this energy. The energy dependence of the Bloch scattering states is expected to be smooth enough in order to be consistent with the realistic band structure. Solving the Bloch equation at few $\varepsilon$ within the energy interval of interest and putting together all the scattering solutions, we obtain a moderate basis which can be used in simulations instead of the complete set of TBM atomic orbitals. In practice we use $\{\Re\chi_\nu(\varepsilon)\}$, $\{\Im\chi_\nu(\varepsilon)\}$ at all reference energies and construct a real-valued orthonormal basis set $\{\Phi_\nu\}$ : $\langle\Phi_\nu|\Phi_\mu\rangle = \delta_{\nu\mu}$, where the scalar product is understood as a sum over the atomic orbitals in the unit-structure. A one-particle state of the device is calculated in the form of the basis expansion

$$\Psi(n) = \sum_{\nu=1}^{N_b} \Phi_\nu \xi_{\nu n}, \qquad (3)$$

where $\Psi(n)$ is the vector of $N_{TBM}$ quantum amplitudes in the $n$-th unit-structure, $N_b$ is the basis size, and the "wave functions" $\xi_{\nu n}$ are to be found from the transport simulations with the low-dimensional model Hamiltonian

$$h_{\nu\mu}(n) = \langle\Phi_\nu|H_0 + V_n|\Phi_\mu\rangle; \ w_{\nu\mu} = \langle\Phi_\nu|W|\Phi_\mu\rangle. \qquad (4)$$

The outlined procedure is straightforward and fairly simple. Test calculations confirm that a sequence of Bloch eigen states also reproduce the scattering solutions at intermediate energies. However, the band structures for two wires Eqs. (1) and (4) are generally not equivalent in the energy interval of interest. The reduced model is found to contain unphysical branches, which in transport simulations would cause erroneous states of the device. In ballistic regime, the contribution from this states can be easily identified and eliminated [12]. Here we present a more general equivalent transport model (EM) without unphysical effects.

## III. Variational construction of the EM

The unphysical branches in the band structure of the reduced scattering model should be expected. Unlike the effective mass model, the tight-binding Hamiltonian is not bounded by the band edge and there is no energy variational principle to guarantee the correct spectrum in this energy interval. Adding more states to the basis set improves the accuracy of the physical solutions, but also leads to new branches which could appear at any energy including the band edge area. In order to construct a model with correct transport characteristics, we develop a variational procedure which guarantees correct choice of the new basis states. The mathematical and numerical details of our variational approach will be published elsewhere. Here we just present the summary of the method and show some results as an illustration.

For a given basis $\{\Phi_n\}$, we introduce a variational functional $N(\varepsilon_1, \varepsilon_2, k, [\Psi])$ which has a meaning of the number of branches at wave number $k$ within energy interval $[\varepsilon_1; \varepsilon_2]$. Here $\Psi$ is a new basis function from the orthogonal complement of $\{\Phi_n\}$. At any $k$, the branches are calculated as the eigenvalues of the matrix representation $H(k)$ of the Bloch operator with respect to the basis $\{\Phi_n\} \otimes \Psi$. The branch energies $\varepsilon_n(k)$ thus become a functional of $\Psi$. If $\{\chi_n\}$ is the basis for an appropriate subspace of the complement, one can use the expansion $\Psi = \sum_n C_n\chi_n$ and obtain the function $N(\varepsilon_1, \varepsilon_2, k, \{C_n\})$ which can be used in numeric.

We require $N(\varepsilon_1, \varepsilon_2, k, [\Psi])$ to be 1) analytical differentiable functional; 2) easily computed together with its lowest derivatives and 3) reach local minimum at $\Psi$ with less number of states in $[\varepsilon_1; \varepsilon_2]$ compared to $\{\Phi_n\}$ model. Then, the variational functional for the whole band structure can be taken as a sum of contributions from several wave numbers $k_i$

$$F[\Psi] = \sum_i f_i N(\varepsilon_1, \varepsilon_2, k_i, [\Psi]) \qquad (5)$$

with the weighting factors $f_i > 0$. To complete the construction, we need to specify $N(\varepsilon_1, \varepsilon_2, k_i, [\Psi])$ and $\{\chi_n\}$. The latter are taken as nonzero eigenstates of the singular operators $(1 - P_\Phi)W^+ P_\Phi W(1 - P_\Phi)$ and $(1 - P_\Phi)H_0 P_\Phi H_0(1 - P_\Phi)$, where $P_\Phi = \sum_n |\Phi_n\rangle\langle\Phi_n|$ is the projector to the initial functional space of the model. This choice simply corresponds to the orbitals with the strongest coupling to the initial $\{\Phi_n\}$ in spirit of the perturbation theory. Finally, the variational functional at fixed $k$ is found in the form

$$N(\varepsilon_1, \varepsilon_2, k, [\Psi]) = \langle\mathrm{Tr}\, G(z, k)\, (z - (\varepsilon_1 + \varepsilon_2)/2)\rangle_z, \qquad (6)$$

where $G(z, k)$ is the resolvent of $H(k)$ and $\langle\ldots\rangle_z$ stands for the arithmetical mean for complex valued $z$ located at circular contour centered at $(\varepsilon_1 + \varepsilon_2)/2$ with radius $(\varepsilon_2 - \varepsilon_1)/2$. This completes our construction and Eqs. (5) and (6) can be shown to satisfied the above criteria for the variational functional. Further details will be presented elsewhere.

## IV. Numerical illustration

Our procedure is summarized as follows. (1) Calculate enough scattering state to guarantee that the physical branches of the NW band structure are well reproduced within energy interval of interest. (2) Minimize the functional Eq. (5) on the appropriate small dimensional subspace of the orthogonal complement. This gives a new basis function $\Psi$ such that the corresponding $N_b + 1$ dimensional model has one less unphysical subband in the band structure. (3) Repeat item (2) until there is no more unphysical branches. (4) Express the original creation/annihilation operators at the atomistic orbitals in terms of that for the basis functions and obtain the equivalent transport model Hamiltonian. At this stage, one can incorporate into the EM any source of scattering including inelastic effects.
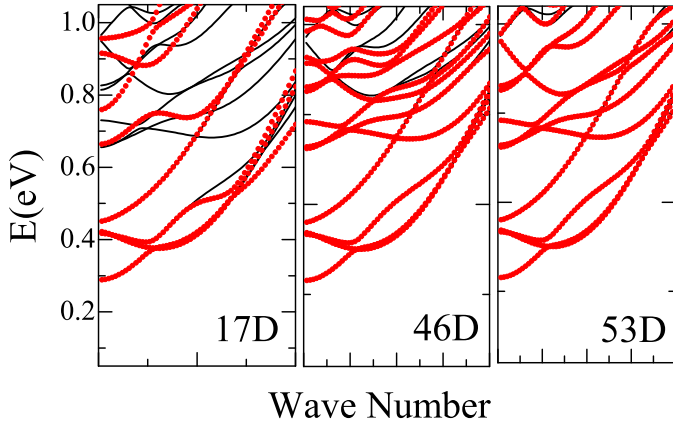
Fig. 1. Valence band structure of [100] SiNW with rectangular cross section $2.2 \times 2.2$ nm. Black lines show the exact band structure and red marks are for three EMs with 17, 46 and 53 basis functions.
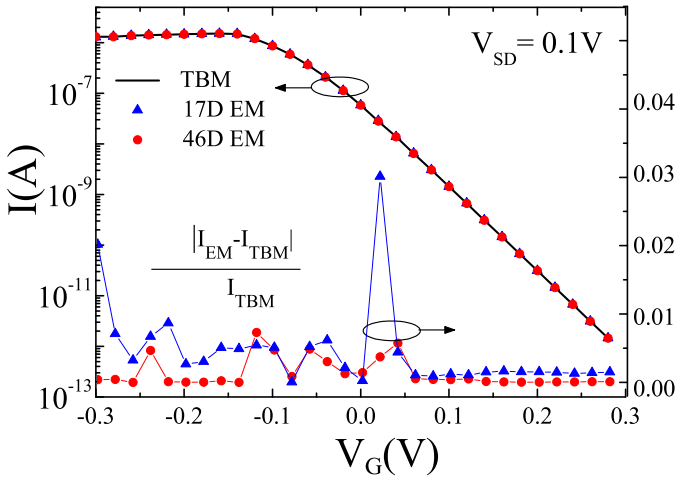


Fig. 2. IV characteristics of p-SiNW calculated in two EMs from Fig. 1 and the original $sp^3s^*$ TBM. The low part of the figure demonstrates numerical accuracy of the EM data.

As a test, we performed atomistic transport simulations in n-SiNW and p-SiNW GAA devices of 30 nm length at room temperatures with dopant concentration in the source/drain regions of $10^{20}$ cm$^{-3}$ for n-Si and $2 \times 10^{19}$ cm$^{-3}$ for p-Si. We use the $sp^3d^5s^*$ and $sp^3s^*$ tight-binding models for n-SiNW and p-SiNW respectively. Fig. 1 shows an example of the band structure in three EMs for [100] p-SiNW with rectangular cross section $2.2 \times 2.2$ nm. The larger EM provides wider part of the band structure at the bottom of the valence band. Thus, the numerical accuracy can be estimated solely from the EMs with no further reference to the original TBM. Fig. 2 presents the computed IV characteristics at applied bias $V_{SD} = 0.1$ V. The results from 17-dimensional and 46-dimensional EMs from Fig. 1 are compared with the exact TBM calculation and $\sim 1\%$ level of accuracy is confirmed in both cases. In fact, the difference between three IV-curves in this figure is within the numerical accuracy of the self-consistent drain current calculations. In this sense, the results are identical. We conclude that the EMs with the band structure within
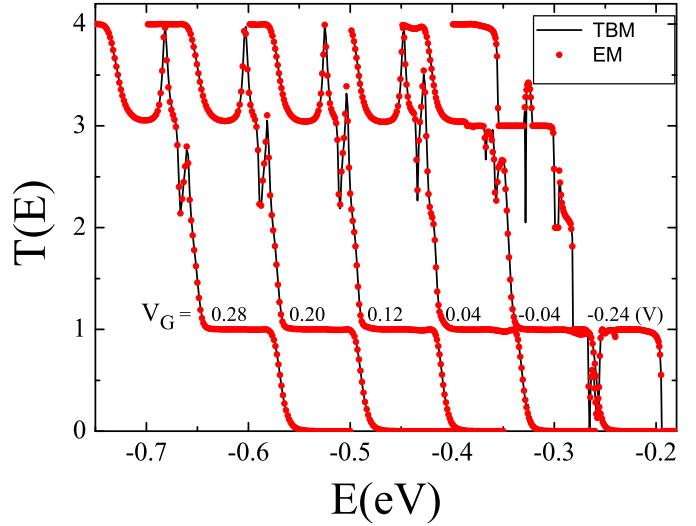


Fig. 3. Transmission functions of p-Si NW at various gate voltages in Fig. 2. 17 D EM (red marks) are compared with the exact TBM (black lines)

$\sim 0.2 - 0.3$ eV interval near the band edge can be safely used in the atomistic device simulations. Figs. 3 and 4 show the computed transmission function at various gate voltages and an example of the charge distribution at 32 Si atoms in the NW cross section. Excellent agreement with the exact data is found even for the smallest 17 D EM. The transport simulations in this case are very cheap and it take seconds to compute the (ballistic) device state at one iteration. The calculations were repeated taking into account the electron-phonon scattering at the level of self-consistent Born approximation in NEGF. In this case, accurate calculation of the phonon absorption subbands require larger band structure of the EM, especially in the off current regime. The results of this study will be published elsewhere.

The same approach was used to construct the EMs from the primary $sp^3d^5s^*$ TBM basis for quantum transport in [100],[110] and [111] n-SiNW MOSFETs with diameters ranging from 2 nm to 4 nm. Fig. 5 shows an example of the conduction band structure in $4 \times 4$ nm [111] n-SiNW with 7780 original atomistic orbitals in a single unit-structure. Again, the cheapest 36-dimensional model is found to provide transport characteristic with 1 % accuracy. In fact, even a smaller EM can be used with only the lowest six nearly degenerate subbands in Fig. 5 reproduced correctly. The accuracy of the calculations drops down to about 10 percents in this case. Fig. 6 shows the IV-characteristics for various n-SiNW MOSFETs with different diameters and lattice orientation. In all cases, $\sim 1$ % level of accuracy is confirmed. In particular, we estimated the subthreshold swing 67, 75, 84 for [100] NWs, 66, 75, 88 for [111] NWs and 72, 77, 87 for [110] NWs (all in mV/dec) depending on the wire diameter.

## V. Summary

We developed a low dimensional atomistic model of quantum transport in nanowire MOSFETs. Our method effectively
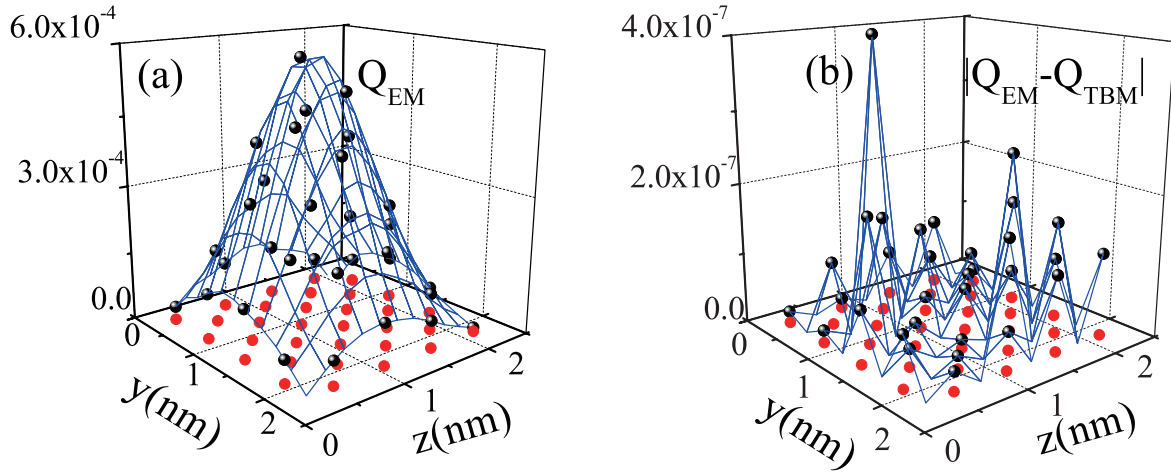
Fig. 4. Example of the mobile charge distribution within one atomic layer in [100] p-SiNW. Red points indicate actual position of 32 Si atoms in (yz)-plane orthogonal to the transport direction. The right panel shows absolute error in the EM data.
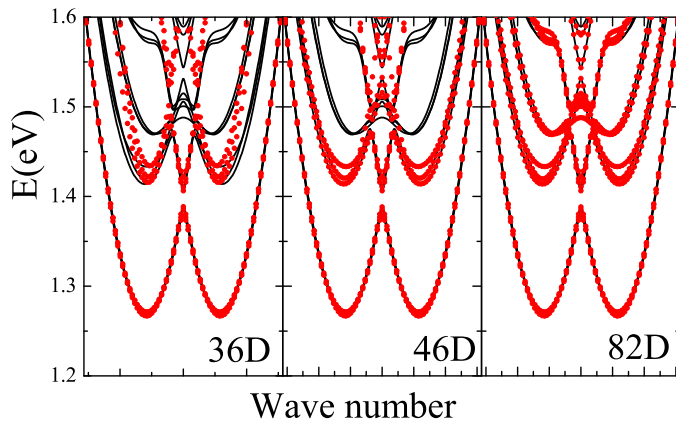


Fig. 5. Conduction band structure of [111] SiNW with rectangular cross section 4×4 nm. Black lines show the exact band structure and red marks are for three EMs with 36, 46 and 82 basis functions.



Fig. 6. IV characteristics of various n-Si NWs in EMs constructed from a primary sp3d5s* TBM.

sorts out a huge number of atomistic orbitals in the device area to extract a small portion of quantum states responsible for the device behaviour. Small size of the equivalent transport model greatly facilitates the atomistic device simulations and makes realistic modeling of inelastic scattering processes in NW MOSFETs also feasible.

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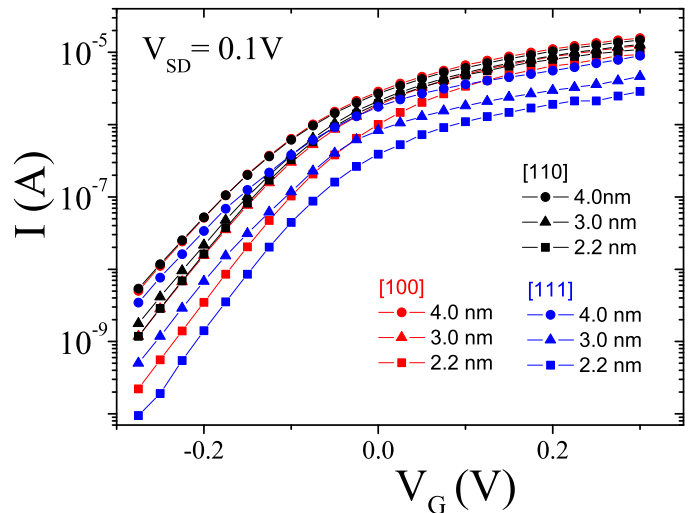[6] N. Singh, et al., *High-performance fully depleted silicon nanowire (diameter ¡ 5nm) gate-all-around CMOS devices* IEEE Electron Device Lett., vol.27, pp.383-386, 2006.
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