Electron-phonon interaction in Si nanowire devices: Low field mobility and self-consistent EM NEGF simulations

Gennady Mil'nikov[1,2] and Nobuya Mori[1,2]
[1]Department of Electrical, Electronic and Information Engineering
Osaka University, Suita, Japan
[2]CREST, JST, Chiyoda, Tokyo 102-0075, Japan
Email: {gena | mori}@si.eei.eng.osaka-u.jp

***Abstract*—The paper presents a method for quantum transport simulations in nanowire (NW) MOSFETs with inelastic scattering processes incorporated. An atomistic tight-binding Hamiltonian with realistic electron-phonon interaction is transformed into an equivalent low-dimensional transport model which can be easily used in full-scaled NEGF simulations. The utility of the method is demonstrated by computing IV characteristics in n-Si NW devices.**

I. Introduction

Recent technological progress has stimulated a growing interest to quasi-one-dimensional quantum transport in nanowire (NW) structures. Experimental studies of Ge/Si NWs have shown excellent gate control, high drain current and reduced sensitivity to temperature [1], [2]. This opens novel opportunities for the design of nanoscale devices and for exploring quantum transport in low-dimensional systems [3]. Theoretical modeling of such nanoscale devices are required to take into account realistic band structure of mobile carries and inelastic scattering effects [4]. The non-equilibrium Green's function (NEGF) formalism with a tight-binding type of atomistic Hamiltonian provides a general framework for such studies [5], [6]. However, complexity of the electronic Hamiltonian and large number of possible electron-phonon (e-ph) scattering processes make the atomistic transport simulations prohibitively difficult.

In the present work we have developed a method to overcome this difficulty. We construct a low-dimensional representation of one-electron states within an energy interval relevant to the transport phenomena and obtain an equivalent model (EM) which greatly reduces the computational costs of atomistic transport simulations and allows inelastic effects to be incorporated. We employ a strain-dependent $sp^3d^5s^*$ tight-binding model (TBM) [7] for the electrons and a generalized Keating model for phonons [8], [9] in order to calculate the inelastic scattering rates and phonon-limited mobility including couplings between all possible electronic and phononic states. We use these exact results as reference data and show that inelastic interaction can be reproduced by a small number of effective phonon modes with properly chosen coupling parameters. We demonstrate our approach by constructing a computationally cheap inelastic EM in various n-Si NW devices and computing their IV characteristics in the presence of the inelastic e-ph scattering.

II. Electron-phonon interaction and low field mobility

We first consider the electron-phonon interaction in a nanowire close to equilibrium. Under applying a constant electric field E, the distribution function f_{nk} for the electron state in the n-th band with wave vector k is given by $f_{nk} = f^0_{nk} + eE\eta_{nk}$, where $f^0_{nk} \equiv f^0(E_{nk})$ is the equilibrium Fermi distribution function. For a weak electric field the deviation η_{nk} can be found from the linearized Boltzmann equation

$$\frac{\partial f_0}{\partial E_{nk}} v_{nk} = \sum_{m\nu} \int dq\; M(nk, mk') \left[\eta_{nk}(1 - f^0_{mk'}) - \eta_{mk'} f^0_{nk}\right] - M(mk', nk) \left[\eta_{mk'}(1 - f^0_{nk}) - \eta_{nk} f^0_{mk'}\right], \quad (1)$$

where $M(nk, mk')$ is the scattering rate between electron states (n, k) and $(m, k' = k + q)$ and $v_{nk} = \hbar^{-1}\partial E_{nk}/\partial k$ is the group velocity. Once equation (1) has been solved, the mobility is given by

$$\mu = e\frac{\sum_{nk} v_{nk}\eta_{nk}}{\sum_{nk} f^0_{nk}}. \quad (2)$$

Performing such calculations in a realistic nanostructure requires considerable computer resources. The electron-phonon interaction is introduced by expanding a strain-dependent TB Hamiltonian $H = H(\boldsymbol{R}^0_a) + (\partial H/\partial \boldsymbol{R}_a)\,\delta\boldsymbol{R}_a$ with respect to quantized normal modes of the atomic displacements $\delta\boldsymbol{R}_a = \boldsymbol{R}_a - \boldsymbol{R}^0_a$. The contribution from a particular phonon mode (νq) to the total rate is given by

$$M^{\nu q}(nk, mk') = \frac{|\langle\Psi_{mk'}|T^{\nu q}|\Psi_{nk}\rangle|^2}{2\omega_{\nu q} M_{\rm Si}} \left[N_{\rm B}\delta(E_{mk'} - E_{nk} - \omega_{\nu q}) + (1 + N_{\rm B})\delta(E_{mk'} - E_{nk} + \omega_{\nu q})\right], \quad (3)$$

where $T^{\nu q} = \sum_a (\partial H/\partial \boldsymbol{R}_a)\, \boldsymbol{e}^{\nu}_a(q)$ is the effective interaction within one unit-cell of the wire, Ψ_{nk} are the unit-cell normalized Bloch states, and $(\omega_{\nu q}, \boldsymbol{e}^{\nu}_a(q))$ are the phonon frequencies and the corresponding eigenstates. Figure 1 shows an example of the phononic band structure in a [100] Si NW obtained from the generalized Keating model [8], [9]. In order to integrate

978-1-4799-5288-5/14/$31.00

the delta-functions of energy conservation in Eq. (3), the grid of q-points in the first Brillouin zone must be taken dense enough. Typically, ~ 400–600 q points are required to achieve convergence and the total number of scattering processes may be as large as ~ 10^6–10^7 making the mobility calculation very heavy.

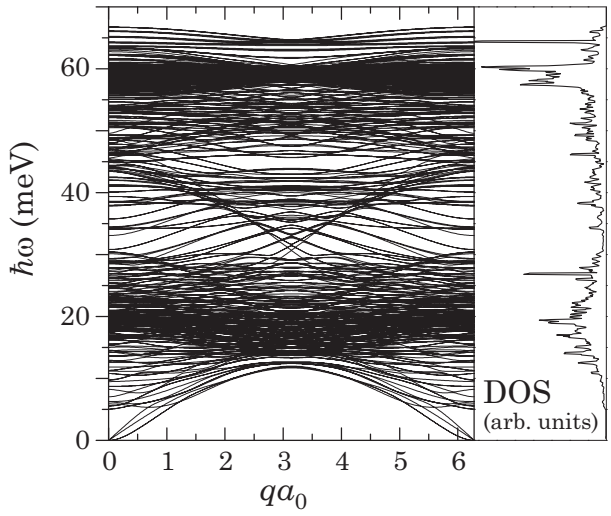

Fig. 1. Phononic band structure of a [100] Si NW with a rectangular cross section $2.2 \times 2.2\,\mathrm{nm}^2$. The DOS is shown in the right panel.

III. Calculation of electron mobility in EM representation

The first step of our method is to reduce the original TBM representation. For any TB model with N_{TBM} orbitals per unit cell, the EM method [10] offers a regular procedure to construct $N_{\mathrm{EM}} \ll N_{\mathrm{TBM}}$ basis functions which give the same physics within a desired energy interval. Thus, the one-electron states can be calculated in the form

$$\Psi_{nk} = \Phi\psi_{nk} \tag{4}$$

where Φ is the constant $N_{\mathrm{TBM}} \times N_{\mathrm{EM}}$ real-valued basis matrix with orthogonal columns $\Phi^T\Phi = 1$ and the EM Bloch states ψ_{nk} are found from a N_{EM}-dimensional eigenvalue problem. Figure 2 shows examples of the band structure in three n-Si NWs used in the simulations. The red points show the results from the EM (N_{EM} = 44 (a), 54 (b) and 57 (c)) which reproduce $\Delta E \approx 0.55$ (a), 0.35 (b) and 0.3 eV (c) at the bottom of the conduction band. In fact, not all the states in Fig. 2 are needed to compute the room temperature mobility. Similar results can be obtained by using smaller EMs with $\Delta E \approx 0.2$ eV. The freedom in choosing EMs of different size and reliable energy interval provides a general tool to optimize the EM calculations and test convergence and accuracy of the results [10].

The matrix elements can now be evaluated in the EM representation $\langle\Psi_{mk'}|T^{\nu q}|\Psi_{nk}\rangle = \langle\psi_{mk'}|t^{\nu q}|\psi_{nk}\rangle$, where $t^{\nu q}$ is a constant interaction matrix obtained by the basis transformation of the nonzero blocks of $T^{\nu q}$. The computational time is reduced by a factor of $(N_{\mathrm{EM}}/N_{\mathrm{TBM}})^2 \sim 10^{-4}$ making the calculations in Eqs. (1-3) trivial. Figure 3 shows two examples of the relaxation time $\tau_t^{-1} = (\partial f_0/\partial E_{nk})\, v_{nk}/\eta_{nk}$ obtained by solving the Boltzmann equation in a [100] n-Si NW with rectangular cross section $2.2 \times 2.2\,\mathrm{nm}^2$ which only takes ~ 1 hour on an ordinary PC. The fact that τ_t is close to the total scattering rate $\tau_0^{-1} = \sum_{mk'} W(nk, mk')$ strongly suggests that one can disregard the phonon dispersion and obtain a simpler model with similar inelastic transport properties.

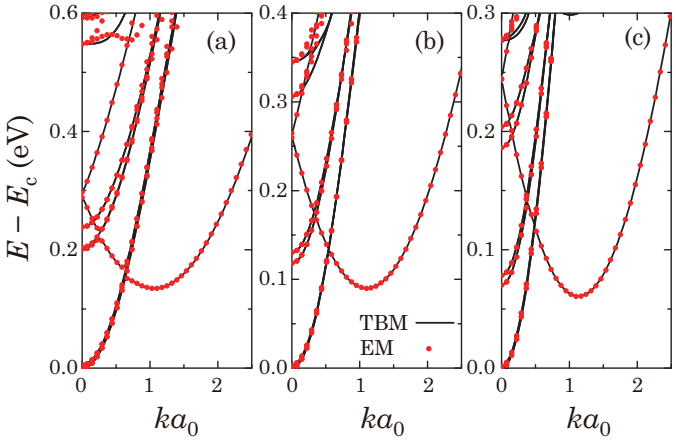

Fig. 2. Conduction band in n-Si NWs with a rectangular cross section 2.2×2.2 (a), 3×3 (b), and $4 \times 4\,\mathrm{nm}^2$ (c) along [100] crystal direction. The red points represent the EM used in the simulations.

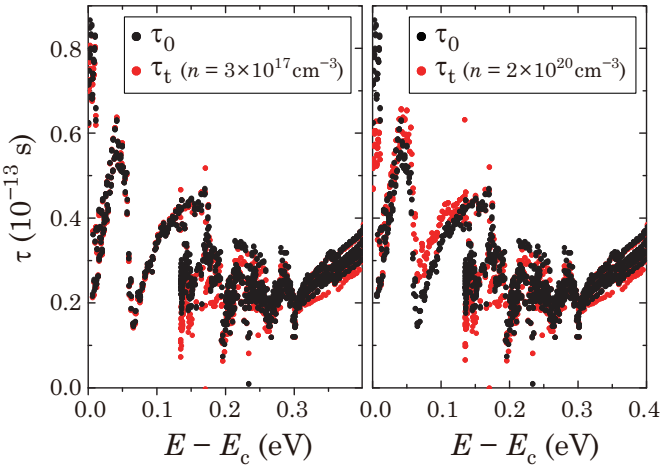

Fig. 3. Relaxation time τ_t (red circles) for low and high carrier concentration in a [100] n-Si NW with a rectangular cross section $2.2 \times 2.2\mathrm{nm}^2$, computed by solving the Boltzmann equation. The black circles refer to the total rate $\tau_0^{-1} = \sum_{mk'} W(nk, mk')$.

IV. Model of random optical phonons

In scope of the NEGF method, the full Green's functions and inelastic self-energies need to be computed and storied at many energies points. Such full-scale atomistic simulations in the original TBM picture simply cannot be done and the EM method offers a promising way to solve the problem. For example, in a ~ 30-nm-length Si NW, the total number of EM quantum states can be made as small as $2–3 \times 10^3$ which

allows the Dyson and Keldysh equations with arbitrary self-energy terms to be solved easily without much time or storage problems. On the contrary, constructing the self-energy terms $\Sigma^{\mathrm{e-ph}}$ themselves becomes the most consuming part of such EM NEGF simulations. Indeed, computing the self-energy involves operations similar to the ones for the scattering rates in Eq. (1) and these must be repeated at many energy points at each step of the self-consistent iteration.

Here we propose an inelastic EM model which generates analytical block-diagonal e-ph self-energy terms and thus optimizes the NEGF simulations. The model is obtained by substituting the actual phonons in the system by a set of simple equidistant dispersionless modes and adjusting the coupling parameters in order to reproduce the exact electron-phonon scattering rates and phonon-limited mobility. To realize this program, we assume a block-diagonal electron-phonon interaction

$$H^n_{\mathrm{e-ph}} = \sum_{\nu q} \frac{T^\nu e^{iqa_0 n}}{\sqrt{2M_{\mathrm{Si}}\omega_\nu}} \{b_\nu(q) + b^+_\nu(-q)\}, \qquad (5)$$

where T^ν is the EM interaction operator ($N_{\mathrm{EM}} \times N_{\mathrm{EM}}$ matrix) for the ν-th phonon mode, n numerates unit-cell and a_0 is its size in the transport direction. Equation (5) is almost the same as the exact electron-phonon interaction term except that we neglect the phonon dispersion in T^ν, ω_ν and omit a minor part of the interaction which comes from the atomic deviations $\delta\boldsymbol{R}_a$ in neighbor cells. Instead of trying to estimate each particular term T^ν we introduce equidistant fictitious phonons which are required to "accumulate" the effect of many original modes with similar frequency. For example, in computing the scattering rates we meet the terms $\sim \sum_\nu \omega_\nu^{-1} T^\nu_{ij} T^{\nu\,*}_{kl}$ where i, j, k, l are the EM indices for electronic states. The contribution from many modes around a fictitious phonon with frequency Ω can be approximated by

$$\sum_{\omega_\nu \approx \Omega} \frac{1}{\omega_\nu} T^\nu_{ij} T^{\nu\,*}_{kl} \delta(\Delta E \pm \omega_\nu) \approx \frac{1}{\Omega} T^\Omega_{ij} T^{\Omega\,*}_{kl} \delta(\Delta E \pm \Omega). \qquad (6)$$

As follows from the definition of T^ν after Eq. (3), various terms in Eq. (6) have generally very different amplitudes and phases. For a dense enough phonon spectrum, the quantity $T^\Omega T^\Omega$ in the r.h.s. is analogous to the average of a product of two random symmetric matrices and can be approximated by

$$T^\Omega_{ij} T^{\Omega\,*}_{kl} \to A^\Omega \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right). \qquad (7)$$

We note that Eq. (7) remains invariant under arbitrary orthogonal transformation of the EM basis. Since the terms T^Ω enter any physical results only in the form of Eq. (7) the parameters A^Ω specify the electron-phonon interaction completely. For example, the matrix element for the scattering by the fictitious phonon Ω is now given by (see Eq. (3))

$$M^\Omega \sim \frac{\left|\langle\psi_{mk'}|T^\Omega|\psi_{nk}\rangle\right|^2}{\Omega} = \frac{A^\Omega}{\Omega}\left[1 + \left|\langle\psi^*_{mk'}|\psi_{nk}\rangle\right|^2\right]. \qquad (8)$$

The inelastic $\Sigma^{\mathrm{e-ph}}$ in the NEGF formalism are calculated in a similar way. For example, the contribution from a mode Ω in the self-consistent Born approximation is given by

$$\frac{i}{4\pi M_{\mathrm{Si}}\Omega} \int d\varepsilon \left[\mathrm{Tr}G(E-\varepsilon) + \tilde{G}^T(E-\varepsilon)\right] D^\Omega(\varepsilon) \qquad (9)$$

where D^Ω is the usual equilibrium function for frequency Ω and $\tilde{G}$ is the block diagonal part of the corresponding Keldysh Green's function. Equation (9) gives analytical block diagonal inelastic self-energies for the system of NEGF equation which can be easily solved.

V. Model parameters and EM NEGF simulations

We now assume a set of phonon modes Ω_n with yet unknown coupling constants A_n. We use equidistant modes in order to reduce the number of mutually coupled Green's functions. Our strategy will be to use the exact mobility calculations as a reference and adjust the coupling parameters A_n in order to reproduce the electron-phonon scattering rates. We thus obtain a numerically cheap inelastic transport model which mimics all the properties of the original TBM and can be employed on similar grounds for the full-scale NEGF simulations.

In practice, we find the coupling parameters which minimize the quantity

$$S = \sum_i \Big[\sum_{nk} F(E_{nk} - E_i)\Delta\tau_0(nk)\Big]^2, \qquad (10)$$

where $\Delta\tau_0$ is the deviation of the scattering rate from the exact result and F is a zero centered weight function, which is introduced in order to avoid too strong influence of any particular point (nk) and smoothen the contribution from many states around the reference energy E_i. We use $F = f_0(1 - f_0)$,

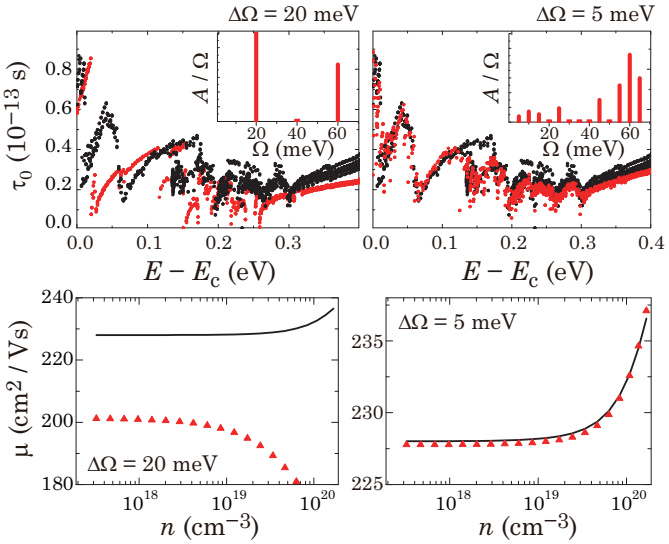

Fig. 4. Constructing the EM with equidistant dispersionless phonons for $\Delta\Omega = 20$ and 5 meV. Upper panels: optimized scattering time τ_0 (red circles) versus the exact data from Fig. 3 (black circles). The insets show the effective strength A/Ω of the electron-phonon interaction. Lower panels: the room temperature mobility as a function of the carrier concentration. The red triangles refer to the equidistant phonon model and the black lines to the full spectrum in Fig. 1.

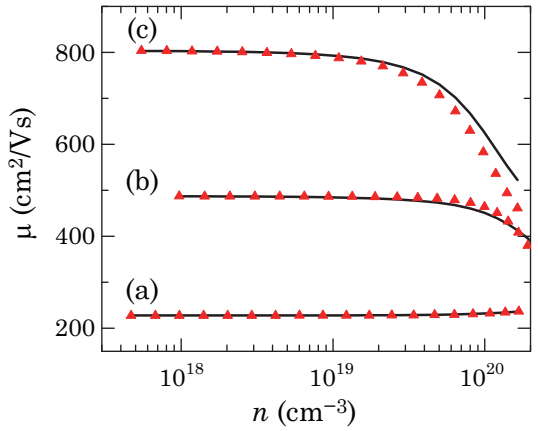

Fig. 5. The room temperature mobility as a function of the carrier concentration in [100] Si NWs in Fig. 2. The black lines show the exact result for the full phononic spectrum. The red triangles refer to the optimized model of 13 equidistant optical modes with $\Delta\Omega = 5\,\mathrm{meV}$.

where f_0 is the Fermi function for $T = 100\,\mathrm{K}$ with 10–20 reference Fermi energies. Figure 4 shows $\tau_0(nk)$ as a function of energy $E(nk)$ in two optimized models with $\Delta\Omega = 20\,\mathrm{meV}$ (3 modes) and $\Delta\Omega = 5\,\mathrm{meV}$ (13 modes). The corresponding room temperature mobility is shown in the lower panels. The model with $\Delta\Omega = 5\,\mathrm{meV}$ is found to be in quantitative agreement with the exact results and can be used in the NEGF simulations. Similar accuracy has been found in the optimized model for n-Si NWs of larger cross section (see Fig. 5).

Figure 6 presents the calculated IV characteristics in a [100] n-Si NW MOSFET at room temperature with dopant concentration of $10^{20}\,\mathrm{cm}^{-3}$ at applied bias $V_{SD} = 0.1\,\mathrm{V}$.

Figure 7 also shows an example of the mobile charge distribution at two contacts and illustrates convergence of the self-consistent Born iterations. The reduction of the drain

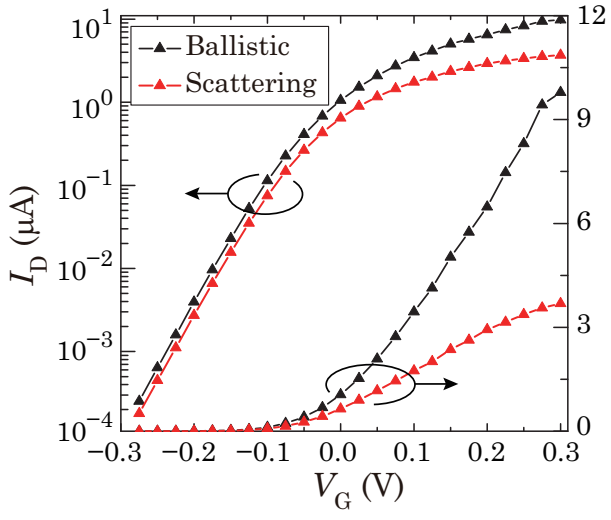

Fig. 6. Transport characteristic I_d–V_G at $V_{SD} = 0.1$ V of a n-Si NW FET with rectangular cross section $2.2 \times 2.2\,\mathrm{nm}^2$. The black lines with triangles refer to the ballistic current and the red lines with triangles to the current with electron-phonon scattering.

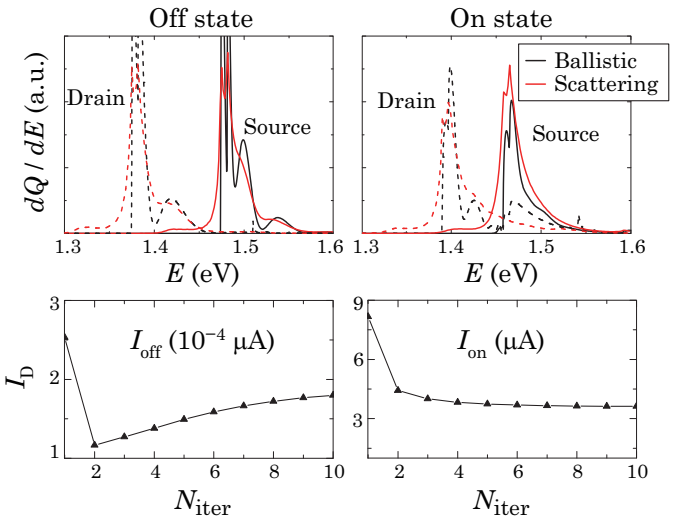

Fig. 7. Mobile charge spectrum (upper panels) and self-consistent Born iterations for the drain current (lower panels) in a [100] n-Si NW with a rectangular cross section $2.2 \times 2.2\,\mathrm{nm}^2$. The ballistic charge spectrum in the same potential is shown for comparison.

current and the phonon subband structure are found to be in a qualitative agreement with the results of the perturbation theory which further justifies the applicability of the inelastic EM with optimized equilibrium parameters. We finally note that the EM approach makes it possible to perform the full-scale NEGF simulations with all the phonon modes included and thus obtain a numerical estimate for the accuracy of the present method away from equilibrium. Such test calculations are currently in progress.

VI. Summary

The method is formulated to construct a low-dimensional model Hamiltonian which reproduces both ballistic and non-ballistic transport in NWs with atomistic resolution. The model makes it possible to utilize the full power of the NEGF formalism and study inelastic scattering processes in realistic nanostructures.

References

[1] N. Singh, A. Agarwal, L. K. Bera, T. Y. Liow, R. Yang, S. C. Rustagi, C. H. Tung, R. Kumar, G. Q. Lo, N. Balasubramanian, and D.-L. Kwong, IEEE Electron Device Lett., **27**, 383 (2006).
[2] J. Xiang, W. Lu, Y. Hu, Y. Wu, H. Yan, and C. M. Lieber, Nature, **441**, 489 (2006).
[3] N. Neophytou, S. G. Kim, G. Klimeck, and H. Kosina, J. Appl. Phys., **107**, 113701 (2010).
[4] M. Luisier and G. Klimeck, Phys. Rev. B, **80**, 155430 (2009).
[5] A. Pecchia and A. Di Carlo, Rep. Prog. Phys., **67**, 1497 (2004).
[6] M. Lundstrom and J. Guo, *Nanoscale Transistors: Device Physics, Modeling, and Simulation*, Springer, New York, 2006.
[7] Y. M. Niquet, D. Rideau, C. Tavernier, H. Jaouen, and X. Blase, Phys. Rev. B, **79**, 245201 (2009).
[8] D. Vanderbilt, S. H. Taole, and S. Narasimhan, Phys. Rev. B, **40**, 5657 (1989).
[9] W. Zhang, C. Delerue, Y.-M. Niquet, G. Allan, and E. Wang, Phys. Rev. B, **82**, 115319 (2010).
[10] G. Mil'nikov, N. Mori, and Y. Kamakura, Phys. Rev. B, **85**, 035317 (2012).