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# Developing a Full 3D NEGF Simulator with Random Dopant and Interface Roughness

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The importance of discrete dopant in the source/drain, straight dopant in the channel, and imperfections in the $Si/SiO_2$ interface became very important at nanometer device dimensions. The effect of random dopants and surface roughness do not average on such small devices. 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 important for those small devices. One of the well established techniques for Nano-CMOS device simulation is the Non Equilibrium Green's Function (NEGF) approach to quantum transport. Two dimensional NEGF models 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. A more realistic situation can be achieved in 3D but unfortunately the 3D quantum mechanical NEGF description of the transport 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 simulation of in ballistic nanotransistors. Here we present the development of a full 3D NEGF simulator, which runs in parallels, and is able to compute electron density, current and transmission for different device configurations. The simulator allows the used of different boundary conditions in the cross section of the device including reflected, wrapped around, and zero density boundaries. A recursive algorithm, 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 $G^r$ retarded green function and $G^<$ the less than green function 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 [2].. In this work we have concentrated on the sub threshold regime, where the coupling with the Poisson equation is not essential. Our main focus is the impact of the location of unintentional dopant, and their relative configuration on the transmission and electron density. The effect of the surface roughness on the electron density has also been studied for different randomly generated surface roughness configurations. A slab of 2nm x 2nm x 6nm undoped *Si* has been used in the simulations. Å mesh spacing is used for generating the space mesh. The energy mesh contains around 600 points. Fig 1 and Fig. 2 show the potential and current density landscapes for two transversal plane (y is the transport direction) in the case of 2 non aligned charges along the channel. Figs. 3, 4 show the same distribution in the case with interface roughness. The potential and electron density for two different cross sections are shown in fig. 5 in the presence of roughness. Fig. 6 shows the transmission as a function of energy for 5 different cases. Note than in the case of 3 impurities the transmission start early than in the case of 2 impurities showing a constructive interference.

## REFERENCES

[1] A. Martinez, A. Svizhenko, M. P. Anantram, J. R. Barker, A.R. Brown and A. Asenov, IEDM Tech. Dig., 627 (2005).

[2] R. Venugopal, Z. Ren, S. Datta and M. Lundstrom, *Simulating quantum transport in nanoscale transistors: Real versus mode-space approaches,* J. App. Phys. **92**, 3730-3739 (2002)

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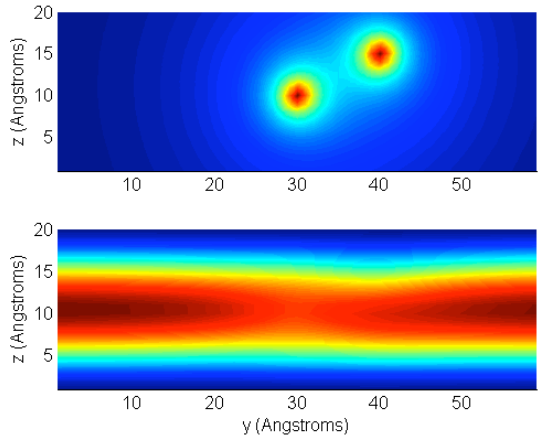


Fig. 1. upper and lower panels present the potential and current landscape respectively for the case of two non alignment charges for the zy plane

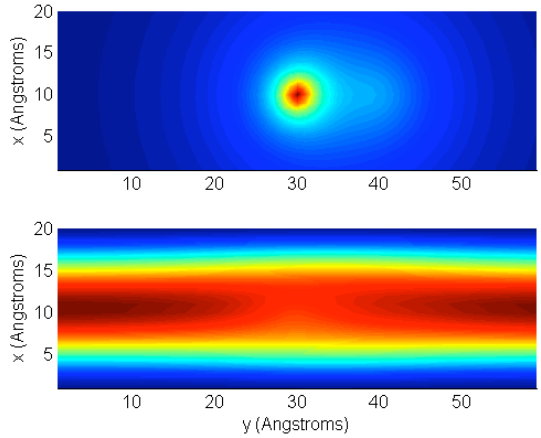


Fig. 2. Same as fig. 1 but for the xy-plane

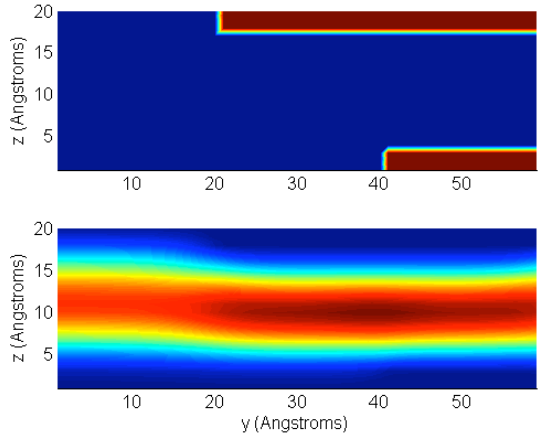


Fig. 3. Same as fig 1 but for the case with interface rougness

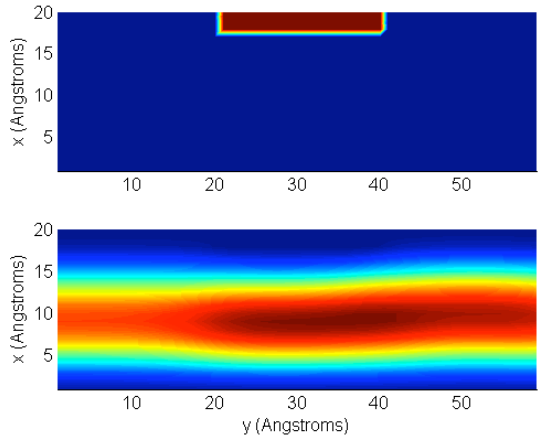


Fig. 4. The same as fig. 3 but in the xy-plane

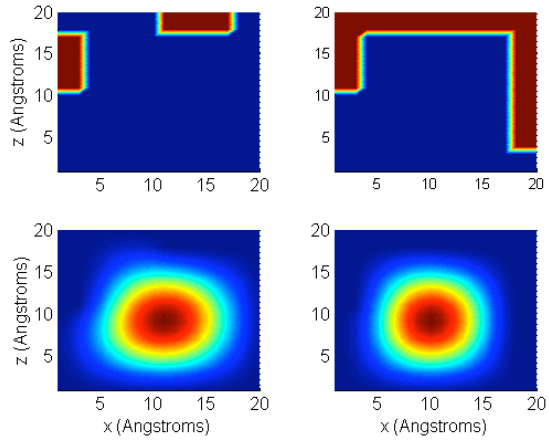


Fig. 5. The two upper panels show the interface roughness for two different cross sections and the lower panels stand for the corresponding electron densities

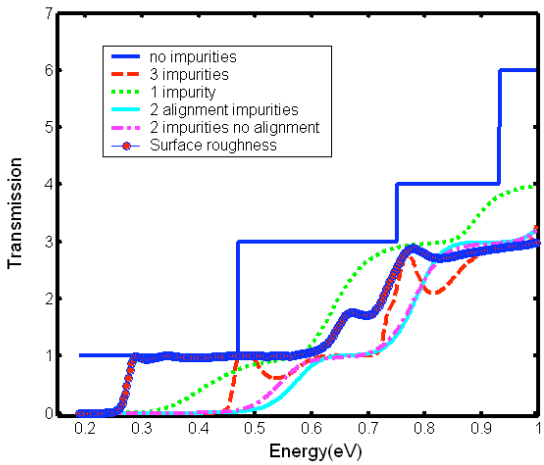


Fig. 6. The transmission function for some of the cases simulates. The case without impurities and surface roughness is also shown.