Modeling of FDSOI and Trigate devices : What can we learn from Non-Equilibrium Green's Functions ?

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As the characteristic size of the devices is now reaching the sub-15 nm range, it has become essential to assess the effects of quantum corrections on the electrical performances. The Non-Equilibrium Green's Functions (NEGF) method is one of the most versatile framework for that purpose. It can deal with quantum confinement, elastic and inelastic scattering in a seamless way. Although numerically intensive, NEGF has benefited from recent advances in computational methodologies and from the increasing availability of high-performance computers. It has now reached a level of maturity where it can be applied to industrial technologies and complement semi-classical modeling [1].

We have computed electron and hole mobilities in Fully-Depleted Silicon-on-Insulator (FD-SOI), 7.5 nm thick film devices manufactured at STMicroelectronics and Trigate (nanowire-like) devices etched on SOI made at CEA/LETI. The electron band structure is modeled with the effective mass approximation (EMA) and with a non-parabolic two bands $\mathbf{k}\cdot\mathbf{p}$ model (2KP). The hole band structure is modeled with a three bands $\mathbf{k}\cdot\mathbf{p}$ model (not including spin-orbit). The role of phonons, surface roughness (SR) and remote Coulomb scattering (RCS) has been analyzed as a function of the bias conditions. Comparisons were made with a Kubo Greenwood (KG) solver.

Electron and hole mobilities in FDSOI thin films are plotted in Figs. 1–4, at different back gate (substrate) bias $V_{\rm bg}$. The back gate controls the transition from front to back interface inversion, which helps to disentangle the different scattering mechanisms. We achieve a consistent description of the electron and hole mobilities with front interface SR rms $\Delta = 0.37$ nm, back interface SR rms $\Delta = 0.33$ nm, and density of RCS charges $n_{\rm RCS} = 3.5\times10^{13}$ cm^{-2} at the SiO_2/HfO_2 interface. The SR rms are significantly smaller than in a KG approach. The peak of mobility at $V_{\rm bg} = 8$ V (electrons) and $V_{\rm bg} = -8$ V (holes) coincides with the transition from front to back interface inversion and is strongly limited by carrier-phonon interactions (see Fig. 5). The data point to an enhancement of the electron-phonon and hole-phonon interactions in thin films, which is similar for electrons and holes, and which is usually accounted for by an increase of the acoustic deformation potential (e.g., $D_{\rm ac} = 14.6$ eV for electrons instead of $D_{\rm ac} = 10$ eV in bulk). We are presently investigating this problem from a refined tight-binding perspective to get a better insight into the underlying physics.

Detailed data for the different scattering mechanisms (Fig. 5), for trigate devices (Fig. 6), and comparisons between KG and NEGF will be discussed at the conference. We will also show how NEGF provides valuable information about carrier localization in these devices, which exhibit a rich physics at low temperature.

This work was supported by the French National Research Agency (ANR project Quasanova). The NEGF calculations were run at the TGCC/Curie machine using allocations from PRACE and GENCI.

References

[1] Y. M. Niquet, V. H. Nguyen, F. Triozon, I. Duchemin, O. Nier and D. Rideau, accepted for publication in Journal of Applied Physics, arXiv:1310.1704 [cond-mat.mes-hall].

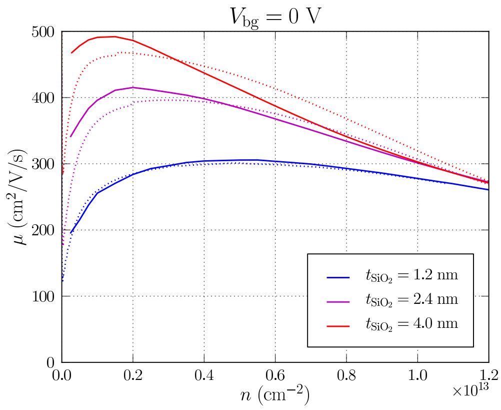

Fig. 1. Experimental (dotted) and 2KP NEGF (solid) electron mobility in 7.5 nm thick FDSOI films as a function of carrier density n. The gate stack is made of an interfacial layer of SiO_2 with thickness t_{SiO_2}, and of a 1.8 nm thick layer of HfO_2. The buried oxide (BOX) is 25 nm thick and the back gate voltage is $V_{bg} = 0$ V. The enhancement of RCS with decreasing t_{SiO_2} reduces the mobility.

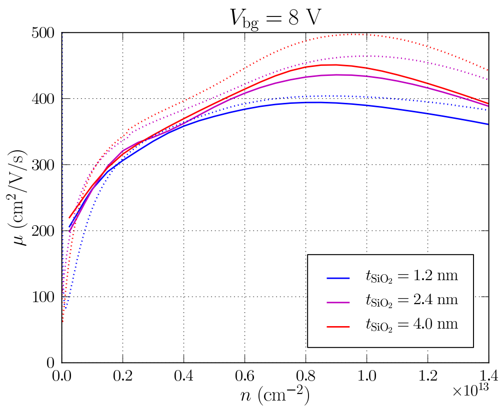

Fig. 2. Same as Fig. 1, but at a back gate voltage is $V_{bg} = 8$ V. There is a transition from back interface inversion at small n to front interface inversion at high n that helps to disentangle the different scattering mechanisms (see Fig. 5).

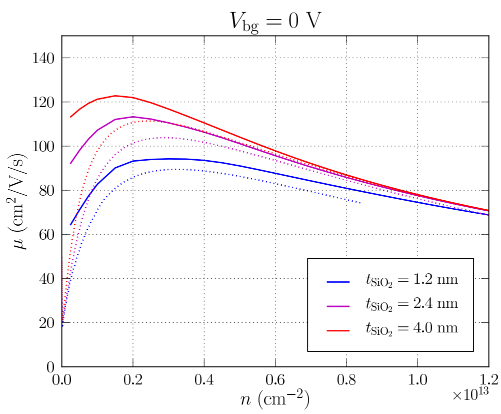

Fig. 3. Same as Fig. 1 for holes ($V_{bg} = 0$ V).

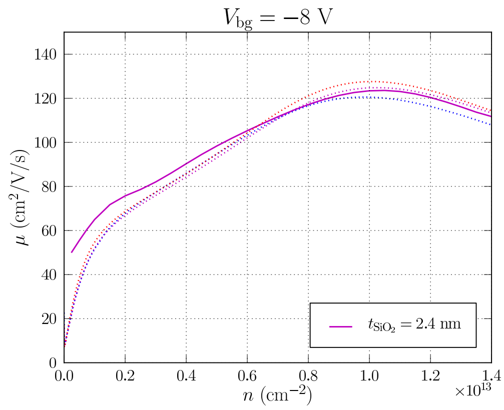

Fig. 4. Same as Fig. 2 for holes ($V_{bg} = -8$ V).

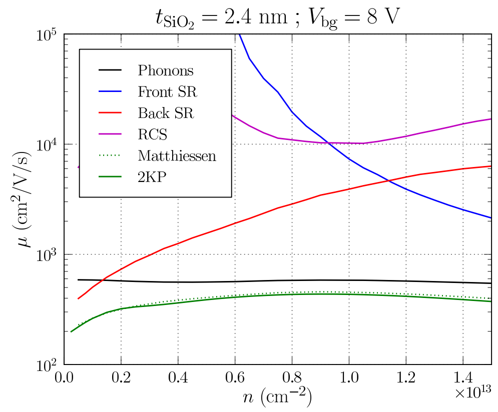

Fig. 5. The different contributions to the electron mobility at $V_{bg} = 8$ V, computed along the lines of Ref. [1]. Matthiessen's rule holds within 5% with that methodology

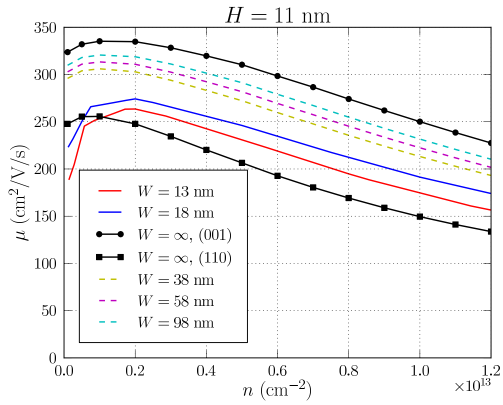

Fig. 6. Electron mobility computed with the EMA in trigate devices with height $H = 11$ nm and various widths W. The mobility in (100) and (110) films (the top and lateral facets of the trigate) is also plotted. Trigates behave like (110) films at small W/H and like (001) films at large W/H.