Treatment of point defects in nanowire MOSFETs using the Nonequilibrium Green's function formalism

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This work describes the point defect treatment in nanowire MOSFETs. The 3D Poisson equation is self-consistently coupled to the Schrödinger equation. We adopt the mode-space representation in which the 3D Schrödinger equation is divided into a 2D equation, including the confinement of the cross-section, and a 1D equation describing the ballistic transport based on the nonequilibrium Green's function formalism (NEGF). We use the simplest form of the tight-binding theory, with one orbital per atom, and considering only the first-neighbor-interactions. In this framework, equivalent to the ellipsoidal energy band approximation, influence of point defects on electronic transport is discussed.

Point defects are characterized by a long range interaction Coulomb potential plus an on-site potential. Coulombian tail, which results from the electrostatic interactions of the defect with the electrons of the remaining system, can be treated as a macroscopic variation which does not disturb the 2D wavefunctions: scalar product of the first eigenstate with and without defect is very closed to 1 (≅0.95). We can then include this new potential directly in the self-consistent mode-space approach without coupling the electron subbands. On the other hand, a full 3D treatment is needed to consider the on-site point defect potential, for which Fourier transform significantly changes the 2D modes in the slices of the nanowire surrounding the defect. Therefore, once achieving the self-consistence with the Coulomb potential, the device is subdivided into two regions at the point defect location (vertical dotted line of figure 1a). By summing over all the quantum confinement modes, we calculate the surface Green's functions of each region. Matrix sizes are greatly reduced compared to a full 3D description and perturbation due to the on-site potential is treated by applying the Dyson's equation to the surface Green's function containing the defect. We finally calculate the total transmitted current through these two regions.

This model has been tested on a 3 nm squared cross-section silicon wire. Source and drain doping concentration is 10^{26} m^{-3} and the channel is undoped. Simulation results demonstrated that the Coulombian tail has the more significant impact on the drain current compared to the on-site potential defect. Considering an acceptor impurity (negative Coulomb potential) Figure 1a shows the first subband profile along the source-drain axis, assuming two different point defect locations and the defect free case. A point defect introduced in the center of the cross-section (inset of Figure 1a), near the source, greatly modifies the subband profile. On the other hand, the defect introduced in the corner of the same cross-section is rapidly screened by the silicon valence electrons and the effects of its Coulomb potential are weaker. This behavior is confirmed by the corresponding drain current versus gate voltage characteristics shown in Figure 1b. The current from the defect free case is higher whereas the one given by a defect located in the center of the cross-section is the lowest. Between these two extrema, the presence of a defect in the border line of the cross-section is less dramatic in term of current decrease: subthreshold current equals 50% of the perfect lattice case.

A full journal publication of this work will be published in the Journal of Computational Electronics.

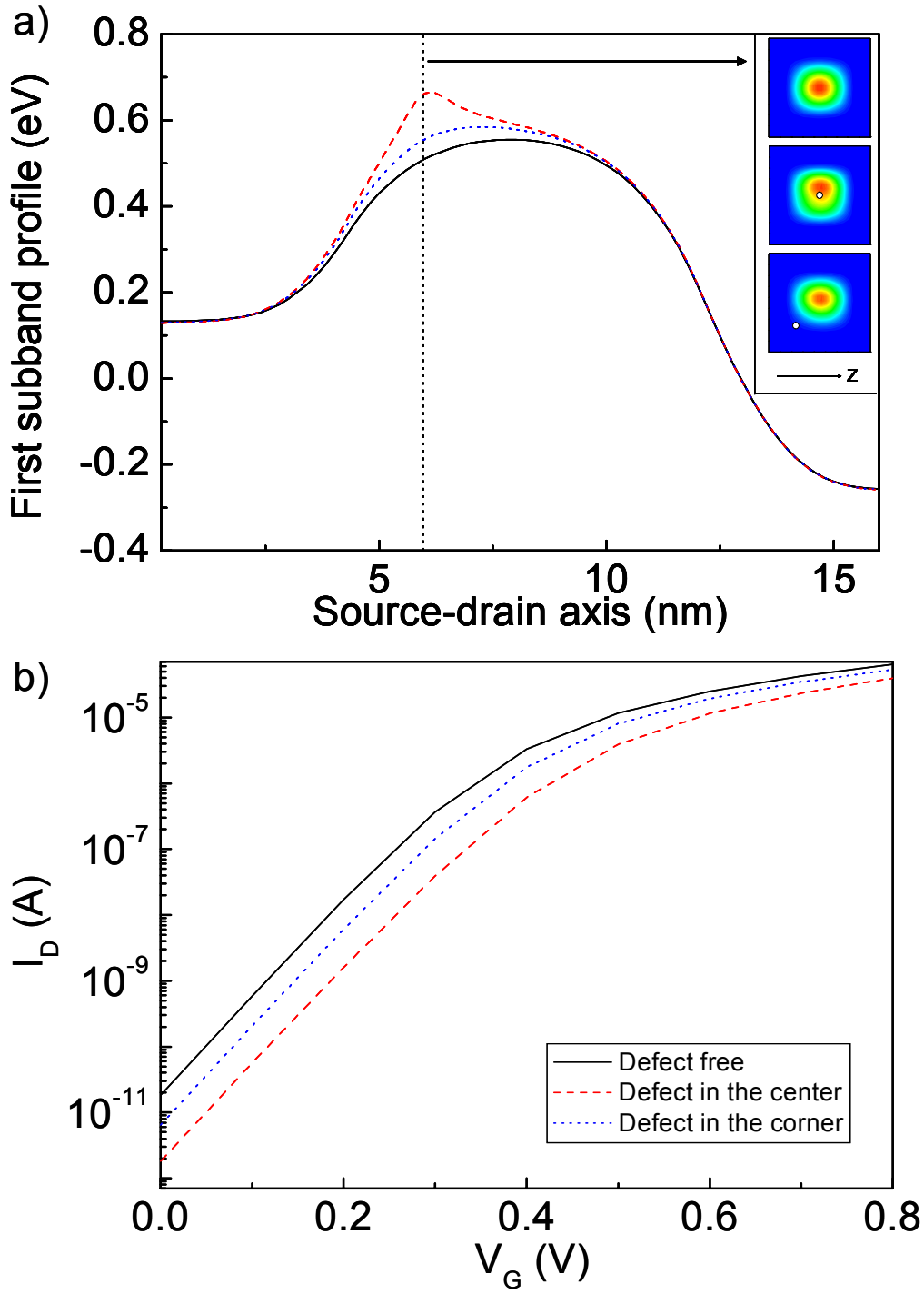

Figure 1: (a) First subband profiles along the source-drain *x*-axis in the defect free case (solid line), assuming a Coulomb potential of a point defect introduced in the center of the cross-section (dashed line) and introduced in the corner of the same cross-section (dotted line). Vertical dotted line indicates the defect *x*-position. The inset shows the associated 2D square modulus of the first eigenstates within the defect slice, where white points indicate the defect location. (b) Corresponding drain current versus gate voltage characteristics. $V_{Drain/Source}$=0.4 V and channel length=8 nm.

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