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Impact of crystal structure of hafnia on the transport properties of model HfO2-Si-HfO2 NSOI-FET: DFT + scattering theory approach

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【序】

We performed calculations of carrier transport in nanometer-thin atomistic Si-on-insulator (NSOI) FET models [1]. We studied the impact of different polymorphs of hafnia [2], considered the best high-*k* dielectric able to replace silica in Integrated Circuit building, on these transport properties. In particular, combining DFT and scattering theory, we have focused on the role that stress plays on the presence or not of interface states in the Si bandgap.

【実験】

We used DFT for atomic relaxation and electronic structure calculation (Generalized Gradient and Local Density Approximations) as implemented in VASP Package. Core electrons are replaced by ultra-soft pseudopotentials (USPP). Ceperley Alder exchange-correlation potential was used within LDA, while Perdew-Wang 91 was used within the GGA. The PW basis set was truncated at 396 eV and 700 eV for augmentation charge cutoff. A 4x1x4 Monkhorst-Pack *k*-point grid was used to relax our initial interface structures until the maximum force was lower than 0.05 eV/Å.

Si experimental cubic unit cell vectors (a = 3.8403 Å) has been adopted as the in-plane fixed lattice parameters for interface building. Such choice stems from the fact that since HfO_2 is deposited on top of Si it is expected that at least the first few monolayers of the oxide should adjust the Si unit cell. Moreover, keeping fixed the Si lattice vectors we can compare transport in the presence of different interfaces without the need to account for the complex relation between conductance and bulk strain in the channel.

NSOI models were built as symmetric HfO_2/Si/HfO_2 structures (Fig. 1) made of 37 atoms in both tetragonal and anatase cases. A vacuum gap (~30 Å) separates the structures from their periodic images along the normal to the interfaces. In order to calculate the electronic current through the device the unit cell was multiplied by eight along the transport direction, resulting in structures containing 296 atoms.

【結果と考察】

We have found that while the tetragonal polymorph creates scattering states,

mostly near the Si band valence band edge, through the presence of stretched Si-Si bonds at the interface, the anatase polymorph, being a better lattice match to Si, does not create interface states in the Si band gap. As result electron transport is more efficient for Si in contact with *a*-HfO_2 than in contact with *t*-HfO_2. For holes, transport is slightly more efficient for Si in contact with *t*-HfO_2. However, the ohmic hole transport characteristics found for the Si/*t*-HfO_2 interface suggests lower hole current at higher source-drain bias than in Si/*a*-HfO_2. We have also found that interface states can be harmful in two ways: by creating a possible source-drain leakage path in the sub-threshold region, thus lowering the on/off current ratio, and by degrading mobility in the channel.

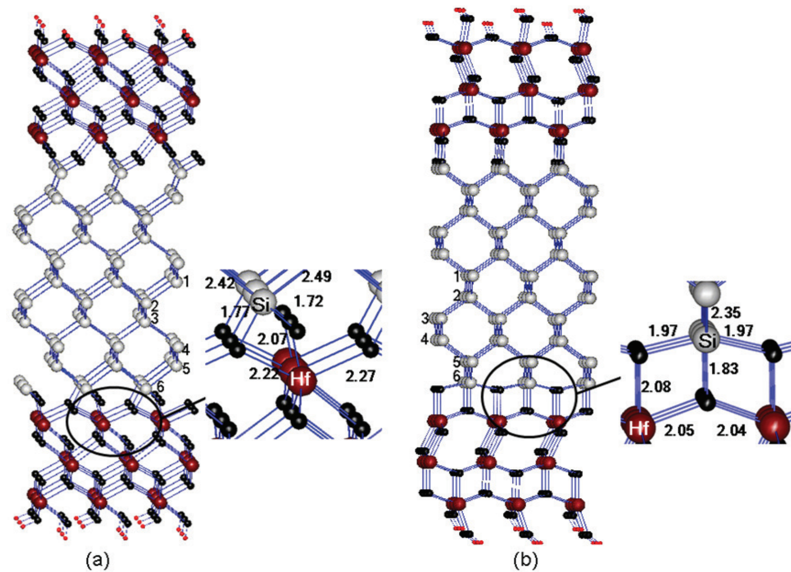

Fig.1

Bibliography

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