NEGF Simulations of Scaled Double Gate MOSFETs using extracted masses from DFT calculations

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According to the 2006 update of the ITRS [1] ultrathin-body multi-gate transistors are expected to replace the conventional MOSFETs at 22 nm technology generation and beyond. One of the favoured candidates is the double gate (DG) MOSFET architecture due to its superior transport and electrostatic integrity. The ultimate scaling of the UTB DG MOSFETs beyond the 10 nm channel length mark requires body thickness below 5 nm. At such body thicknesses, the silicon channel losses its translation symmetry in the confinement direction and the reciprocal lattice becomes 2D. Si 2D bandstructure confined in the $\langle 100 \rangle$ direction becomes direct and the longitudinal and transversal masses of Γ, L and X valleys will depend on the channel thickness. Therefore, the predictive modelling of next generation UTB device performance has to take the channel thickness dependence of the bandstructure into account.

In this work, we employ a hierarchical simulation approach to study the impact of the Si-channel thickness dependence on the ultimate scaling of DG MOSFETs to the sub-10 nm channel lengths. First principles Density Functional Theory (DFT) [2] simulations of the confined bandstructure have been carried out for Si slabs with different thicknesses passivated by hydrogen (Fig. 1). The B3LYP DFT crystal orbital method using a 88-31G* basis was used in CRYSTAL03 code [3] yielding a good agreement for the bulk transversal (m_t) and longitudinal (m_l) effective masses. The simulated bandstructures for three different Si channel thicknesses are illustrated in Fig. 2. The variations of electron transversal and longitudinal masses on the thickness (Fig. 3) have been extracted by fitting the E(**k**) dependence of the LUMO state. The variation of confined masses are in good agreement with more scattered results from the DFT method published previously [4].

The extracted thickness dependent masses have been used to calculate the I_D-V_G characteristics of DG MOSFETs with corresponding body thicknesses using a 2D Non-Equilibrium Green's Functions (NEGF) simulator [5,6] in a ballistic regime. In order to illustrate the impact of the thickness dependence of the effective masses, the results were compared with simulations assuming constant bulk effective mass values. The effect associated with the impact of the thickness dependence of the longitudinal and transversal masses on the device characteristic have been studied.

DG MOSFETs with 10, 6 and 4 nm gate lengths having body thicknesses of 6.1, 2.6 and 1.3 nm and oxide thicknesses of 0.6, 0.5 and 0.5 nm, respectively, follow the prescriptions of the ITRS [1]. The simulation domain for a device with the 10 nm gate length is shown in Fig. 4. All transistors have a S/D doping of 2×10^{20} cm^{-3} and an undoped channel. The corresponding 2D potential and electron density distributions in the mid channel plane are shown in Figs. 5 and 6. The simulated I_D-V_G characteristics of the 10 nm DG MOSFET illustrated in Fig. 7 indicate that there is practically no change at V_D=0.8 V when the bulk transversal effective mass is replaced by its confined value but the threshold voltage slightly increases at V_D=0.05 V. Figs. 8 and 9 show I_D-V_G characteristics of the 6 nm gate length transistor with a body thickness of 2.6 and 1.3 nm, respectively. There is a small change of 5 and 10 mV/dec in the subthreshold slope (SS) between the confined and corresponding bulk masses in the 2.6 and 1.3 nm body devices, respectively. The SS change from 88 to 65 mV/dec indicates a better electrostatic control in the thinner channel transistor when the device body narrows from 2.6 nm to 1.3 nm. Fig. 10 shows the I_D-V_G characteristics for the 4 nm gate length device with a 1.3 nm body thickness. The characteristics obtained by using bulk mass have an order of magnitude higher leakage current compared to those obtained by using confined transversal mass. At such channel thickness, the transversal mass increases from its bulk value of 0.19 m_0 to 0.294 m_0 thus reducing the S/D tunnelling. The impact of the confined m_t and m_l in the subthreshold regime can be distinguished in Fig. 11. When only the bulk transversal mass is replaced by its confined value then the SS increases. When, in addition, the bulk longitudinal mass is replaced by its confined value the SS remains unchanged but the threshold voltage decreases. The behaviour of the I_D-V_G characteristics is related to that of transmission coefficients in Fig. 12. Here, a contribution of the first valley only is shown because the second and third valleys are positioned energetically higher (by 0.5 eV) and do not contribute to the transport. At the onset, the transmission obtained using the bulk masses for both m_t and m_l is larger. As energy increases, the transmission obtained using the confined mass for m_t becomes larger, eventually crossing the transmission obtained using the bulk masses only thus exactly mimicking the behaviour observed in the I_D-V_G characteristics of Fig. 11.

In conclusion, the channel thickness dependence of the Si bandstructure starts to affect noticeably the DG MOSFET performance at channel lengths below 6 nm.

References:

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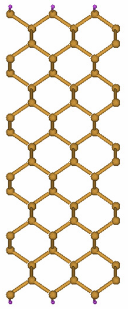

Fig. 1: Atomic structure of a confined Si used in the DFT calculations.

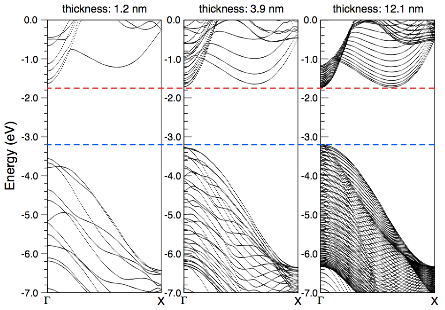

Fig. 2: Bandstructure of the Si slab along the Γ to X direction. The total density has been calculated by 4 **k**-points.

Poster

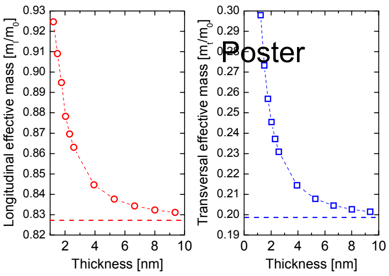

Fig. 3: Longitudinal [m(l)] and transversal [m(t)] electron effective masses versus the slab thickness extracted from calculated bandstructures. The values of extracted bulk masses are indicated by dash lines.

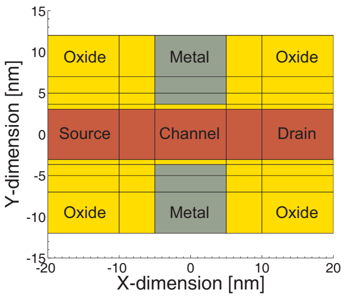

Fig. 4: 2D domain of DG MOSFETs as considered in the NEGF simulator. The source and drain contacts are assumed to be heavily doped to 2×10^{20} cm^{-3}.

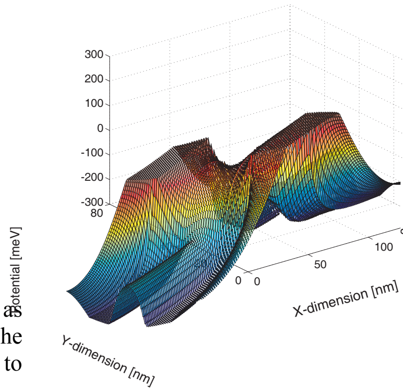

Fig. 5: Potential profile at V_D=0.05 V and V_G=0.2 V in the 10 nm gate length, 6.1 nm thick body DG MOSFET.

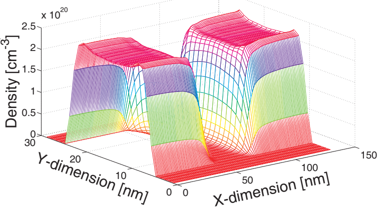

Fig. 6: Electron density at V_D=0.05 V and V_G=0.2 V in the 10 nm gate length, 6.1 nm thick body DG MOSFET.

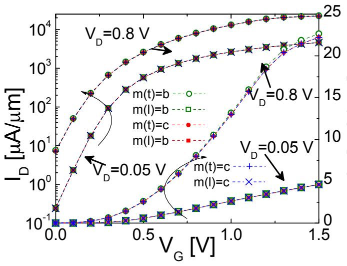

Fig. 7: I_D-V_G characteristics for the 10 nm gate length DG MOSFET obtained from NEGF simulations. The impact of confined (c) masses in transversal [m(t)] and longitudinal [m(l)] transport directions is compared with that of bulk (b) masses.

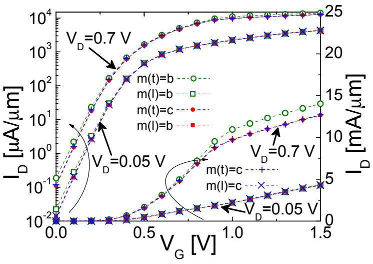

Fig. 8: I_D-V_G characteristics for the 6 nm gate length, 2.6 nm thick body DG MOSFET comparing the effect of confined (c) and bulk (b) Si masses in transversal [m(t)] and longitudinal [m(l)] transport directions.

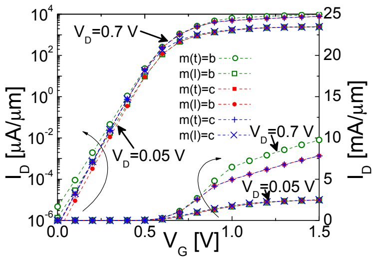

Fig. 9: I_D-V_G characteristics for the 6 nm gate length, 1.3 nm thick body DG MOSFET comparing the effect of confined (c) and bulk (b) Si masses.

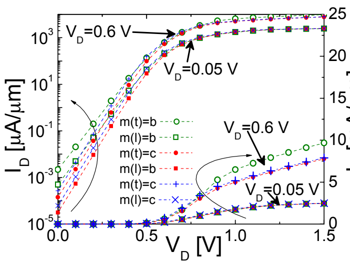

Fig. 10: I_D-V_G characteristics for the 4 nm gate length, 1.3 nm thick body DG MOSFET comparing the effect of confined (c) and bulk (b) Si masses.

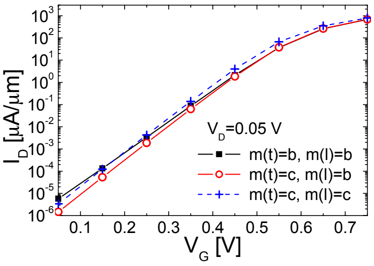

Fig. 11: The detail of I_D-V_G characteristics for the 6 nm gate length, 1.3 nm body DG MOSFET. The effect of systematically replacing bulk values of m(t) and m(l) with their confined values is demonstrated.

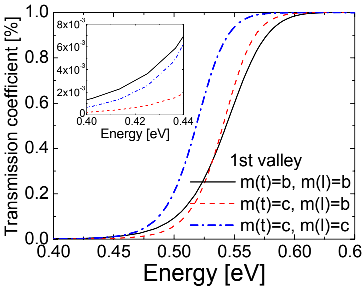

Fig. 12: Transmission coefficients as a function of energy at V_G=0.15 V and V_D=0.05 V in the 6 nm gate length, 1.3 nm thick body DG MOSFET. The inset shows the detailed onset of the transmission.