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STRESS AND STRAIN in Si/HfO_2 INTERFACES

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INTRODUCTION

Scaling electronic devices nowadays is one of the most active research areas in microelectronics. Transistor performance has to be maintained with scaling of its lateral dimensions to smaller size, thus imposing the SiO_2 gate oxide thickness to be reduced proportionally. The growing tunneling current limits SiO_2 gate oxide shrinking to about 1 nm. To retain the current progress of CMOS technology, SiO_2 has to be replaced by another material with higher dielectric constant. Recent analysis has revealed hafnium oxide (HfO_2) as one of the most promising candidates, but interface defects and mobility degradation remain the challenges to overcome. In our atomistic DFT study we designed of HfO_2/Si interfaces for a comparative study Si/SiO_2 systems in order to reveal the important trends in stress and strain and their relation to the electric properties. We use comparative thermodynamic analysis in order to estimate the local stress at the interface and to estimate its components, chemical (intermediate oxidation state) and local mechanical (bond deviation from their optimal values) and polarization. In particular, we have built up and optimized three interfaces Si-HfO_2, consisting of 100, 116, and 120 atoms (see Fig 1a-1c).

COMPUTATIONAL DETAILS

All calculations have been performed using DFT methods implemented in SIESTA [1] and VASP [2] program, which have numerical atomic orbitals and plane wave basis sets, respectively. Both GGA [3] and LDA [4] level of theory have been employed in our calculations; in particular, in SIESTA calculations, PBE (Perdew-Burke-Ernzerhof) [1] XC functional has been employed at GGA level of theory calculations, while CA (Ceperley-Alder) [1] functional has been employed at LDA level of theory. LDA/CA and GGA/PW91 (Perdew-Wang91) [2] calculations have been performed with VASP package.

RESULTS

Our analysis on the three optimized interfaces reveals a high amount of the stress energy, i.e. the extra energy associated to the difference between the energies of the supercells and those of their components (Si, HfO_2, and SiO_2) as described in [5]. In particular, as reference systems we have chosen the 8-atom unit cell for Si, the 12-atom unit cell (4 Hf and 8 O atoms) for monoclinic hafnia (m-{HfO_2}). As the reference system for SiO_2, α-quartz unit cell structure has been chosen for calculations using NAO/GGA/PBE, NAO/LDA/CA, and PW/LDA/CA approaches. First, we have calculated the stress energy deriving from each component (Si and HfO2) to the three Supercells taking into account the starting structures from which the Supercells have been built up; we have let the two subcells, Si and HfO_2, relax keeping fixed the lateral dimensions. To evaluate the components of the stress we used bulk Modulus (K) and its first derivative (K'=

∂K/∂P) calculated from the Birch-Murnaghan's formula at both PW/GGA/PW91 and PW/LDA/CA level of theory. We also estimated the stress components by comparing energies of relaxed and constrained HfO_2 and Si cells implying the lateral parameters of HfO_2/Si supercell to the separate HfO_2 and Si units.

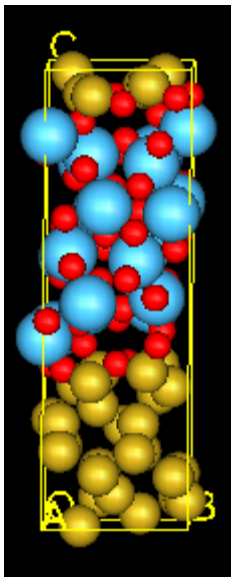

Fig. 1a

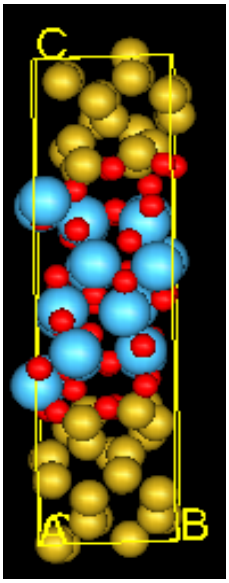

Fig. 1b

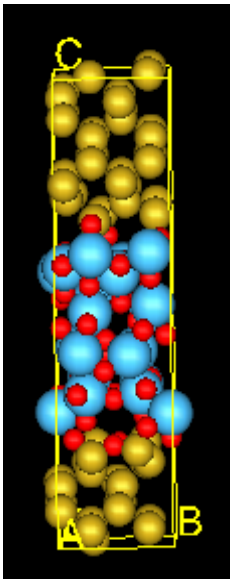

Fig. 1c

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