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Developing a full 3D NEGF simulator with random dopant and interface roughness

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Abstract We have developed a full 3D Non Equilibrium Green's Function quantum transport simulator of nanoelectronic devices. In order to illustrate the capabilities of the simulator we have computed the transmission function for silicon nanowires, in the presence of surface roughness and unintentional dopant atoms. Unlike the case of 2D simulations, in which the channel is blocked by the presence of only one impurity, the 3D current flow can turn in 3D avoiding the local impurity potential. This feature counts for a milder effect of the stray impurities and trapped carriers on the current in nanoscaled devices. Another interesting effect is the interference between the reflections of the electron wave function, from multiple impurities in the channel, which produces visible features in the transmission function. The electron density is deformed by the impurity in the channel, which is an effect of the deformation of the transversal electron wave function around the local impurity potential. Similar phenomenon occurs in the case of surface roughness. The above results illustrate the acute need for a three-dimension description of the transport in nano devices in the presence of atomic scale variations in doping and interface configuration.

Keywords Non Equillibrium Green Function · Nanowires · Interface roughness · Discret dopants

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1 Introduction

Random discrete dopant in the source/drain, stray dopant in the channel, and imperfections in the Si/SiO_2 interface became very important in nanometer scale devices. The effect of random dopants and surface roughness do not average on such small scales. Therefore, the particular configuration of dopants from device to device produce fluctuations in the current and threshold voltage in an ensemble of technologically similar devices as show previously using 2D NEGF simulations [1]. Quantum phenomena are governing the device behaviour at nanoscale dimensions. The Non Equilibrium Green's Function (NEGF) approach to quantum transport has become well established as a simulation tool for nano-CMOS device simulation. Two dimensional NEGF simulators produce reasonable qualitative results however the restrictions to the line charges and 1D interface roughness result in an overestimation of the effect of fluctuations, especially in very small devices. More realistic results can be achieved using 3D simulations but unfortunately the 3D realisation of quantum mechanical NEGF formalism is very computationally expensive and memory consuming. This is because of the fine step energy integration and large matrix inversions requirements. Fortunately faster processors and larger memories are becoming available allowing the 3D NEGF technique to become a realistic choice for the 3D simulation of nanotransistors in ballistic regime.

2 The 3D-NEGF simulator development

Here we present the development of a full 3D NEGF simulator, which runs in parallel, and is able to compute electron density, current and transmission for different device configurations. The simulator allows the use of different boundary

conditions in the cross section of the device including reflected, wrap-around, and zero density boundaries. A recursive algorithm [2], in order to calculate the density of states and electron density has been incorporated. This allows us to calculate efficiently the diagonal terms of the retarded green function G^r and the less than Green function $G^<$ which are needed in order to compute the density of states and the electron density respectively. The calculation of the first off-diagonal terms of $G^<$ is needed in order to compute the current density. The self-energies are calculated following [3].

3 Results and discussion

The capabilities of the new simulator are illustrated in the simulations relevant to the nanowire transistor illustrated in Fig. 1.

We focus on the impact of the location of stray dopants and their relative configuration on the transmission and electron density. The effect of atomic scale interface roughness on the electron density has also been studied for different randomly generated surface roughness configurations. The transistor in Fig. 1 has a 2 nm × 2 nm × 6 nm undoped Si body. Uniform 1 Å mesh is used in the simulation. The energy discretisation contains approximately 600 points. Figure 2 and 3 show the potential and current density landscapes for two transversal planes (y is the transport direction) in the case of 2 non-aligned single negative charges along the channel. The repulsive potential of the two impurities is visible in Fig. 2 which illustrates the potential and the current density distributions in the (y, z) plane at $x = 10$ which is the x-coordinate of the centre of the channel. One of the impurities is very close to the interface. The impurity potential of this impurity does not appear in the Fig. 3 which is a (y, z) plane at $z = 10$. This is because this impurity is located close to the interface far from this plane. In Fig. 2 the current density became smaller at the centre of this plane and is not conserved in the direction of the transport in this plane, this is because the current is meandering out of the plane. This is

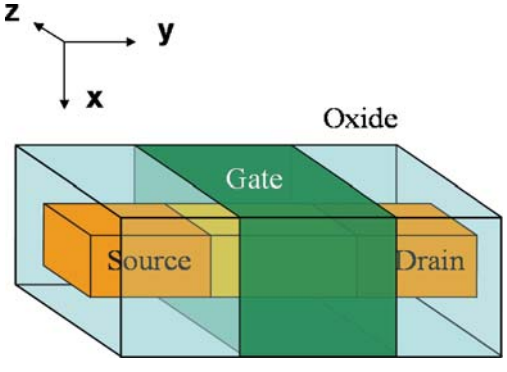


Fig. 1 The structure of the nanowire and the co-ordinated system

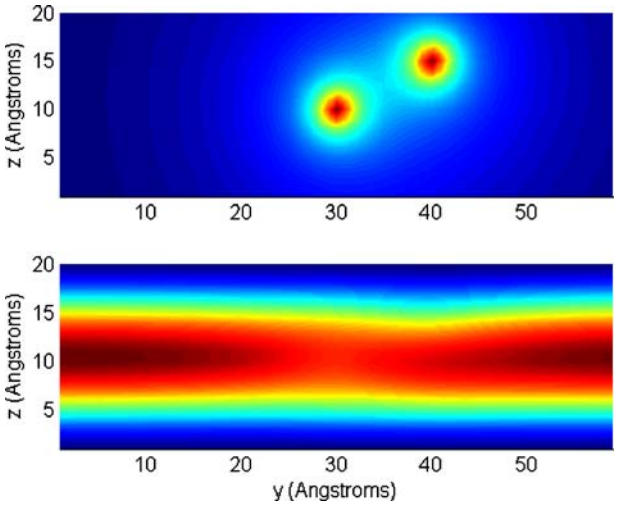


Fig. 2 Upper and lower panels present the potential and current landscape respectively for the case of two non-alignment charges for the zy plane

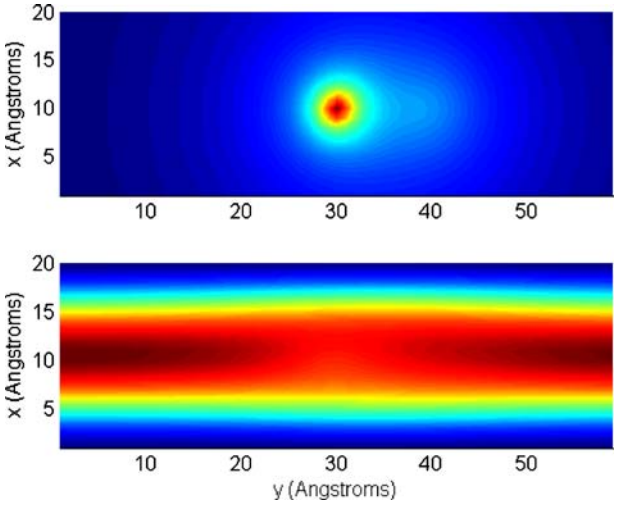


Fig. 3 Same as Fig. 2 but for the *xy*-plane figure caption

a phenomenon, which can not be properly captured in a 2D or 1D simulations. The current density is conserved through every cross section perpendicular to the transport direction as a result of the Hermiticity of the 3D Hamiltonian in the internal points of the device i.e. not at the boundaries of the source and drain. Note that in Figs. 2 and 3 the current density is not totally zero at the position of the impurities which indicates the tunnelling through the impurities potential.

Figures 4 and 5 show the potential and the current density distributions through the same two planes identified in Fig. 2 and 3 but for a particular random generated surface roughness. In Fig. 4 the surface roughness reduces the body thickness around the drain region. This constriction and the corresponding confinement, produces additional energy shift in the z transversal wave function. As a result the current is further squeezed in the z direction. Fig. 5 represents the (x, y)

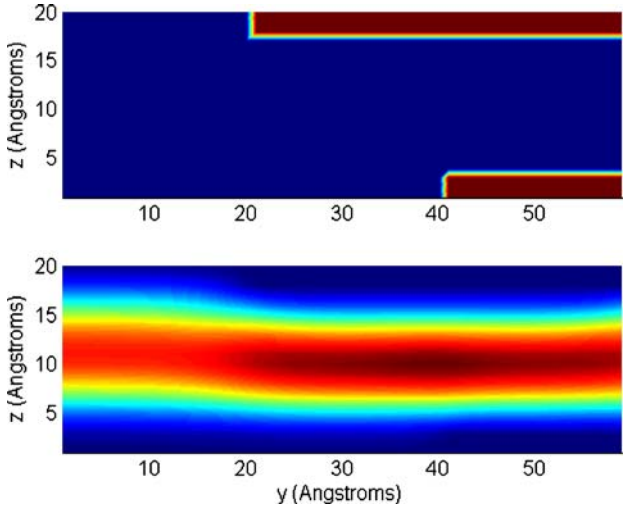


Fig. 4 Same as Fig. 2 but for the case with interface roughness

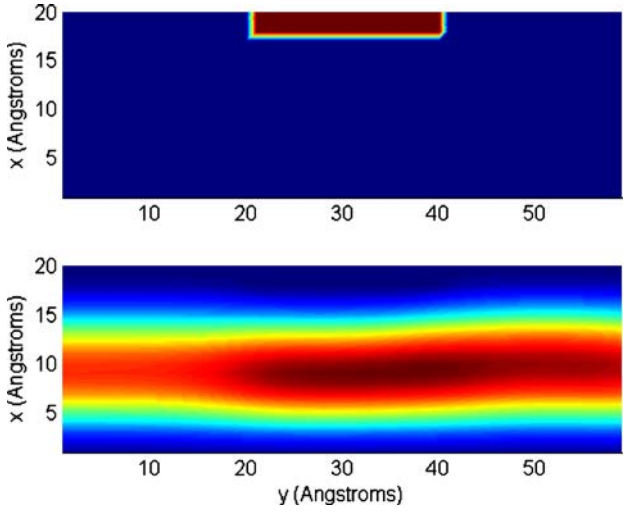


Fig. 5 Same as Fig. 4 but for the *xy*-plane

plane at $z = 10$ in which the effect of the roughness is less severe. Only an extra confinement in the upper interface at the middle of the channel has been introduced. Note that the current has been squeezed in the middle of the channel but still some effects of the confinement, in the perpendicular direction, can be seen close to the drain.

The potential and electron density distributions in the presence of roughness are shown in Fig. 6 for two different cross sections normal to the direction of the current flow. The electron density of the lower left plane shows a non-rectangular deformation, which reflects the roughness configuration. In the lower right panel the density remains rectangular in shape but corresponds to a higher energy transversal state than that of the left panel. This reflects the fact that the conducting channel cross section, in the upper right panel is smaller than that of the left. These variations in the electron density reflect the variation of the transversal wave functions, which invalidates the 1D or mode space transport model.

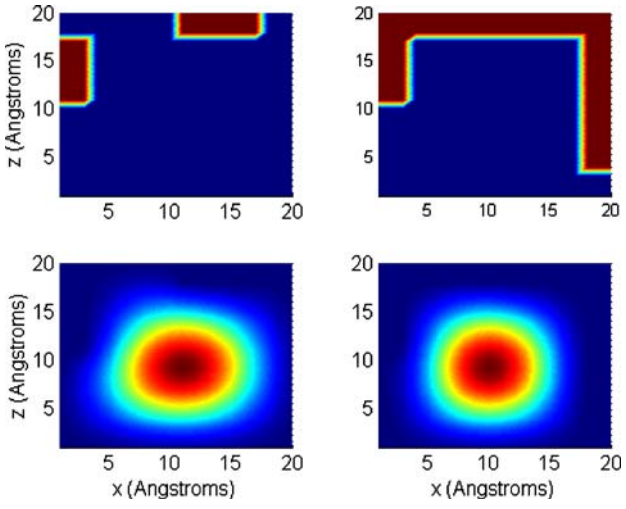


Fig. 6 The two upper panels show the interface roughness for two different cross sections and the lower panels stand for the corresponding electron densities

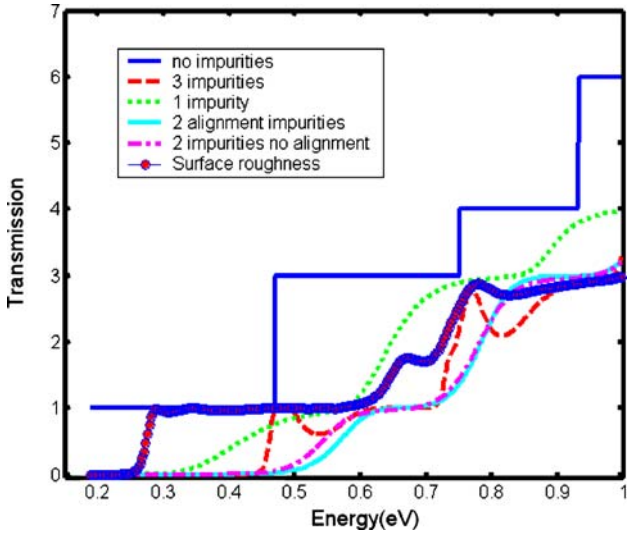


Fig. 7 The transmission function for some of the cases simulates. The case without impurities and surface roughness is also shown

We have calculated the transmission function for different configurations of unintentional dopants and for different amounts of unintentional dopants in the channel. The results have been compared to the device without unintentional dopants.

Figure 7 shows the transmission as a function of energy for 5 different cases. They differ in the numbers and positions of impurities. The transmission for the case of the surface roughness illustrated Figs. 4 and 5 has also been shown. The case without surface roughness and impurities is also shown for comparison. The transmission with one impurity starts around 0.3 eV, while in the other impurity cases the transmission start after 0.45 eV. Note than in the case of 3 impurities the transmission starts earlier than in the case of 2 impurities, showing a constructive interference. The case with three

impurities presents very marked resonances. The two impurities correspond to the worst case. The transmission for the surface roughness case shows the removal of the degeneration of the second transversal state around 0.7 eV. Note the resonances caused by the constriction in the body thickness at the middle of the channel, due to the surface roughness (see Fig. 5). Comparing the transmission of the studied cases of unintentional dopants and interface roughness with the plain case an energy shift of approximately 300 meV is observed. This suggests an approximate threshold voltage shift of such magnitude in the Id-Vg curve. The corresponding change in transmission between the plain case and the roughness case is around 100 mV.

4 Conclusions

Using a full 3D NEGF simulations, we have computed the current and electron density and the transmission function for idealized Si nanowires, in the presence of unintentional dopants in the channel and interface roughness. The current density has a distinct 3D character meandering along the channel. The transversal wave function is clearly distorted in the cross section along the channel, producing a distortion in the electron density. Finally, the transmission obtained for the nanowires, with unintentional impurities, suggests a threshold voltage shift on the order of 300 mV compared with the reference uniform and undoped device.

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