

First-principles calculations of the non-equilibrium polarization in ultra-small Si nanowire devices

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Abstract—The paper presents a method for the first principles calculations of polarization charge in non-equilibrium states of silicon nanowire transistor. The method combines the density-functional perturbation theory and piecewise equivalent model representation which enables us to reduce the numerical burden and eliminate erroneous contributions from the occupied electronic states. In the mean field approximation, the polarization response of the device material is taken into consideration by using appropriate dielectric constants in the Poisson solver. Our results suggest that this approximation generally fails and the electric field in the device area may give rise to a nonzero macroscopic polarization charge which is completely ignored in common device simulations.

I. INTRODUCTION

Recent advances in nanofabrication technology have stimulated growing interest to quasi-one-dimensional transport in nanowire (NW) structures. Silicon NWs have attracted much attention as promising candidates for active building blocks for nanoscale electronics and they can nowadays be fabricated by lithography or chemical growth with good control over their shape and composition. Therefore, it becomes important to understand the transport properties of small SiNWs in order to help in addressing practical issues in the design of ultra-small SiNW devices and predict their transport characteristics. The modelling of quantum transport in such systems requires a detailed description of the electrical properties at atomistic level including the effects of strain or localized charged defects. The first-principles calculations based on the density functional theory (DFT) provide comprehensive microscopic information but their application to the transport studies requires considerable computational resources. In common approach, the atomistic description (tight-binding or DFT) is only used for computing mobile charge distribution in current-carrying states of quantum device and the polarization response of the device material is incorporated into the Poisson equation in the mean-field approximation. However, the dielectric constant in a strongly confined nanostructure is expected to deviate significantly from the bulk material. Moreover, in the nanoscale regime, one can no longer assume the local charge neutrality of the induced polarization density and generally has to consider a non-equilibrium polarization charge distribution in the device channel. The density-function perturbation theory provides a well established approach for calculating the dielectric response in bulk media but its application to semi-

conductor nanostructures is much more challenging and, to our knowledge, no such calculation has been performed so far. In the present work we have generalized recently developed equivalent model (EM) method [1] as to become applicable to the perturbative calculations with the DFT Hamiltonian in the real-space representation (RSDFT) [2]. The EM has been originally developed as a tool to construct a low dimensional representation for atomistic transport Hamiltonians which is only valid within a narrow energy interval of mobile carriers. Small size of such EM representation greatly reduces the computational burden and allows the non-elastic effects to be incorporated [3]. On the other hand, numerical studies of the non-equilibrium polarization require accurate calculation of a huge number of matrix elements between Bloch states in a much wider energy range of complex band structure (band folding). We extend our method to such cases by constructing a set of small EMs which can successively cover arbitrary energy range. We develop a perturbative approach for such calculations and demonstrate that the piecewise EM representation can be used for computing the polarization response in realistic NW.

II. EFFECTIVE TRANSPORT MODEL IN REAL-SPACE DENSITY FUNCTIONAL THEORY

The atomistic device Hamiltonian for the first-principles transport simulations is obtained by the real-space finite-difference pseudopotential method (RSDFT) [2]. Compared to the conventional plane wave basis representation, the RSDFT approach does not require the time-consuming fast Fourier transformation and effective parallel algorithms can be implemented for solving the Kohn-Sham sparse matrix equations with smooth Troullier-Martins nonlocal pseudopotentials [4]. The method has been proven to be suitable for large scale parallel DFT calculations in nanoscale systems of tens of thousands atoms. The RSDFT calculation in a single unit structure with periodic boundary conditions is performed in order to obtain a self-consistent periodic atomistic local potential in the ideal wire. The corresponding device Hamiltonian can be represented in the form of tri-diagonal block matrix (see Fig. 1)

$$H_{mn} = H_0 + V_n; H_{m+1} = W; H_{n+1n} = \tilde{W}, \quad (1)$$

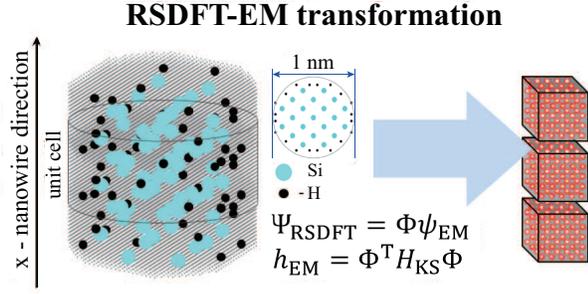


Fig. 1. The RSDFT-EM transformation with a low-dimensional atomistic EM basis $\{\Phi\}$ which reproduces the exact solution of the Kohn-Sham equation. The distribution of mobile and polarization charge is effectively computed by making use of the low-dimensional transformed Hamiltonians h_{EM} .

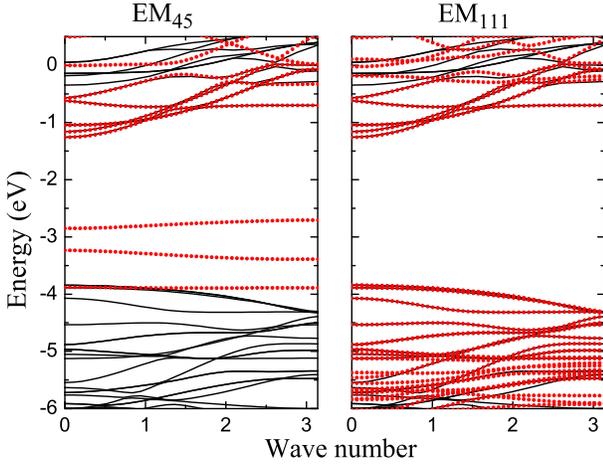


Fig. 2. The band structure of EMs in a thin SiNW with diameter $D = 1$ nm (red points). The solid lines correspond to the exact band structure. The left panel shows a 45-dimensional EM for the mobile carriers at the bottom of the conduction band. The right panel shows a larger EM for both electrons and holes which covers ~ 4 eV transport energy range.

where the size N_{RSDFT} of blocks H_0 and W is determined by the number of grid points in the unit structure. The diagonal matrix V_n represents an extra external potential. The coupling term W originates from the long-range kinetic operator in discrete space and the non-local interaction in separable form which simplified required matrix operations.

The basis orthogonality problem does not arise in the RSDFT formalism and standard non-equilibrium Green's function (NEGF) technique can be used for device modelling [5]. In this work we only consider ballistic transport and our task is to compute self-consistently the total microscopic charge and the external potential V_n in the device area $n = 1, 2, \dots, N$. The potentials at $n < 1$ (source) and $n > N$ (drain) are assumed constant and define two leads with different Fermi energies $\mu_{S,D}$ leading to the electric current through the device channel. Solving the NEGF equation one obtains the drain current and the mobile charge distribution $n_e(\mathbf{r})$ which must be consistent with the Poisson equation

$$\sum_{\mathbf{r}'} \Delta_{\mathbf{r},\mathbf{r}'} V_{\mathbf{r}'} = 4\pi (n^+(\mathbf{r}) - n_e(\mathbf{r}) - \delta n_v(\mathbf{r})), \quad (2)$$

where $\Delta_{\mathbf{r},\mathbf{r}'}$ is the Poisson operator $\nabla_{\mathbf{r}} \epsilon(\mathbf{r}) \nabla_{\mathbf{r}}$ in the discrete space, n^+ is the dopant concentration and δn_v is the polarization charge density.

The size of the original RSDFT Hamiltonian in Eq. (1) can be drastically reduced in the equivalent model (EM) representation

$$\Psi_{\text{RSDFT}} = \Phi \psi_{\text{EM}} \quad (3)$$

with a rectangular basis matrix Φ constructed in such way that Eq. (3) remains valid for any scattering solutions within a desired energy interval [1]. The EM basis transformation generates an “equivalent” chain model with the same microscopic properties as the original system (Fig. 1). There are generally infinite number of EMs and their size (number of columns in basis Φ) depends not on the original mesh density but only on the complexity of the band structure in the target energy interval. Figure 2 shows an example of two different EMs in a SiNW from Fig. 1 which correspond to mobile electrons (left panel) and both electrons and holes (right panel).

The EM method is based on a simple idea that a smooth set of Bloch Hamiltonians $H(k)$ can be well represented by a moderate number of representative points in the Brillouin zone under condition that the resulting model ensures minimum density of states. Thus, the EM construction can be reduced to a minimization of a certain functional in the form [1]

$$F[\Phi] = \sum_k \tilde{N}_{\varepsilon_1(k), \varepsilon_2(k), k}, \quad (4)$$

where $\tilde{N}_{\varepsilon_1, \varepsilon_2, k}$ represents a “smoothened” number of Bloch energies $\varepsilon_{nk} \in [\varepsilon_1, \varepsilon_2]$ [1].

A few modifications have been introduced to the original formulation of the EM method in Ref. [1]. In particular, the starting guess for the variational calculation is taken in the form $H(k_0)\Phi\psi_{nk_0}$ where ψ_{nk_0} is an unphysical state automatically detected in the course of iteration. We allow for k -dependent energy parameters $\varepsilon_{1,2}(k)$ in the variational functional Eq. (4) which are adjusted at each step in order to guarantee that the branch where ε_{nk_0} belongs does not cross any of the energy intervals $[\varepsilon_1(k); \varepsilon_2(k)]$ which ensures effective elimination of the unphysical branch. The exact solutions at necessary representative points are computed by the FEAST algorithm [6] and the variational space is constructed by projecting the auxiliary set $H_0\Phi \oplus (W + \tilde{W})\Phi$ to the orthogonal complement (RSDFT)/(EM) which can be performed without large operations $O(N_{\text{RSDFT}}^2)$, $O(N_{\text{RSDFT}}^3)$. This enables us to construct any suitable EM representation for the first-principles study of non-equilibrium states.

III. NON-EQUILIBRIUM POLARIZATION IN LINEAR RESPONSE THEORY

In this work we mainly consider the polarization charge δn_v in Eq. (2). In sub-micron regime, this term can be ignored since the induced polarization is well described by the appropriate dielectric constant $\epsilon(\mathbf{r})$ in the Poisson operator. However, in nanoscale regime the mean field approximation may fail and fully quantum microscopic approach is needed. The NEGF approach is not suitable for this purpose since it does not guarantee mutual cancellation of states in the valence

band. However, under normal conditions, the external field in the device area is relatively weak and one can compute the electron-density linear response within the density-functional perturbation theory [7].

We take the whole device area ($n = 1, 2, \dots, N$) as one supercell and consider an infinite sequence of such supercells. The polarization charge in this auxiliary system is given by

$$\delta n_v(\mathbf{r}) = 4\text{Re} \sum_{n \in \text{v.b.}} \Psi_n^*(\mathbf{r}) \delta \Psi_n(\mathbf{r}) \quad (5)$$

where the first order correction to the eigenstates of the unperturbed system is found from

$$(\varepsilon_n - H_{\text{KS}}) \delta \Psi_n(\mathbf{r}) = \delta H_{\text{KS}}(\mathbf{r}) \Psi_n(\mathbf{r}) \quad (6)$$

and the perturbation term δH_{KS} includes external potential as well as a contribution from the exchange-correlation part of the Kohn-Sham Hamiltonian. Equations. (5) and (6) give the usual result for linear polarization [7]

$$\delta n = 4\text{Re} \sum_{\substack{n \in \text{v.b.} \\ m \in \text{c.b.}}} \Psi_m(\mathbf{r}) \Psi_n^*(\mathbf{r}) \frac{\langle \Psi_m | [\delta H_{\text{KS}}, H_{\text{KS}}] | \Psi_n \rangle}{(\varepsilon_n - \varepsilon_m)^2}. \quad (7)$$

We now assume that the polarization response is local i.e. it does not depend on the potential outside the device area. This assumption is consistent with the Neumann boundary conditions in the Poisson equation and its validity can be checked at the end of calculations. Then one can modify the external potential outside the device area such that

$$\delta V_{n+N} - \delta V_n = \Delta V, \quad (8)$$

where ΔV is a constant shift $\sim O(\mu_D - \mu_S)$. Since the ‘‘perturbation’’ $[\delta H_{\text{KS}}, H_{\text{KS}}]$ does not violate the translational symmetry, one can use the Bloch eigenstates in the auxiliary system

$$\Psi_{v,n,k}(\mathbf{r}) \equiv \frac{1}{\sqrt{N}} \Psi_{v,(k+2\pi n)/N}(\mathbf{r}), \quad (9)$$

where $\Psi_{v,k}$ are the original normalized Bloch states in ideal wire and $n = 0, 1, \dots, N-1$ is the band folding quantum number. Evaluating the commutator, we obtain the final expression for the non-equilibrium polarization charge distribution

$$\delta n(\mathbf{r}) = \frac{4}{N_k N^2} \text{Re} \sum_k \sum_{nm} \sum_{v \in \text{v.b.}} \sum_{\mu \in \text{c.b.}} \frac{\Psi_{\mu,m,k}(\mathbf{r}) \Psi_{v,n,k}^*(\mathbf{r})}{\varepsilon_{v,n,k} - \varepsilon_{\mu,m,k}} \times \left[\langle \Psi_{\mu,m,k} | \delta H_{\text{KS}} | \Psi_{v,n,k} \rangle + \Delta(v, \mu, n, m, k) \right], \quad (10)$$

where the wave number runs over N_k sampling points $k = 2\pi n_k / N_k$; $n_k = 0, 1, \dots, N_k - 1$. The matrix element in Eq. (10) is defined by a sum over the grid points in the device area and the surface term $\Delta(v, \mu, n, m, k)$ can be written in the form

$$\Delta(v, \mu, n, m, k) = \frac{\Delta V}{\varepsilon_{v,n,k} - \varepsilon_{\mu,m,k}} \left[\langle \Psi_{\mu,m,k} | \tilde{W} | \Psi_{v,n,k} \rangle e^{-i(k+2\pi n)/N} - \langle \Psi_{\mu,m,k} | W | \Psi_{v,n,k} \rangle e^{i(k+2\pi n)/N} \right]. \quad (11)$$

The surface contribution $\sim |\mu_S - \mu_D| / \{(\varepsilon_c - \varepsilon_v)N\}$ depends on the device size and applied basis and it is normally much smaller compared to the calculations in bulk material.

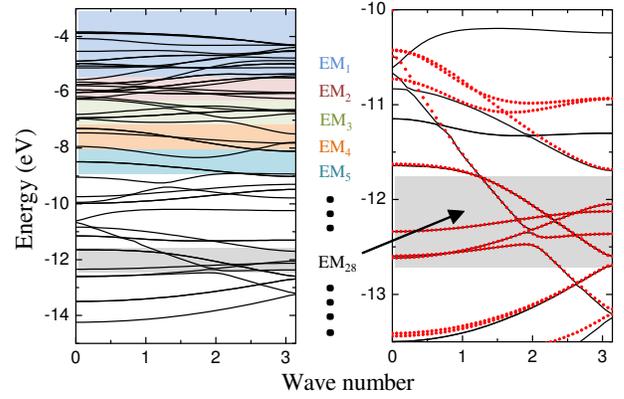


Fig. 3. The piecewise EM representation in the valence band of a SiNW with diameter $D = 1$ nm. Each member of the set in the left panel covers a narrow ~ 0.3 eV energy window. The right panel shows a particular member of this set (red points). The solid lines represent the exact band structure.

IV. NUMERICAL ILLUSTRATION

Computing the Bloch states and evaluating all the matrix elements in Eq. (10) may be very challenging. The developed EM method can be used to make such computations feasible. In the present work, we use the EM representation in two different ways. First, an EM for the conduction band is implemented in order to facilitate the first-principles NEGF calculation of the mobile carrier and charge distribution. Clearly, this model does not work for most of Bloch states in Eq. (10). In principle, one can enlarge the EM target window at the price of larger computational cost (see Fig. (1)). However, our experience shows that taking contributions only from the upper states underestimates the polarization charge and accurate calculations require all the branches in the valence band. In order to optimize the computer performance, we have constructed a set of small EMs such that each model is only used for electronic states within an energy window with 0.3 eV width. Figure 3 shows schematically such a set of EMs for the whole valence band in SiNW and a particular member of this set (EM₂₈) for energies around -12.5 eV (right panel). The advantage of such approach is that by keeping all the Bloch eigenvalue problems small, one can reduce the matrix operations to the size of the corresponding EM and effectively evaluate Eq. (10) at many sampling points in the Brillouin zone.

As a test, we have applied the developed approach to model ballistic transport in a nSi MOSFET with ultra thin channel $D = 1$ nm shown in Fig. 4 with $L_G = 6$ nm and $t_{\text{ox}} = 0.5$ nm. Other parameters are $V_{\text{SD}} = 0.1$ V, $T = 300$ K, dopant concentration in the source/drain regions is taken as 10^{20} cm⁻³. EM₄₅ has been used for the mobile carriers since it fully reproduces the quantum states within ~ 0.8 eV at the bottom of the conduction band which is more than enough at room temperature. Usage of larger EM does not change the results but it helps to confirm the numerical accuracy of the first principle calculations in the EM representation.

To evaluate the polarization charge in Eq. (10), we use a set

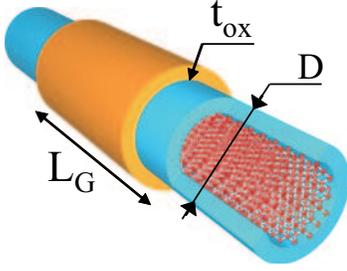


Fig. 4. SiNW MOSFET used in the simulations.

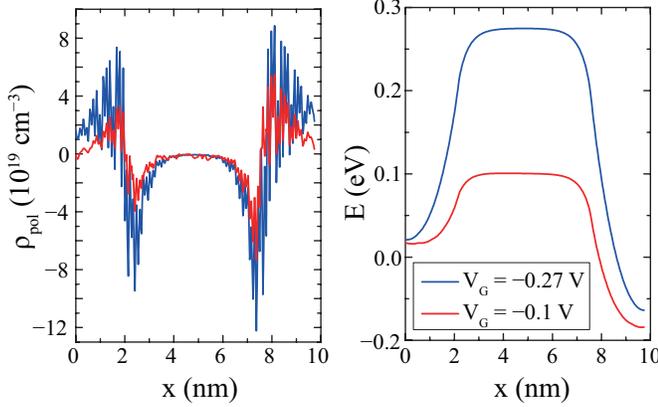


Fig. 5. Averaged polarization charge density along the n-SiNW MOSFET channel for two values of the gate voltage in Fig. 3 (left panel). The right panel shows the corresponding potential profiles.

of 70 small EMs (typical size 35–40) for a sequence of energy intervals which cover the whole valence band and the lowest 10 eV energy range in the conduction band. We have confirmed that contribution from higher energies does not change our results. Figure 5 shows the polarization charge distribution at two values of the gate voltage. The absolute value of δn_v is seen to be comparable with the mobile charge density and it cannot be reproduced by simply adjusting the dielectric parameters. Figure 5 also confirm that δn_v is well localized, although in the device with such short channel our calculations become less accurate at stronger field ($V_G = -0.27$ V).

Figure 6 shows the calculated IV characteristics. The black curve corresponds to the mean field approximation ($\epsilon_{Si} = 11.9$) which is compared with the result of the first-principles calculations of polarization charge. The IV curve for $\epsilon_{Si} = 1$ without polarization is shown for comparison. A noticeable decrease of the drain current is caused by the nonzero polarization charge and it cannot be explained simply by the reduced value of dielectric constant ϵ in the wire.

V. SUMMARY

We have presented a method for the first-principles transport simulations in nanowire MOSFETs. We have combined the NEGF simulations for mobile carriers and the density-functional perturbative calculations for the microscopic polarization charge in the device area. We have modified the EM method and developed a parallel code in order to construct a

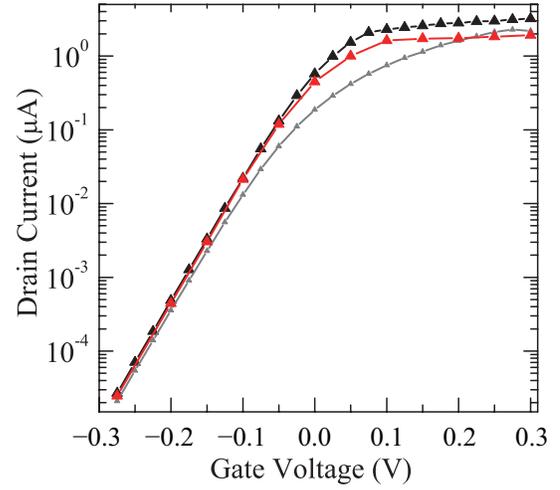


Fig. 6. IV -characteristics in a n-SiNW MOSFET with $L_G = 6$ nm, $t_{ox} = 0.2$ nm and $D = 1$ nm. The first-principles RSDFT method is only used in the silicon core region. The black curve is obtained from standard NEGF simulations using $\epsilon_{Si} = 11.9$ in the Poisson equation. The red curve is obtained by directly computing the polarization charge δn_v in the silicon core from density function perturbation theory. For comparison purpose we also show the IV curve (gray) in a fictitious system without polarization ($\delta n_v = 0$ and $\epsilon_{Si} = 1$).

piecewise low-dimensional EM representation for wide energy range of RSDFT Hamiltonian which is suitable for such calculations. The method have been tested by computing the dielectric response in an ideal SiNW and further applied to the non-equilibrium polarization in a SiNW MOSFET. Our results show that standard mean-field approximation with fixed dielectric parameters may fail since it cannot reproduce induced macroscopic polarization charge separation in the device channel.

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