Phonon-Limited Low-Field Mobility in Silicon Nanowires: NEGF Quantum Transport vs. Linearized Boltzmann

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Introduction Quantum transport simulations of nanoscale devices in a full-band and atomistic basis are computationally very intensive, especially those including electron/hole-phonon scattering in the Non-equilibrium Green's Function (NEGF) formalism [1]. To investigate realistic structures with such an approach, it is necessary to introduce physical and numerical approximations. However, even in these cases, the computational burden remains very high as compared to semi-classical simulations with the drift-diffusion model.

Here, we propose to check and validate the approximations made in dissipative quantum transport (QT) simulations through comparisons with the exact solution of the linearized Boltzmann Transport Equation (LB). Although it does not allow for the simulation of current characteristics as QT, the LB method is particularly well-suited to compute low-field mobilities in bulk and nanostructures. Using the same electron/hole tight-binding parametrization and phonon bandstructure model in the QT and LB approaches, we calculate the electron and hole mobility in bulk Si and ultrascaled Si nanowires as shown in Fig. 1. A careful analysis of the results shows that the QT simplifications work well for electrons, but are less accurate for holes.

Method In the quantum transport case, low-field mobilities are calculated within the NEGF formalism [2] using the dR/dL method [3]. The linearized Boltzmann Transport Equation is solved exactly in the stationary regime [4] to obtain reference mobility values. All the simulations use the same nearest-neighbor $sp^3d^5s^*$ tight-binding model to describe the electron and hole properties in Si [5] and the same valence-force-field (VFF) method for phonons [6]. The electron/hole-phonon interactions are derived from the first order Taylor-expansion of the tight-binding Hamiltonian ($\nabla \mathbf{H}_{ln}$) around the equilibrium lattice positions R_l and R_n. The strain parametrization has therefore a strong influence on the electron-phonon coupling strength.

As depicted in Fig. 2, the NEGF formalism accounts for electron-phonon interactions through scattering self-energies $\mathbf{\Sigma}^{<>}_{nn}(E)$ while the LB approach relies on transition matrix elements $S(b, k_x; b', k_x')$ based on Fermi's Golden Rule . For computational reasons, the scattering self energies are assumed diagonal and use a simplified form factor $\widetilde{\mathbf{V}}$. With LB, all the scattering elements can be taken into account (LB FULL) or only the diagonal ones (LB APPROX), as in the NEGF calculations.

Results As a first step, we compare the bulk mobility of Si computed with NEGF and LB to experimental data. The goal is not only to determine whether the two approaches agree, but also how close they are to reality. Once that confidence in the models is obtained, nanowires can be considered. Note that the calculation of bulk mobilities requires the coupling of transverse momentum, which is not shown in Fig. 2, but performed anyway. Two different strain models are investigated, labeled *old* [7] and *new* [8]. Mobility results are reported in Fig. 3. For electrons, a good agreement between the NEGF and LB approach (both FULL and APPROX) can be observed, especially with the *new* strain model where the values are close to the experimental data. For holes, LB reproduces the experimental values reasonably well, but NEGF greatly overestimates them. This discrepancy needs further investigations.

We now consider free-standing silicon nanowires with different diameters and crystal orientations as schematized in Fig. 1. The QT mobilities are obtained by simulating three different nanowire lengths (20, 30, and 40 nm) at a low applied voltage ΔV=10^{-4} V and low doping concentrations N_A, N_D=10^{16} cm^{-3}. Based on the resulting channel resistance, the dR/dL method is applied. In the LB calculations, the Fermi level matches the QT one. In Fig. 4 and 5 the electron mobilities for two crystal orientations and different diameters are plotted. A good agreement between QT, LB FULL, and LB APPROX is achieved. Figure 6 shows the hole mobility in $\langle 110 \rangle$-oriented Si nanowires with different diameters. The QT mobilities still agree well with LB APPROX, where only the diagonal elements of the scattering matrix are taken into account, but they are too large as compared to LB FULL. This indicates an underestimation of the hole-phonon coupling strength with diagonal self-energies only.

Conclusion A NEGF quantum transport simulator and the linearized Boltzmann Transport Equation have been compared by means of the calculation of low-field mobilities in Si bulk and nanowires. A good agreement between the NEGF and LB results is demonstrated where we apply the same diagonal approximation, validating the simplification made to the electron/hole-phonon form factor. There are still discrepancies to address between NEGF and LB FULL. Once they are solved, the LB approach could be used to efficiently parametrize the electron/hole-phonon coupling strength of the NEGF formalism so that experimental mobility values can be reproduced for materials other than Si.

References [1] M. Luisier, *Proc. ACM/IEEE Conf. Supercomput.* 2010, pp. 1-11. [2] M. Luisier, G. Klimeck, *Phys. Rev. B*, 80, 155430, 2009. [3] K. Rim et al., *Tech. Dig. Int. Electron Devices Meet.* 4346, 2002. [4] W. Zhang et al., *Phys. Rev. B*, 82, 115319, 2010. [5] T. B. Boykin et al., *Phys. Rev. B*, 69, 115201, 2004. [6] Z. Sui, I. P. Herman, *Phys. Rev. B*, 48, 17938, 1993. [7] T. B. Boykin et al., *Phys. Rev. B*, 76, 035310, 2007. [8] T. B. Boykin et al., *Phys. Rev. B*, 81, 125202, 2010.

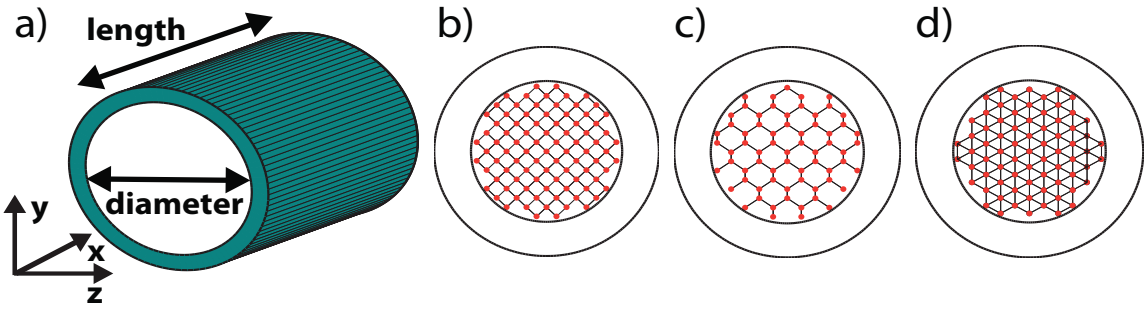

Fig. 1. (a) Schematic view of the nanowire structures simulated in this work. The diameter and length vary between 2.0 and 3.5 nm and 20 and 40 nm, respectively. Three different cross sections are considered (b) ⟨100⟩, (c) ⟨110⟩ and (d) ⟨111⟩.

$$\textbf{NEGF:}\quad \widetilde{\mathbf{V}}^{ij}_{nlln}(\omega_{ph}) = \sum_{\lambda}\int_{-\pi}^{\pi}\frac{dq_x}{2\pi}\cdot\mathbf{V}^{i}_{nl}(\lambda,q_x)\cdot\left(\mathbf{V}^{j}_{ln}(\lambda,q_x)\right)^{*}\quad\text{with}\quad \omega_{ph}-\Delta_E/\hbar\le\omega_\lambda(q_x)\le\omega_{ph}+\Delta_E/\hbar$$

$$\mathbf{\Sigma}^{\lessgtr}_{nn}(E)\approx\sum_{l,i,j}\sum_{\omega_{ph}}\widetilde{\mathbf{V}}^{ij}_{nlln}(\omega_{ph})\cdot\nabla_i\mathbf{H}_{nl}\cdot\left(n_{ph}(\omega_{ph})\cdot\mathbf{G}^{\lessgtr}_{ll}(E\mp\hbar\omega_{ph})+(n_{ph}(\omega_{ph})+1)\cdot\mathbf{G}^{\lessgtr}_{ll}(E\pm\hbar\omega_{ph})\right)\cdot\nabla_j\mathbf{H}_{ln}$$

$$\textbf{LB:}\quad S(b,k_x;b',k_x')\approx\frac{1}{\hbar}\sum_{\lambda}\int_{-\pi}^{\pi}dq_x\left|\sum_{n,l,i}\left(\mathbf{c}_n(b',k_x')\right)^{*}\cdot\mathbf{c}_l(b,k_x)\cdot\nabla_i\mathbf{H}_{nl}\cdot\mathbf{V}^{i}_{nl}(\lambda,q_x)\right|^2\cdot\delta_{k_x',k_x+q_x+Q_x}$$
$$\cdot\left[\left(n_{ph}(\omega_\lambda(q_x))+\frac{1}{2}\mp\frac{1}{2}\right)\cdot\delta(E^{b'}_{k_x'}-E^{b}_{k}\mp\hbar\omega_\lambda(q_x))\right]$$

Fig. 2. Comparison of the electron/hole-phonon equations in the NEGF and Linear Boltzmann approaches for nanowires. The indices i,j refer to spatial coordinates $\{x,y,z\}$, n, l to the atomic positions while b/λ indicates the electron/phonon mode. The variables k_x/q_x represent the electron/phonon wavevector, Q_x a primitive phonon wavevector, $E/\hbar\omega$ the electron/phonon energy, n_{ph} the equilibrium phonon distribution (Bose-Einstein), $\mathbf{G}$ is the electron Green's Function and $\mathbf{c}$ the electron eigenvectors resulting from the tight-binding Hamilton matrix $\mathbf{H}$. The term $\nabla\mathbf{H}$ describes the derivative of the tight-binding Hamilton matrix, $\mathbf{V}$ is the electron/hole-phonon scattering form factor, and $\widetilde{\mathbf{V}}$ its approximated value in the NEGF calculations [2]. In LB, the squared absolute value allows for either taking all the scattering elements ($n_1n_2\rightarrow n_1l_1l_2n_2$, LB FULL) into account or applying the same diagonal approximation ($nn\rightarrow nlln$, LB APPROX) as in the NEGF formalism.

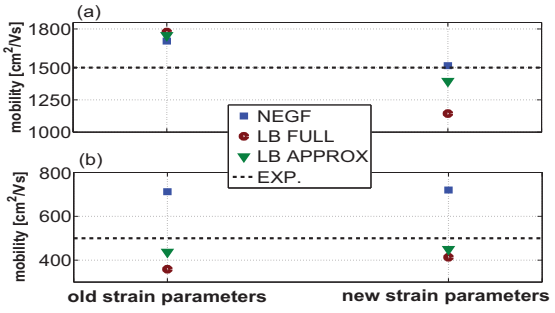

Fig. 3. (a) Electron mobility in bulk silicon. Comparison between the *old* [7] and *new* [8] strain model and the experimental value of pure silicon (dashed line). The blue squares refer to the NEGF simulations, red circles to LB FULL, and green triangles to LB APPROX. (b) Same as (a), but for holes.

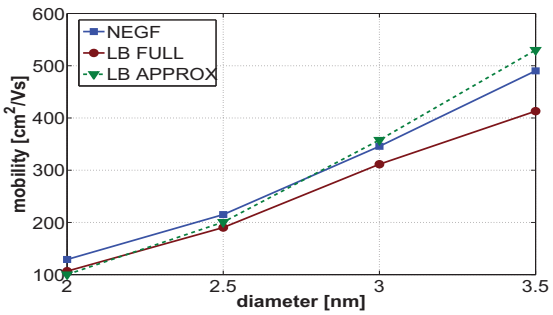

Fig. 4. Electron mobility in a ⟨100⟩-oriented silicon nanowire for diameters comprised between 2 and 3.5 nm. The blue line with square refers to NEGF, the red line with circles to LB FULL, and the green line with triangles to LB APPROX. In all these simulations, the *old* strain model is used.

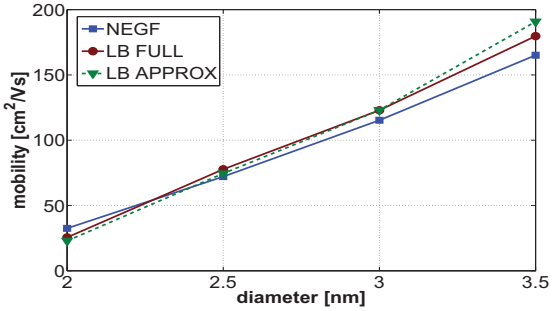

Fig. 5. Same as in Fig. 4, but for electrons along the ⟨111⟩ crystal orientation.

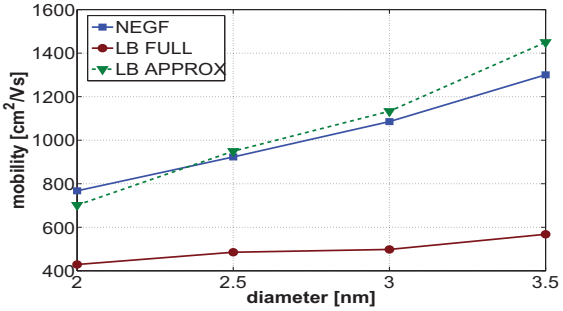

Fig. 6. Same as in Fig. 4 and 5, but for holes along the ⟨110⟩ crystal orientation.