DEFECT PROPERTIES AT THE HfO_2/SiO_2 INTERFACE FROM AB INITIO CALCULATIONS

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Due to the continuous decrease in feature size, silicon devices are approaching a number of fundamental limits. In particular, the gate oxide in modern integrated circuits has reached atomic dimensions. The use of a different gate oxide with higher dielectric constant could permit similar transistor performance with drastically reduced leakage currents due to the greater physical thickness of the gate dielectric. HfO_2 and its alloys with SiO_2 are most likely potential candidates for replacing SiO_2 as the gate dielectric[2]. The interface between this oxide and the silicon channel usually includes a very thin SiO_2 layer. Segregation of HfO_2 nano-particles inside the $HfSiO_x$ matrix is commonly observed experimentally. Defects at the HfO_2/SiO_2 interface are thought to be responsible for leakage current, breakdown and degradation of micro-electronic devices. Therefore, determining the structure of the HfO_2/SiO_2 interface and characterization of different types of defects induced by the growth and post-deposition annealing of these systems, as well as positioning of the defect energy levels with respect to the silicon band gap are of considerable interest.

In this work, an embedded cluster methodology developed by our group[3,4] for the study of defects in SiO_2 has been extended to treat point defects at the HfO_2/SiO_2 interfaces. In this model, the whole system is divided in three regions. First is a quantum mechanical region, in which the atoms are treated using an ab initio quantum mechanical method. This region is surrounded by a interface region, which provides smooth connection to the rest of the system treated classically. The main challenges of this work have been the ternary character of the compound and its heterogenious structure. We have developed a robust set of consistent classical inter-atomic potentials, which accurately reproduce the geometry and the main mechanical and dielectric properties of the different phases of HfO_2 and of $HfSiO_4$ as well as their phonon spectra. The main advantages of the new potentials are that they correctly reproduce the relation between the three phases of HfO_2 and predict correct dielectric constants of the three compounds. These potentials were used for building different models of HfO_2/SiO_2 interfaces and for embedded cluster calculations using the GUESS code[3,4]. We have also developed embedding potentials which provide a smooth transitions between the quantum and classical regions. The quantum mechanical calculations were carried out using the B3LYP density functional. They correctly reproduce the band gap of the bulk material and the properties of oxygen vacancies in different charge states. A distribution of defect levels arising from oxygen vacancies has also been characterized using this approach. We have calculated the properties of oxygen vacancies at the HfO_2/SiO_2 interface and characterised their structure and spectroscopic properties.

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