Student Paper

First-Principle Study of Silicon Vacancies near 4H-Silicon Carbide/Silicon Dioxide Interface

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In this work, we model an ideal 4H-Silicon Carbide (SiC)/Silicon dioxide (4H-SiC/SiO2) interface using Density Functional Theory (DFT)-based molecular dynamics. We then simulate the effect of Si vacancies present in Silicon Carbide side of the 4H-SiC/SiO2 interface on the electronic bandgap of SiC. While previous calculations have investigated Si vacancies in bulk SiC, our simulations look at those present a few monolayers below the interface [1].

Silicon Carbide is an indispensable material for present and future high-power and high-temperature electronics. Various factors that make it attractive include its wide bandgap, ability to grow a native oxide (SiO_2) using well-established thermal oxidation and high thermal conductivity. However, the mobility of electrons at 4H-SiC/SiO_2 interface, as in a MOSFET, is exceptionally poor. This is mainly attributed to the high density of interface traps arising from the oxidation process. These traps not only reduce the number of available carriers for conduction, but also act as Coulomb scattering centers thereby degrading channel mobility.

In the past, theoretical and experimental investigations have been carried out to identify the atomic make-up of 4H-SiC/SiO2 interface defects. While the true nature of these traps still remains a subject of considerable debate and investigation, near-interface Silicon vacancy in SiC side of the interface has emerged as a candidate defect due to the recent Electrically Detected Magnetic Resonance (EDMR)-based spectroscopic measurements [2]. The effect of such Si vacancies on the interfacial electronic structure of SiC is explored in this is paper using Density Functional Theory (DFT), as implemented in the software Quantum Espresso [3].

Interface Model Generation: The model for an ideal 4H-SiC/SiO2 interface is generated using DFT-based quantum molecular dynamics (QMD) and geometry optimization. In order to create an amorphous SiO2 structure, a supercell of crystalline α-quartz containing 36 atoms is heated to 4000K. The molten SiO2 is then rapidly quenched to 300K through 3000K, 2000K and 1000K. At each temperature, the system was allowed to evolve for 1ps according to plane-wave DFT-based molecular dynamics. The time step used in molecular dynamics was 1fs. The cutoff energy of plane-waves used in the DFT calculation was 820 eV. Brilliouin zone sampling was done at the Gamma point. The core electrons were represented using norm-conserving pseudopotentials. The DFT calculations were performed under the Generalised Gradient Approximation (GGA) using exchange-correlation given by PBE (Perdew-Burke-Ernzerhof) scheme. It should be noted that QMD simulations are computationally demanding and are performed for only 5ps.

The SiO2 structure generated above is then placed carefully over a 72 atom SiC unit cell, whose crystal properties were obtained from literature [4]. Density functional geometry optimization was performed on the combined system until the force acting on each atom was less than 0.05eV/A. At the end of the simulation, we obtained an ideal 4H-SiC/SiO2 interface devoid of any dangling bond as shown in Figure 1(a). The bonding properties of amorphous SiO2, given in Table 1, are in close agreement with similar interface obtained previously [5]. The Density of States (DOS) of the interface structure, calculated using DFT, is shown in Figure 1(b). The surface dangling bonds were terminated using Hydrogen atoms. A clean bandgap can be observed even though it is underestimated, a well-known problem of using DFT.

Investigation of Silicon vacancies: Neutral Silicon vacancies were then introduced into the ideal interface at two non-equivalent Si sites, labeled *h* and *k*. Geometry optimization was then performed on these structures to obtain relaxed configurations as shown in Figure 2. The DOS for interface containing Si vacancy was calculated using DFT (Figure 3). Both the Si vacancies can be seen to introduce new states in the SiC bandgap.

In conclusion, we modeled an ideal, structurally relaxed 4H-SiC/SiO2 interface using quantum molecular dynamics. We found that the results gave rise to Si-O-Si and O-Si-O bond angles that differ from the ideal α-quartz crystal, indicating amorphous oxide. The DOS of the ideal interface was extracted using density functional calculations. We then introduced neutral near-interface Si vacancies at various sites on SiC side of the interface to identify their effects on the interfacial DOS. We observed that new states are introduced in the SiC bandgap as a result of these defects.

References

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TABLE 1: Comparison of bond angle and bond length distribution of amorphous SiO2 and α-quartz

Property	Mean	Std.dev	α-quartz
Si-O-Si angle	135.39 °	13 °	144 °
O-Si-O angle	108.72 °	5.85 °	109.5 °
Si-O bond length	1.66 A	0.03 A	1.66 A

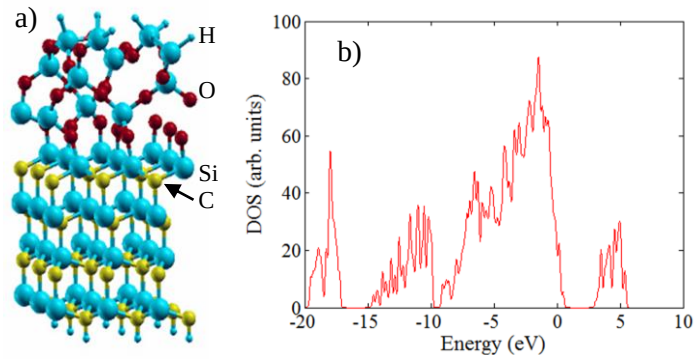

Figure 1: a) The abrupt interface and b) its density of states.

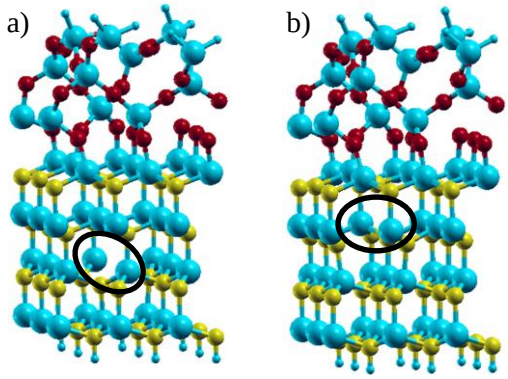

Figure 2: Si vacancy at, a) *h*-center and b) *k*-center. Vacancy is circled.

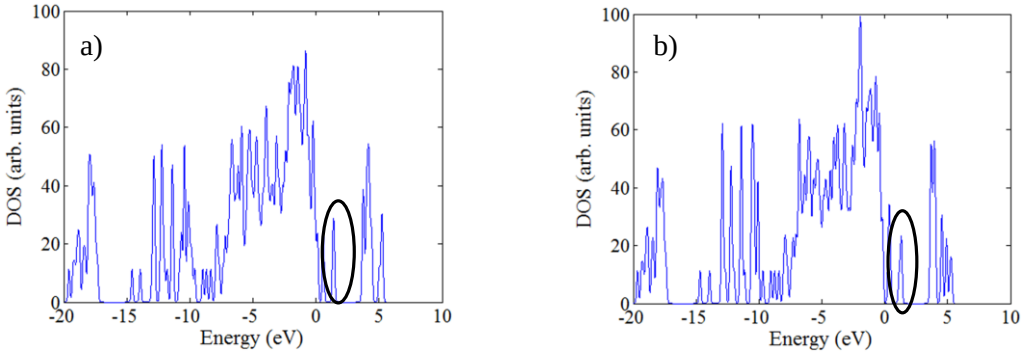

Figure 3: Interfacial DOS for Si vacancy at, a) *h*-center, b) *k*-center. New states are circled