Simulation of impurities with an attractive potential in fully 3-D real-space Non-Equilibrium Green's Function quantum transport simulations

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Abstract—**The impact of one unintentional channel dopant on the performance of an n-channel Si nanowire MOSFET has been investigated using 3D Non-Equilibrium Green's Function simulations. Both donors and acceptors have been studied. The attractive donor potential is screened by conducting electrons through resonant states. The resultant inverted-sombrero potential has a twofold effect: lowering of the source-drain barrier and creating resonant states in the potential well, both of which increase the current. At low gate voltage the donor induced current increases two orders of magnitude compared to the impurity-free device. At high gate voltage, the current difference slowly disappears. In the case of an acceptor in the channel the current is reduced over the whole gate bias range.**

Keywords: discrete impurities, nanowire transistor, Non-Equilibrium Green's function, screening, transmission resonances.

I. Introduction

The Non-Equilibrium Green's Function (NEGF) formalism has been extensively used to study the performance of nanowire transistors [1]. The fluctuations in the I_D-V_G characteristics caused by the repulsive potential of a stray charge have also been investigated [2] for nanowire MOSFETs. However, the effects of an attractive potential have never been studied using a fully-3D self-consistent Poisson-NEGF scheme. The proper inclusion of the effect of all types of discrete dopants and trapped charges in 3D NEGF simulations is of great importance for the proper simulation and understanding of atomic-scale variability in nanowires and other types of MOSFETs.

There is a major difference between an attractive and a repulsive potential in the context of quantum transport simulations. The impact of the repulsive potential is mainly associated with charge exclusion and a certain degree of tunnelling through it. The attractive potential creates quantum confinement but does not necessarily confine conducting electrons in the Coulomb potential well. If the wavelength of the electron is of the same order of magnitude as the spatial variation of the impurity potential, the potential could reflect the electron. The screening self-consistently changes the local electric field around a donor. Screening has been extensively studied in the literature [3, 4] from many-body point-of-view but none of the methods include local field corrections from conduction electrons in a non-perturbative way in the context of a nanowire. The screening of a localised charge in a semiconductor can be roughly divided into two parts: one associated with the polarization of the valence electrons taken into account by the static dielectric constant [5], and the other by the excess of conducting electrons, which interacts with the long-range screening potential. The transport electron screening of the attractive donor potential happens through resonance and zero transmission states of the potential [6, 7], which are highly localised in energy. The corresponding resonant energies are very sensitive to small changes in the shape of the potential. This fact can make the convergence of the Poisson-NEGF scheme very cumbersome to achieve. In the cases of very narrow wires the screening is mainly 1-D. Therefore, the screening is much weaker than the 2-D and 3-D or bulk-type one.

In this paper, for the first time, we present a detailed study of the effect of an attractive potential, associated with a donor-type impurity in the channel, on the performance of a *n*-channel nanowire transistor. The model device and the simulation technology are described in section II. The results and discussion are presented in Section III and the conclusions are drawn in Section IV.

II. Model and Device

The 3D NEGF equations [2] are used to describe the quantum electron transport and are solved self-consistently with the 3-D Poisson equation. We use the effective-mass Hamiltonian to compute the retarded Green's function matrix, G^R, which is used to calculate the *less-than* Green's function, $G^<$, directly related to the electron and current density:

$$n(E,x) = iG^<(E,x,x) \tag{1}$$

$$J(E,x) = -i\frac{e\hbar}{2m}(\nabla - \nabla')G^<(E,x,x')\Big|_{x=x'} \tag{2}$$

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The effective masses are extracted from tight-binding calculations [8]. The recursive algorithm and boundary conditions for solving the NEGF are presented elsewhere [1, 9].

The electron density from the NEGF is used to self-consistently calculate the electrostatic potential through the solution of Poisson's equation. In the iterative process we calculate auxiliary quasi-Fermi levels (which in our case have no physical significance) using the new electron density and the old potential [10]. These quasi-Fermi levels are used in solving the non-linear Poisson equation, giving the new electrostatic potential. After that, a new density is computed using the NEGF equations and fed to the subsequent solution of the Poisson equation. The solution is iterated until density and current converge. This method is stable if damping is applied to both the potential and density solutions.

As an initial condition we use the electrostatic potential obtained from a density gradient solution of the Drift-Diffusion (DD) equations [11]. The DD solver has Neumann boundary conditions in the source and drain instead of the Dirichlet boundary conditions usually used in the DD formalism [12, 13], and is therefore consistent with the open boundary conditions required for the Green's function solution. The self-energies are calculated using the algorithm given in [14].

The investigated gate-all-around nanowire transistor has a 2.2×2.2 nm^2 cross-section, and has one impurity in the channel. The source/drain doping is 10^{20} cm^{-3}. Fig. 1 shows a schematic view of the transistor. All simulations in this paper were carried out close to equilibrium at V_D=1 mV in order to study the charge density around the impurity. We considered three devices, two of which have a discrete donor in the channel and the third one has a discrete acceptor [denoted *Acceptor*]. The donor atoms differ in their location: one is located at the middle of the cross section [denoted *DM*] and the other is close to one of the four SiO_2 interface planes [denoted *DA*]. The unintentional impurities have been introduced as one electron charge (+ve donor, -ve acceptor) divided by the discretisation volume associated with a node, in our case 0.2×0.2×0.2 nm^3. We have checked that the solution of the discretised Poisson equation reproduces the $q/(\varepsilon_{Si} r)$ Coulomb potential for the undoped bulk case, where ε_{Si} is the dielectric constant of the semiconductor.

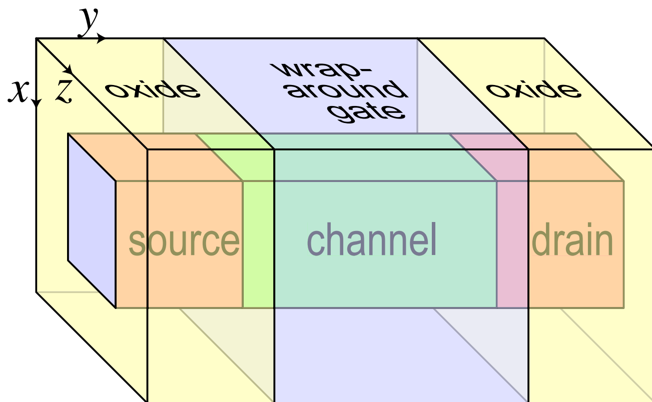

Figure 1. Schematic view of the nanowire.

III. Results and Discussion

The potential and density in a channel cross-section containing the impurity at V_G=0.4 V for the *DM* and *DA* cases are shown in Fig. 2. The potential plot shows the locations of the impurities in the cross-section for both devices. Note, that in the *DA* case, the peak in electron density is misaligned with the potential associated with the dopant position due to the quantum confinement effect. Fig. 3 shows a 3-D isoline plot of the potential and the electron density in the nanowire for the *DM* and *DA* cases. The behaviour of the equipotential contour lines along the interface close to the impurity (case *DA*) is due to the polarisation in the dielectric and the induced charge in the metal.

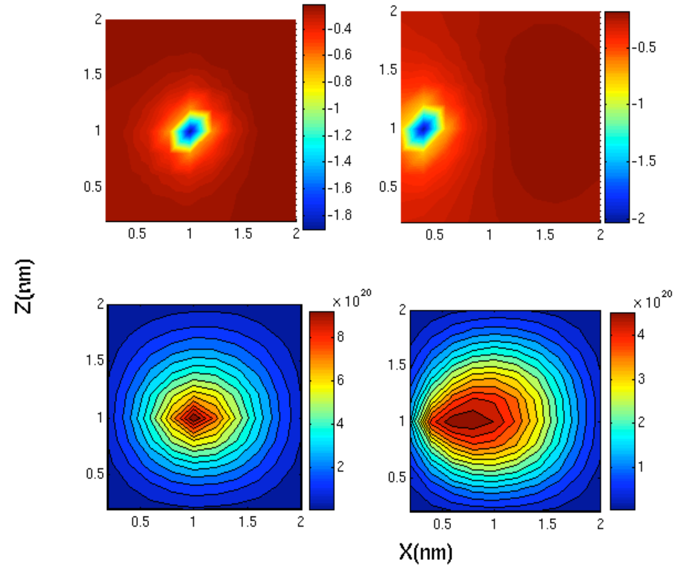

Figure 2. (above) potential and (below) density at the impurity location cross-section.

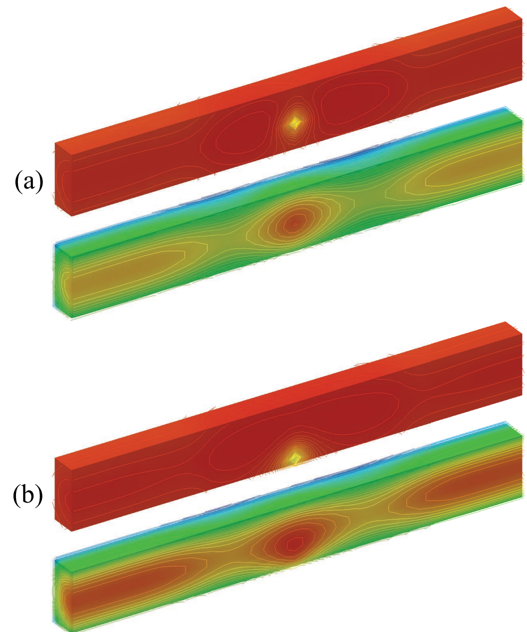

Figure 3. 3D potential and density for (a) DM and (b) DA cases, cut through the middle of the device.

For a set of different gate voltages the electrostatic potential along the channel in the middle of the cross-section, for the *DM* and *DA* devices, is shown in Figs. 4 and 5 respectively. Note the inverse 'sombrero' shape of the potential. This shape produces quasi-bound states similar to these in resonant tunnelling structures.

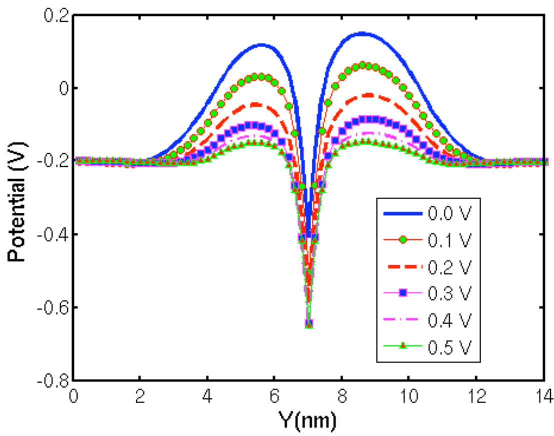

Figure 4. Potential for DM case along the wire at different V_G

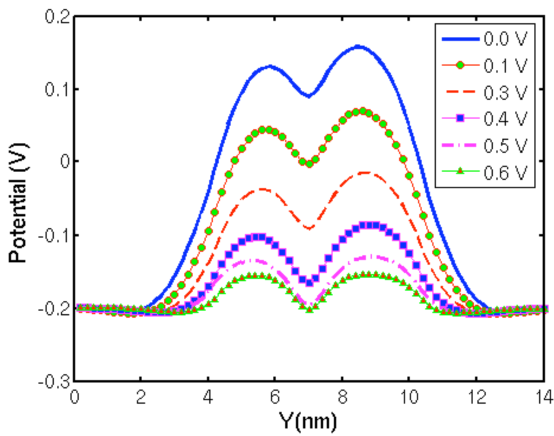

Figure 5. Potential for DA case along the wire at different V_G

The transmission coefficients for the cases *DM* and *DA* at several gate voltages are shown in Figs. 6 and 7 respectively. The transmission coefficients contain one resonance (or quasi-bound state) at the onset of each sub-band's conductance. This potential introduces transmission channels, which increases the current in these devices when compared with the impurity-free device. At high drain bias, backscattering of the carriers from the impurity potential reduces the current.

The resonances corresponding to the device with the donor close to the interface are less sharp because the impact of the donor potential on the source-drain barrier is less severe. This effect is more pronounced in the first sub-band, as shown in Figs 6 and 7.

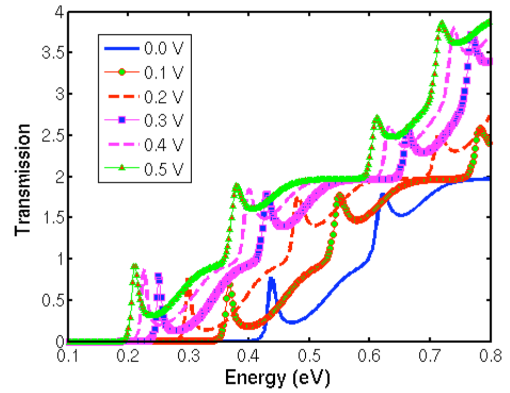

Figure 6. Transmission for the device with the dopant at the middle of the channel (DM case) at different V_G

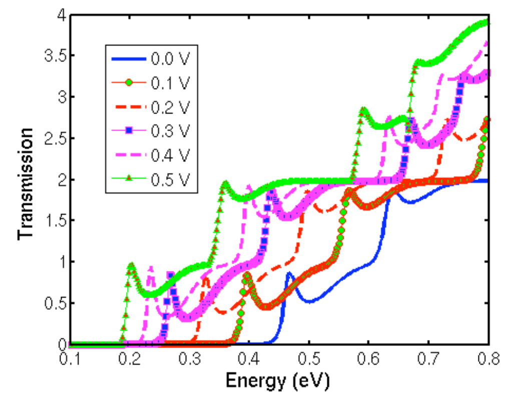

Figure 7. Transmission for the device with the dopant close to the interface (DA case) at different V_G

Figs. 8 and 9 show the electron concentration corresponding to the same gate voltage and dopant configuration positions of Figs. 4 and 5 respectively. At low gate bias the electrons are repelled from the channel, and the electron density at the impurity is very low. At high gate bias the potential barrier of the channel decreases. As a consequence, the electrons penetrate into the channel and start to contribute to the screening of the impurity. For the *DA* case the screening is not so strong because the impurity is close to the interface and the electron density there is smaller due to quantum confinement.

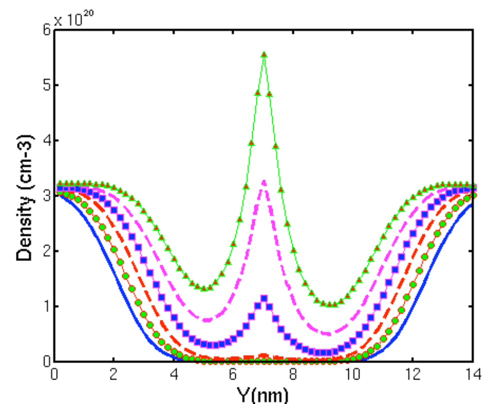

Figure 8. Density along the wire for the device with the dopant at the middle of the channel (case DM) at different V_G

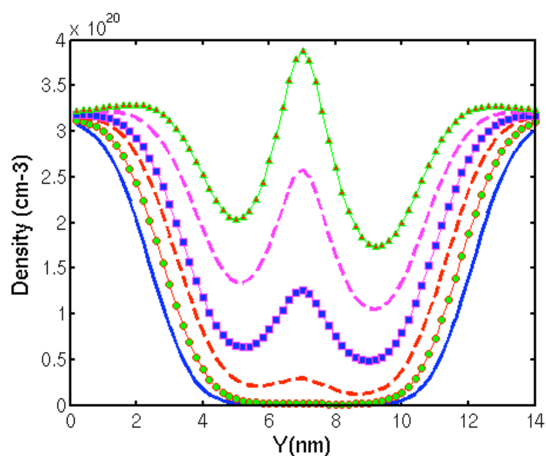

Figure 9. Density along the wire for the device with the dopant close to the interface (case DA) at different V_G

The I_D-V_G characteristics of the *DM*, *DA*, and *Acceptor* devices are shown in Fig. 10. The device without impurity is also shown for comparison. The off-current is substantially increased in the cases of *DM* and *DA* when compared with the impurity-free device. This is due to two effects: firstly, the lowering of the gate barrier because of the presence of the attractive impurity charge and, secondly, because of the type of resonant tunnelling structure induced by the impurity potential. At high bias the *DM* and *DA* cases yield similar current. This is due to the energy broadening of the resonance peak and the reduction in back scattering for the *DA* compared to *DM* case. This fact can be observed when comparing the transmission coefficients of the *DM* and *DA* cases shown in Fig. 6 and 7 at high gate bias. The *Acceptor* device has the lowest current as should be expected, due to the repulsive barrier of the acceptor.

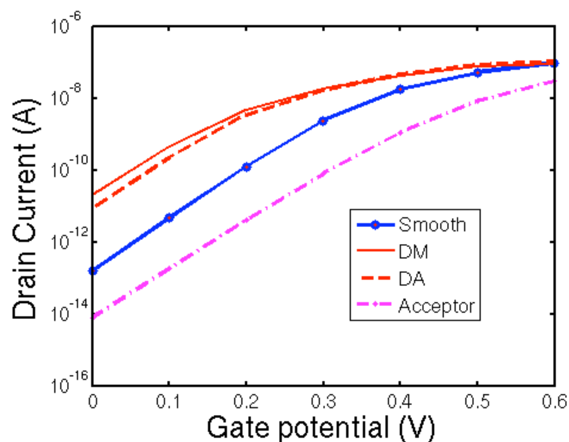

Figure 10. I_D-V_G for Smooth, *DM*, *DA* and *Acceptor* cases

IV. Conclusions

Using a fully-3D real-space NEGF formalism, we have studied the impact of one unintentional dopant located in the channel on the performance of a narrow gate-all-around nanowire transistor. Attractive and repulsive potential (donor and acceptor-type impurities) have been studied. The convergence of the NEGF-Poisson equations is more cumbersome in the case of donor impurities, and therefore requires a careful selection of the initial guess and a heavy adaptive damping scheme in the iterative calculation of potential and density. We have observed resonances in the case of the donor-type potential, which represent the major contribution to screening, and that are also responsible for backscattering, which affects the on-current in the donor-impurity-type devices. As expected the leakage is large in both donor cases due to the barrier reduction and resonances. One interesting phenomenon is the shift of the screening charge with respect to the location of the donor, when it is close to the interface. This is a consequence of the quantum confinement in the presence of the interface barrier, which repels the charge away from the interface. The *Acceptor* case device produces a significantly lower on-current, due to the increased potential barrier in the channel.

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