

# Density Functional and Monte Carlo-Based Electron Transport Simulation in 4H-SiC(0001)/SiO<sub>2</sub> DMOSFET Transition Region

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**Abstract**— The potential presence of a transition layer at the SiC/SiO<sub>2</sub> interface may affect the electronic characteristics of SiC devices. Several experiments indicate the presence of C-O-Si bridges [1-3] at the interface. We investigated and compared the effect of possible interface structures on the total, and projected density, of states of the SiC/SiO<sub>2</sub> system with the use of density functional theory (DFT). We also utilized the Monte Carlo carrier transport modeling technique to obtain the average velocities and mobilities of each structure. The ionized impurity limited mobility of likely structures has been calculated. We constructed various structures with the forms of SiO<sub>x</sub>C<sub>y</sub>, and Si<sub>1-x</sub>C<sub>x</sub>O<sub>2</sub> in both SiC, and SiO<sub>2</sub> sides of the interface. According to our calculations, strong possible candidates for generating the traps near the conduction band are SiO<sub>x</sub>C<sub>y</sub> structures formed by replacing carbon atoms in SiC with oxygen. The overall mobility, and the ionized impurity limited mobility decrease as the number of O(C) in the SiC side of the SiO<sub>x</sub>C<sub>y</sub> structures increase. Moreover, the calculated ionized impurity limited mobility is less than 30 cm<sup>2</sup>/Vs in low external field.

**Keywords**— SiC/SiO<sub>2</sub> interface, Monte Carlo transport, density of states (DOS), density functional theory (DFT), mobility

## I. INTRODUCTION

As a result of its large bandgap and thermal conductivity, Silicon Carbide (SiC) has promising potential in high power, high temperature electronics. SiC based devices are expected to have fast switching speed and low energy loss at elevated temperatures. In addition, the advantage of having SiO<sub>2</sub> as its native oxide allows the fabrication of SiC-based MOSFET devices. However, the potential of SiC is hindered by the low electron mobility in the MOSFET inversion layer [4, 5]. One possible cause of the problem is the large density of interface trap states at the SiC/SiO<sub>2</sub> interface [6, 7].

High trap density near the conduction band has been attributed to either the defects at the interface or a transition layer in SiC/SiO<sub>2</sub> system. During the oxidation process, a layer of SiO<sub>2</sub> grows naturally on the surface of SiC. The resulting interface of the SiC/SiO<sub>2</sub> system may not be chemically abrupt, and the presence of a transition layer has been reported by various investigators [1-3, 8]. The transition layer is likely to be a ternary phase, called silicon oxycarbide with C-O-Si bridges which were primarily observed using Fourier transform infrared spectroscopy [4]. C-O-Si bridges are either formed by substituting oxygen for carbon in SiC [9, 10, 11], and/or carbon for oxygen in SiO<sub>2</sub> [9, 11]. In both cases a

layer of SiO<sub>x</sub>C<sub>y</sub> is formed. Also, a layer of Si<sub>1-x</sub>C<sub>x</sub>O<sub>2</sub> may be formed by replacing silicon atoms with carbon in the oxide side [9].

In this paper, we constructed the most likely structures for the transition layer; then we calculated the energy, and total (and projected) density of states (p(DOS)) with density functional theory simulator [12] to compare the electronic properties. The projected density of states is the density of states due to small group of atoms in the material. We also retrieved the bandgap of each structure with hybrid functionals. To obtain the electron-phonon limited bulk mobilities, the calculated density of states is imported into a Monte Carlo transport simulator [13]. The effect of Coulomb scattering is investigated by studying the impact of high concentrations of ionized impurities on the calculated mobilities in the presence of a low electric field.

## II. METHODOLOGY

### A. Density Functional Theory (DFT) Calculations

Total and projected densities of state ((p)DOS) curves are obtained via density functional theory (DFT) calculation. These simulations are based on the approximate many body solution of the Schrodinger equation. To perform the DFT calculations for the interface region, we create a large unit cell or supercell shown in Figure 1. The super cell is an abrupt structure of SiC/SiO<sub>2</sub>, formed by putting a 37-atom structure of oxide on a 72-atom structure of 4H(0001)-SiC. In the abrupt structure, all Si atoms on the surface of the bulk SiC are terminated with oxygen atoms and there are no dangling bonds between bulk SiC and SiO<sub>2</sub>. Layers of vacuum have been placed on the top and bottom of the structure to isolate it in the vertical direction. The dangling bonds at the top and bottom of the structures are terminated with hydrogen. The DFT based geometry optimization is performed within the plane-wave basis set until the maximum force becomes smaller than 0.1eV/Angstrom. The relaxation avoids energy levels that might emerge due to the stress on the individual atoms in the system. The cut off energy of the plane wave is set to be 952eV. A DFT solver called Quantum Espresso [12] is used to perform relaxation, band-structure and DOS calculations of the SiC/SiO<sub>2</sub> interface structures. The bandgap of each structure was retrieved in two steps: first the geometry optimization and energy calculations were carried out within the Generalized Gradient Approximation (GGA) framework [13]; then a hybrid functional is used to calculate the exact bandgap of the

structures [14]; the DOS of each super cell is corrected accordingly. With the use of the hybrid functional, the band gap obtained for the original abrupt structure of SiC/SiO<sub>2</sub> is almost 3.2 eV.

### B. Monte Carlo Transport

Monte Carlo methodology is used to obtain the electron transport characteristics in 4H-SiC/SiO<sub>2</sub> interface structures. We developed a Monte Carlo simulator [15] and adapted it to employ the density of states curves extracted from DFT as the input. The Monte Carlo simulator was then used to calculate the electron scattering rates, average velocity, and mobility. In general, the Monte Carlo method is a semi-classical technique, which simulates electrons as classical particles undergoing scattering events separated by drifts in an electric field. Carrier scattering from phonons and the imperfections in the semiconductor periodic lattice, such as impurities, are considered quantum mechanically. The durations of the carrier free flights between two successive collisions and the scattering events involved in the simulation are selected stochastically in accordance with some given probabilities describing the process. Fermi's Golden rule and deformation potential approximation are used for electron-phonon scattering rates for acoustic, optical and polar optical phonons. To calculate the impurity scattering rate, we employed the Brooks-Herring formula. The details are given in [15]. Electrons interact with the crystal through a variety of scattering processes which relax the energy and momentum of the particle. The transition rate from an initial state to a final state is given by Fermi's Golden rule.

### C. DFT and DFT-Based Monte Carlo Calculations

To investigate the physical origins of traps at the SiC/SiO<sub>2</sub> interface, and to examine the effects of different interface configurations on electron mobilities, we used the vast data which are extracted from DFT calculations along with our Monte Carlo transport simulations. DFT results of possible silicon--oxycarbide bridges and substitutions provide the impact of each type of transition structure on the energy band-

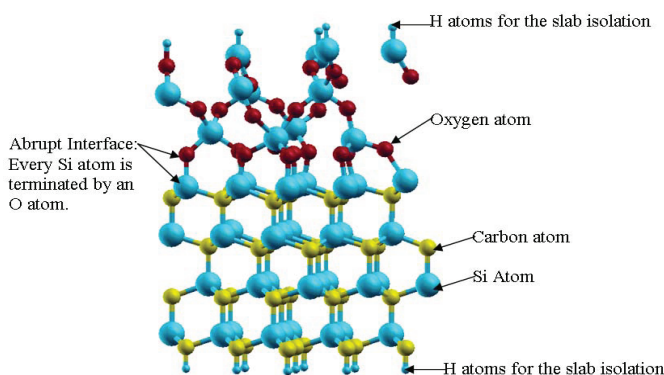


Fig. 1. Atomic configuration of 4H(0001)SiC-SiO<sub>2</sub> structure

structure, total, and projected densities of states. This information is then input into the Monte Carlo simulator, which then uses it to help calculate bulk and ionized impurity limited electron mobilities to shed further light to the properties of the proposed structures.

## III. RESULTS AND DISCUSSIONS

### A. SiO<sub>x</sub>C<sub>y</sub> in SiO<sub>2</sub>

As a first step to investigating possible transition layer morphology, oxygen atoms in SiO<sub>2</sub> are substituted by carbon atoms with several concentrations to make the SiO<sub>x</sub>C<sub>y</sub> structures in the oxide side. To investigate the impact of these substitutions, we compared the total, and projected density of states (pDOS) of C-Si-O bridges in the abrupt structure with the C-Si-C ones that have been created by substituting oxygen for carbon to create the SiO<sub>x</sub>C<sub>y</sub> structures as in Figure 2. Although, these replacements make levels in midgap, they increase the number of states at energy levels that are within the conduction bands as well. (Comment on notation: In the figure, we represent carbon substituted for oxygen as C(O)).

We then simulated the average velocity and mobility of each of those SiO<sub>x</sub>C<sub>y</sub> structures, made in the oxide side, as a function of external electric field using Monte Carlo simulation. There are two inputs to the MC simulator. The first is the volume of the unit/super cell to calculate DOS per volume, and the second is the DFT-DOS curve or values starting from the conduction band edge of a given structure. The calculated electron mobilities are compared with those of bulk SiC. Figure 3 shows the mobility versus field for SiO<sub>x</sub>C<sub>y</sub> structures with one, three, and six C atoms substituted O atoms. The mobility at the electric value of 10000 V/cm has values of 700 cm<sup>2</sup>/s for bulk SiC, 214 cm<sup>2</sup>/Vs for one C(O), and 200 cm<sup>2</sup>/Vs, and 150 cm<sup>2</sup>/Vs for three, and five C(O), respectively. The decrease in mobility may be the result of excessive states in conduction band.

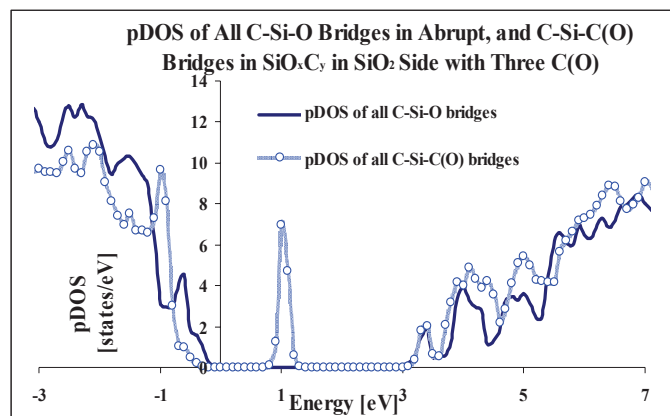


Fig. 2. Comparison between all the C-Si-C(O) bridges in SiO<sub>x</sub>C<sub>y</sub> formed in the oxide side with three C(O) and all C-Si-O bridges in the abrupt structure.

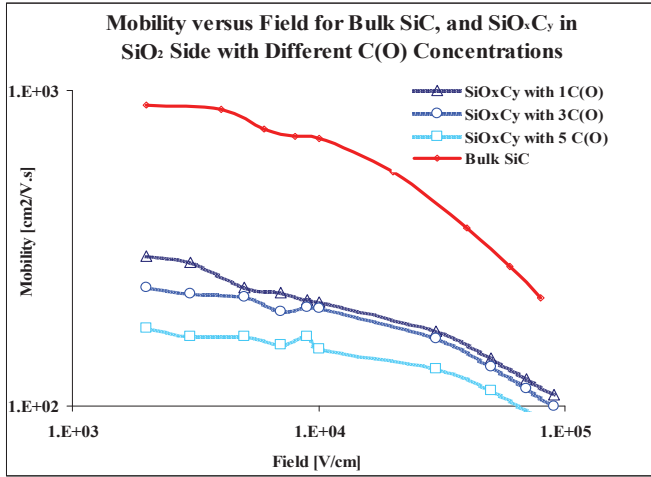


Fig. 3. Electron-phonon limited bulk mobility for bulk SiC, and SiO<sub>x</sub>C<sub>y</sub> structures with various concentrations of C(O) in the oxide side.

### B. SiO<sub>x</sub>C<sub>y</sub> in SiC

Next, defect transition structures are formed by substituting the carbon atoms with oxygen atoms to make the SiO<sub>x</sub>C<sub>y</sub> in SiC side of the interface with different concentrations. This substitution is one of the potential mechanisms behind SiC oxidation [16]. According to our DFT calculation, an O atom replacing a C atom makes an O-V<sub>C</sub> (carbon-vacancy) complex, which pushes the neighboring Si atoms away from O. This kind of substitution in SiC leads to formation of a thin oxygen contaminated Si-rich interface layer which needs a very small structural reconstruction to form SiO<sub>2</sub>. Since the formation energy of the C vacancy is less than Si vacancy [16], and the Si-C bonds are smaller than the Si-Si bonds in Si crystals, the C vacancy is the likely to be the preferred host for an O atom. Furthermore, several experiments indicated the evidence of oxide formation over this type of SiO<sub>x</sub>C<sub>y</sub> structure [2, 10, 17].

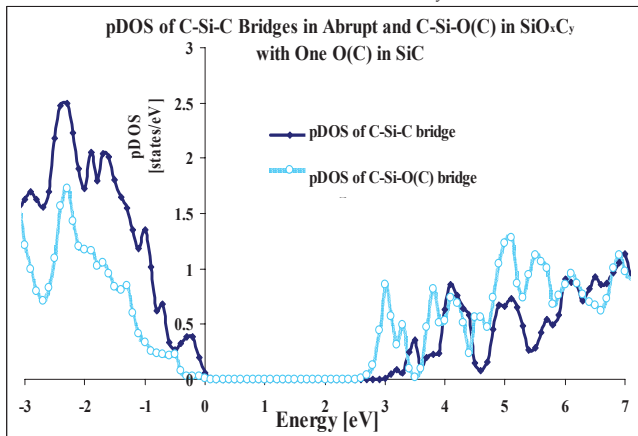


Fig. 4. Comparison between pDOS of C-Si-C, and O-Si-C bridges in abrupt, and SiO<sub>x</sub>C<sub>y</sub> structure with one O(C) in SiC side.

The comparison between C-Si-C bridges in abrupt and O(C)-Si-C bridges in SiO<sub>x</sub>C<sub>y</sub> structures shows that substitution of oxygen for carbon in SiC makes levels near the conduction band. We believe that the conduction band tail of this layer appears in the upper part of the SiC gap as a near-interface state density. Figure 4 shows the contribution of C-Si-C, and O-Si-C bridges in abrupt, and SiO<sub>x</sub>C<sub>y</sub> structures with one O(C) atoms.

We used the Monte Carlo simulator to investigate the effect of SiO<sub>x</sub>C<sub>y</sub> structures in the SiC side on the mobility. As it is seen in figure 5, the mobility at 10000 V/cm field drops from 700 cm<sup>2</sup>/V.s for bulk SiC to 338 cm<sup>2</sup>/V.s for two O(C), and to 280 cm<sup>2</sup>/V.s, and 186, and 143 cm<sup>2</sup>/V.s for three, six, and nine O(C), respectively. Again, the mobility drop may be attributed to the more states in conduction band.

In modern SiC MOSFETs, the peak field effect mobilities (generally measured in the linear region, using drain current versus drain voltage curves when gate-to-source voltage is roughly equal to V<sub>th</sub>) are usually less than 50 cm<sup>2</sup>/Vs. This is thought to be due to Coulomb scattering from trapped interface charges [18, 19]. To examine the effects of different amounts of interface traps on the transport calculations, we calculated the low field mobility as a function of different levels of ionized impurity concentration. The results plotted in Figure 6 show that mobilities are in lower double digits as ionized impurity concentration approaches 10<sup>20</sup> cm<sup>-3</sup>. Assuming a transition region thickness of 1nm, the above-mentioned ionized impurity concentration can be translated into an aerial concentration of 10<sup>13</sup> cm<sup>-2</sup>, which is consistent with total acceptor type trap levels measured for SiC/SiO<sub>2</sub> interfaces [15, 16]. The mobility drops from 28 cm<sup>2</sup>/Vs for the SiO<sub>x</sub>C<sub>y</sub> structure with two O(C) to 25 cm<sup>2</sup>/Vs, and 10 cm<sup>2</sup>/Vs for three O(C), and six O(C), respectively.

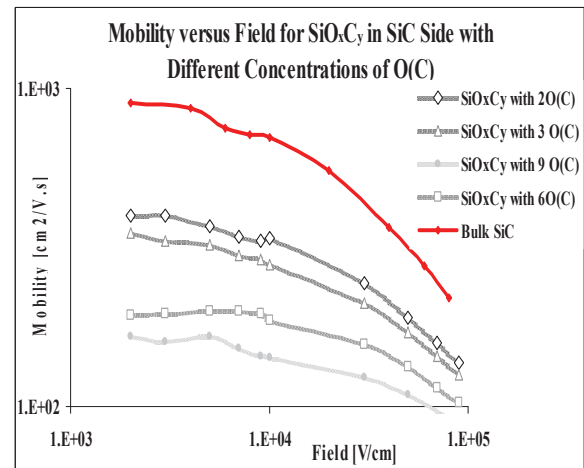


Fig. 5. Electron-phonon limited bulk mobility for bulk SiC, and SiO<sub>x</sub>C<sub>y</sub> structures with several concentrations of O(C) in SiC.

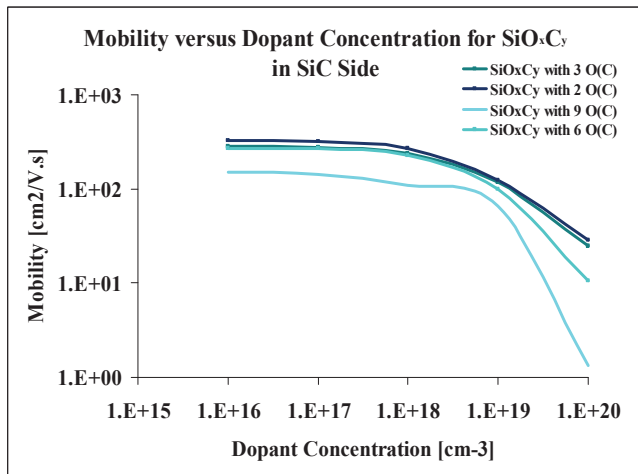


Fig. 6. Electron-phonon and ionized impurity limited mobility as a function of ionized impurity for  $\text{SiO}_x\text{C}_y$  structures with various concentrations of O(C) in SiC side.

### C. $\text{Si}_{1-x}\text{C}_x\text{O}_2$ Structures in $\text{SiO}_2$

To construct the C-O-Si bridges, and hence the most likely interfaces, we first replaced silicon atoms in the oxide side by carbon atoms with different concentrations ( $x=1/3$ , and  $x=1/2$ ) to form  $\text{Si}_{1-x}\text{C}_x\text{O}_2$  layer. The band structure and total DOS are calculated by DFT simulator, and then compared with the abrupt structure. According to our calculations, these substitutions do not introduce levels in the bandgap. The same substitution in pure  $\alpha$ -quartz gives the same outcome. Therefore we rule out the  $\text{Si}_{1-x}\text{C}_x\text{O}_2$  structure as the potential transition layer which may increase the near interface states.

## IV. CONCLUSION

In summary, we constructed likely SiC/SiO<sub>2</sub> interface layers, and calculated the resulting energy states with DFT after geometric relaxation. We found the band diagram, dispersion relation, and density of states with the use of generalized gradient approximation (GGA); then we utilized the hybrid functional to retrieve the proper bandgap of each structure. The retrieved bandgap for 4H-SiC agrees with experimental data. By comparing the total and projected density of states of C-Si-O bridges in various structures, we realized that  $\text{SiO}_x\text{C}_y$  structures made by substituting C atoms with O in the SiC side of the interface may give rise to traps near the conduction band. Defects, both in the SiC and the SiO<sub>2</sub>, lead to mobility degradation in the transition region of approximately 70%. Finally, we calculated the Coulomb mobility stochastically (Monte Carlo simulation); the results indicate that the Coulomb mobility is less than 30 cm<sup>2</sup>/Vs in all cases. Furthermore, the more O(C) substitutions that were formed in  $\text{SiO}_x\text{C}_y$  structures in SiC, the less the mobility would be, as predicated by Monte Carlo calculations.

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