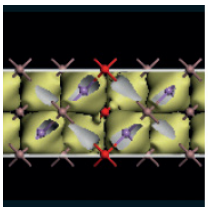

First-principles based simulations of si ultra-thin-body FETs with SiO_2 gate dielectric

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In ultra-thin-body (UTB) field effect transistors (FETs), the gate dielectric layer not only functions as a medium to deliver gate electric fields to the channel region but also gives significant influences on channel electrons. The band-offset between channel and dielectric materials affects the quantum confinement energy levels in the channel, and the charge distributions at the channel and dielectric interface may screen the gate electric fields considerably. However, in the empirical tight-binding method which is a state-of-the-art method to treat UTB FETs at the atomistic level, channel atoms are usually passivated by hydrogen atoms, thus enforcing the hard-wall boundary condition, and oxide atoms are virtual atoms that merely fill up the gate dielectric region. To address the above effects of the gate dielectric in UTB FETs, a first-principles based approach that treats the oxide atoms on an equal footing with the channel atoms is therefore called for.

In this work, we have developed a first-principles, density functional theory (DFT) based non-equilibrium Green's function (NEGF) code to simulate Si UTB FETs, fully taking into account all the real SiO_2 atoms in the gate dielectric.

The schematic structure of the double-gate Si UTB FET that we simulate in this work is shown in Fig. 1. Simulations were done in the following three steps: In the first step, to realize the double gate structure at the atomistic level, SiO_2/Si/SiO_2 unit cell was taken as shown in Fig. 3. Its atomic and electronic structure was obtained by using the openMX DFT package with GGA-PBE functional and a *s2p2d2* atomic orbitals basis set (18 orbitals per atom) for both Si and O atoms. For SiO_2, crystalline β-cristobalite and α-quartz phases were realized, and the bridge-oxygen model was adopted at the Si/SiO_2 interface. After full relaxation, the DFT Hamiltonian (H) and overlap (s) matrices of the unit cell were extracted.

In the second step, imported H and s matrices were reduced in size to greatly alleviate the computational burden but without loss of accuracy [1]. This is a crucial enabling step that makes the calculations possible. Stemmed from the periodic boundary condition along the width (y) of the UTB device, 40 k_y values uniformly distributed in the Brillouin zone were used in our calculations, and $H(k_y)$ and $s(k_y)$ for each k_y were constructed and transformed. For the unit cell having a-quartz for the dielectric (Fig. 3(c)), the full Hamiltonian is reduced to around 60 x 60 from its original size of 3240 x 3240, but the band structure is accurately reproduced as seen in Fig. 4.

In the third step, the Hamiltonian matrices and atom coordinates were imported into our in- house NEGF transport simulator. All the Si and O atoms were involved in the charge density and electrostatic potential calculations. After convergence of NEGF and Poisson self- consistent calculations, ballistic current was calculated.

Fig. 5 shows the calculated current-voltage characteristics of the double-gate, n-type Si UTB FET of Fig.1. The device with gate dielectric of β-cristobalite SiO_2 and that of α-quartz SiO_2 are compared to the device with simple H-passivated Si surfaces and virtual atoms. Our calculations show that the H-passivation results in overestimation of on-state current by 13 % and 33 %, compared to when the β-cristobalite and α-quartz gate dielectrics, respectively, are put into place. The differences in the band structures and local density of states of the three cases as shown in Fig. 4 can account for the difference in the currents, as the group of subbands indicated by the arrow in the figure is lowered in energy for β-cristobalite and α- quartz SiO_2, increasing the density of states and hence lowering the Fermi energy.

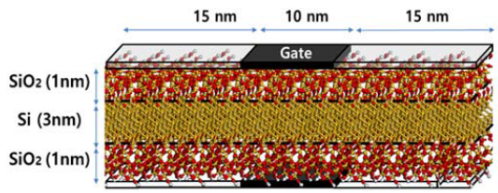

Fig.1 Schematic structure of double-gate Si UTB FET with SiO2 gate dielectric used in the device simulation. The Si channel of 3 nm thickness is confined in the [001] direction and transport along the [110] direction. The source/drain extensions are 15 nm long with the doping density of 10^{20} cm^{-3} and the channel region is intrinsically doped.

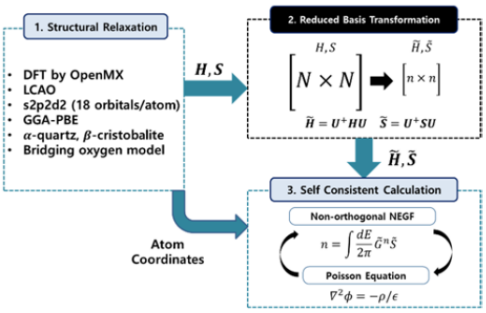

Fig.2 The simulations steps. From the fully relaxed structure, Hamiltonian (H and S) is extracted and fed to the NEGF-Poisson self-consistent routines to compute the drain current. A reduced basis transformation is performed for H and S for efficient calculations but without loss of accuracy.

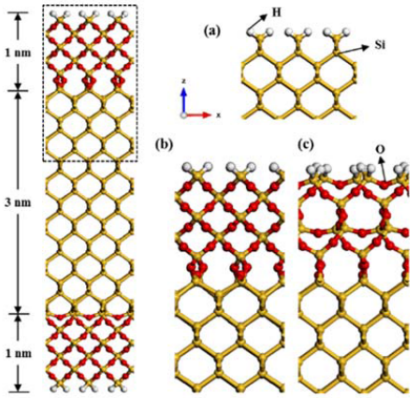

Fig. 3 Atomic models of SiO_2/Si/SiO_2 super cell used in the DFT relaxation. The 3 nm thick Si region consists of 23 atomic layers grown in the [001] direction, with which 1 nm thick crystalline SiO_2 of (b) β-cristobalite or (c) α-quartz phase is interfaced. The periodic boundary conditions are imposed in the x and y directions while vacuum layers with sufficient thickness are included in the z direction for the supercell calculation. Hydrogen passivated surfaces are shown in (a).

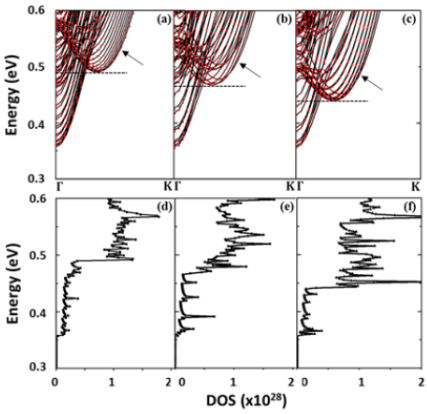

Fig. 4 The conduction band structures of the SiO_2/Si/SiO_2 unit cells shown in Fig. 3 along the Γ to K direction, with (a) H passivated surface, (b) β-cristobalite SiO_2, and (c) α-quartz SiO_2. Solid lines and dots represent the bands calculated by the original DFT and reduced-sized Hamiltonians, respectively. The conduction band edges are aligned for a comparison purpose. (d), (e), and (f) are the local density of states corresponding to (a), (b), and (c), respectively.

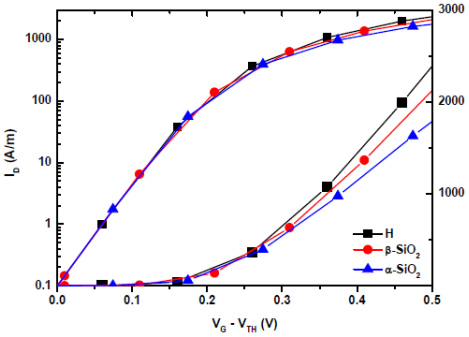

Fig. 5 The calculated current-voltage characteristics of the double-gate, n-type Si UTB FET of Fig.1. The devices with H-passivated surface, β-cristobalite SiO_2, and α-quartz SiO_2 are compared. The drain voltage of 0.5 V is applied and the off-current is set to 0.1 μA/μm.

[1] M. Shin, W. J. Jeong, and J. Lee, J. Appl. Phys., vol. 119, no. 15, 154505, 2016.