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3D real-space quantum transport simulation of nanowire MOS transistors: Influence of the ionized doping impurity

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A R T I C L E I N F O

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A B S T R A C T

We report a numerical study of both donor- and acceptor doping impurity effects in the quantum transport of silicon nanowire metal-oxide-semiconductor (MOS) transistors. The code is based on a full three-dimensional (3D) real-space non-equilibrium green function (NEGF) formalism self-consistently coupled with the 3D Poisson equation. The general results show that the influence of an impurity strongly depends on its type. Indeed, an acceptor or a donor will create a repulsive or attractive potential, giving rise to tunneling effect or resonances, respectively. Our calculations analyze the impact on electron density, transmission coefficient and drain current (I_D) which undergoes variations up to 50%. This pinpoints the importance of intrinsic fluctuations due to doping in ultimate nano-transistors whose magnitude cannot be neglected in the next generations of integrated circuits.

As the traditional scaling of transistors is running out of steam, the microelectronics industry urgently needs new devices to replace the conventional metal oxide semiconductor field-effect transistors (MOSFETs) [1]. Among different plausible architectures, nanowire transistors are the most promising candidates. Despite their enhanced transport properties, which suggest a possibility to outperform performances of conventional metal-oxide-semiconductor (MOS) transistors, these devices suffer from a high sensitivity to intrinsic fluctuations at the nanometer scale. One of the main issues is the discreteness of the doping impurity, which can dramatically modify the current characteristics [2]. In this work, we then report a theoretical study of the point-defect impact by examining the dependence of the current, the potential, and the electron transmission coefficient. The code is based on a full three-dimensional (3D) real-space non-equilibrium green function (NEGF) formalism [3,4] self-consistently coupled with the 3D Poisson equation [5,6]. The Hamiltonian of the system is expressed within the effective mass approximation whose parameters have been fitted on a quantum wire full-band structure computed from a sp^3 third neighbors tight-binding model [7]. Fig. 1 shows the nanowire MOS transistor studied in this work. Source and drain are continuously n–doped with a concentration of $10^{20}\,\mathrm{cm}^{-3}$ and the channel is intrinsic. We consider a single ionized impurity located at the end of the source as illustrated in Fig. 2. The presence of a donor or an acceptor involves substantially different transport phenomena. Fig. 3 shows the influence on the electron density in the off-regime (small V_G). The general exponential density decrease in the channel is the consequence of the tunneling effect through the channel potential barrier. This trend is nevertheless strongly modified according to the considered impurity. More precisely, an ionized acceptor creates a repulsive potential that repels conduction electrons and results in a larger decrease of the density in the channel. On the other hand, a donor induces an attractive potential that increases the density and lengthens the source region. This evolution is also clearly visible in the transmission coefficient (Fig. 4). The difference between a perfect device and the one with an acceptor is quite significant, with a reduction of the transmission in the last case due to the positive Coulomb potential energy. On the contrary, device with a donor gives roughly the same transmission as the one of a perfect device. The currents are therefore very close ($I_D = 1.13 \times 10^{-11}$ A with a donor compared with $I_D = 0.9 \times 10^{-12}$ A). The fact that the current obtained in the presence of a donor is slightly higher than the one without is due to the reduction of the channel barrier. In the on-regime (high V_G), the impact of an acceptor remains unchanged whereas the attractive potential of a donor defines confined states in the vicinity of the defect, giving rise to quasi-localized energy levels and resonant tunneling. This effect is illustrated in Fig. 5 showing electron density resonances that result from the interaction between the quasi-localized state and the continuum. This behavior appears also in the transmission coefficient where anti-resonances dips are visible (Fig. 6).

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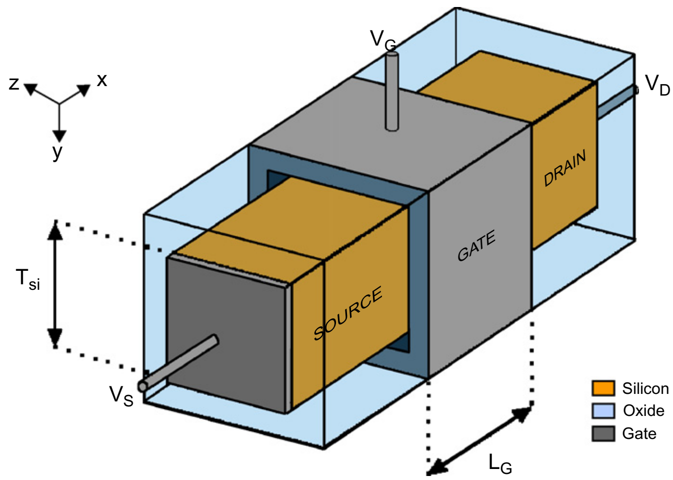

Fig. 1. Schematic view of a Si nanowire MOSFET with a surrounding gate electrode. The dimensions of the Si wire under the gate electrodes are $[T_{Si} \times T_{Si} \times L_G]$. In all the present work $L_G = 9$ nm, $T_{si} = 2$ nm and the oxide thickness is equal to 1 nm. Source/drain length is 5 nm.

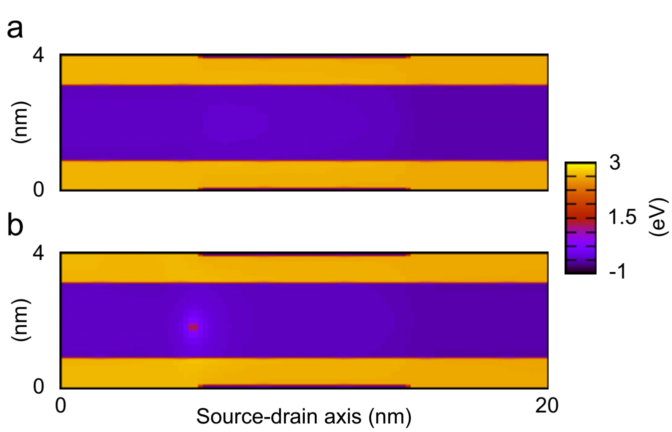

Fig. 2. Potential energy in a slice along the transport direction: (a) without impurity and (b) with an acceptor ionized impurity introduced at the beginning of the channel. The gate voltage $V_G = 0.5$ V and the applied source–drain bias (V_{DS}) is 0.1 V.

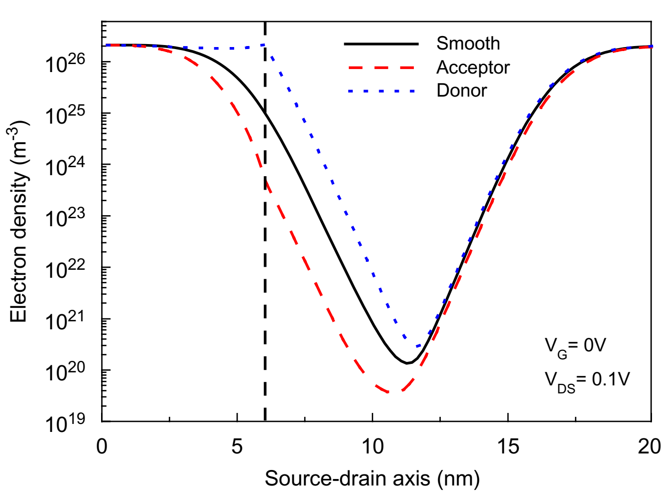

Fig. 3. Off-regime electron density along the source–drain axis for the configurations of Fig. 2. The repulsive/attractive potential of the acceptor/donor impurity clearly decreases/increases the charge density in the channel. $V_G = 0$ V.

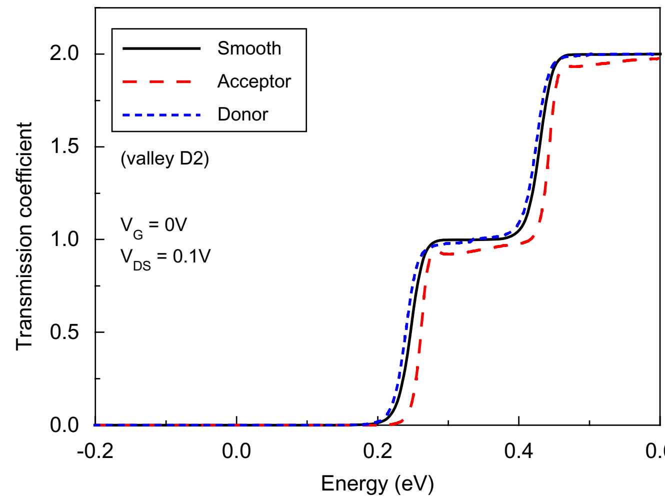

Fig. 4. Transmission coefficient corresponding to the potential energy shown in Fig. 3. The overall step-like shape behavior represents the effect of the quantum of conductance (e^2/h).

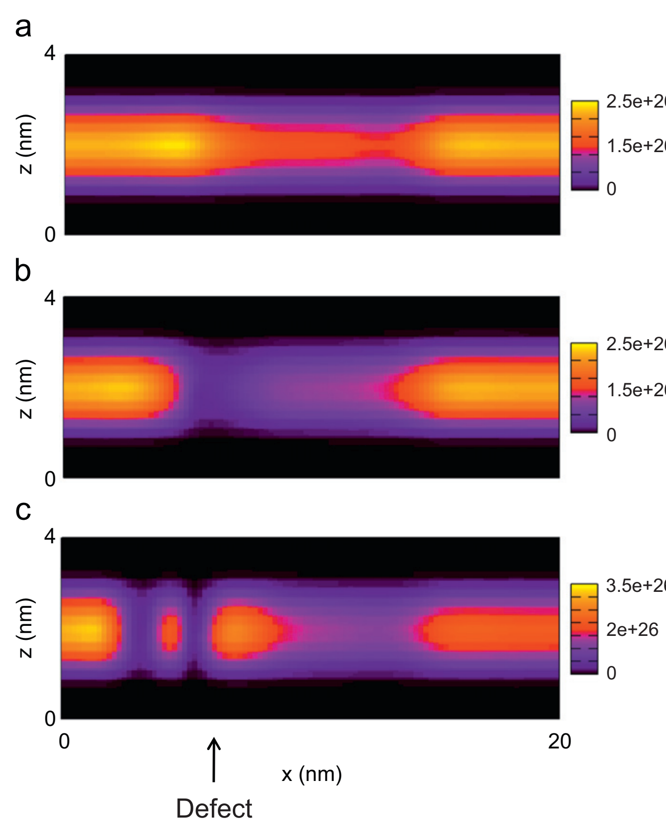

Fig. 5. Electron density in a slice along the transport direction (a) without defect, (b) with an acceptor, and (c) with a donor. $V_G = 0.6$ and $V_{DS} = 0.1$ V.

However, at room temperature these resonances does not have an important impact on the total current ($I_D = 1.6 \times 10^{-5}$ A with a donor compared with $I_D = 1.66 \times 10^{-5}$ A in a perfect device). On the contrary, an acceptor gives rise to major perturbations inducing a current decrease of more than 50% ($I_D = 7 \times 10^{-6}$ A). As a conclusion, variations of the total drain current in nanowire MOSFET induced by a single impurity substantially depend on its type. An acceptor can lead to strong modifications with current variations of more than 50%. A donor generates quasi-localized

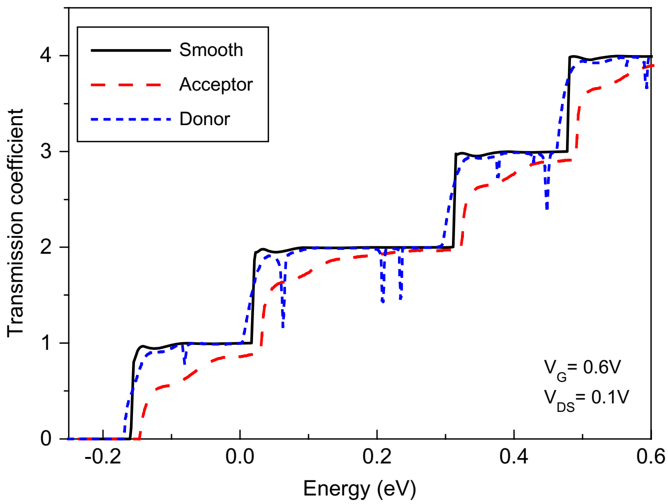

Fig. 6. Transmission coefficient on the on-regime. The presence of anti-resonance dips in the case of an ionized donor clearly illustrates the interaction between the impurity and the continuum coming from the reservoirs. $V_G = 0.6$ and $V_{DS} = 0.1$ V.

states and then anti-resonances, which can be understood via a careful observation of the electron density and transmission coefficient. Further studies have to be done in order to analyze the impact of the dopant position. Nevertheless, the present results already suggest that fluctuations in the device characteristics due to single impurity should have important effects in future circuit designs.

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