Density Functional Theory Based Simulation of Carrier Transport in Silicon Carbide and Silicon Carbide-Silicon Dioxide Interfaces

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Abstract— We present density functional theory based calculations of band structure and density of states curves for bulk silicon carbide (SiC) and possible silicon carbide-silicon dioxide (SiC-SiO$_2$) interfaces. We then show carrier transport calculations in these structures using Monte Carlo techniques. This is for understanding the origins of the bandgap traps arising from the SiC-SiO$_2$ interface, which are of relatively high concentration in SiC MOSFETs compared to those in Si MOSFETs. It is also for investigating the effects of different atomic configurations on channel mobility, on-resistance, and thus losses in SiC power MOSFETs that are used as low-loss switching devices in high power high temperature applications.

Keywords-Silicon carbide; Monte Carlo transport; density of states; silicon carbide-silicon dioxide interface; silicon carbide interface traps.

I. INTRODUCTION

Silicon carbide is emerging as a material of choice for high power high temperature applications due to its favorable intrinsic electrical properties such as high breakdown field, high thermal conductivity, low noise and wide bandgap. Silicon carbide also has the advantage of having a native oxide which is silicon dioxide. As silicon along with its native oxide, silicon dioxide, has propelled today's integrated circuits, we expect silicon carbide similarly to open new paradigms in power electronics, and to be the driving force behind highly efficient low-loss power systems. As a matter of fact, SiC MOSFETs recently became commercially available. However, they lack the latest mature fabrication methods developed for silicon devices, and thus exhibit current-voltage characteristics that are not on par with silicon carbide's full potential (high mobility and low channel resistance). But SiC power MOSFETs are still advantageous over their silicon counterparts in high power and voltage applications in terms of efficiency and relatively lower losses. The main culprits that prevent SiC MOSFETs from reaching their full potential are the bandgap traps arising due to the silicon carbide-silicon dioxide interface. These traps result in low subthreshold swings, high threshold voltages, and most importantly low field effect mobilities (giving rise to high channel on-resistances). Therefore, it is of utmost importance to understand the silicon carbide-silicon
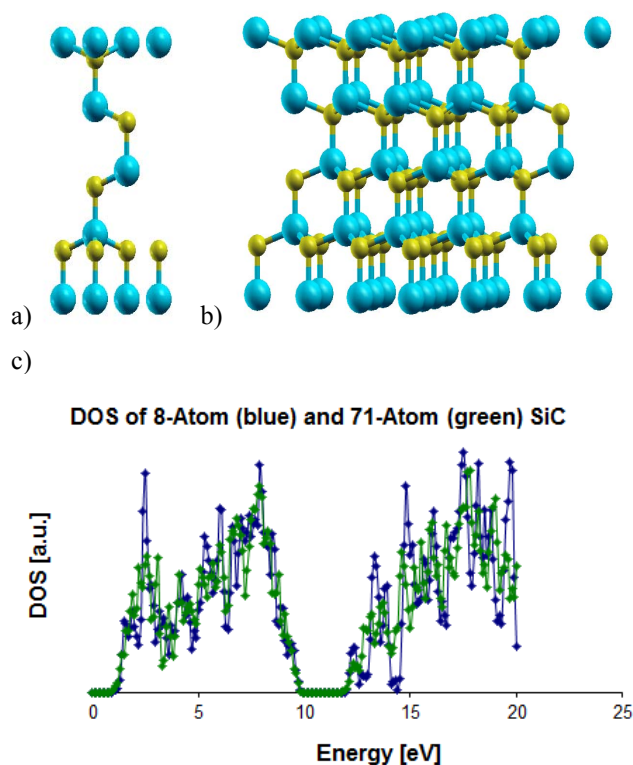

Figure 1. a) and b) show 8 and 72 atom unit cells we use for SiC DFT calculations, respectively. c) Densities of states curves calculated by Quantum Espresso [1] for the above structures.

dioxide interface at the atomic level for finding passivation methods for these traps and defects, as well as for investigating the effects of different structures on electron-phonon and Coulomb scattering limited mobilities that eventually dictate Joule losses in SiC power MOSFETs. To this end, we simulate different SiC-SiO$_2$ interfaces including possible defects, vacancies, interstitials, etc. using density functional theory (DFT) based methods [1]. We later import densities of states calculated for these structures into our Monte Carlo (MC) transport simulator [2] to obtain electron-phonon limited

mobilities as well as effects of Coulomb scattering with various concentrations of scatterers on these mobilities.
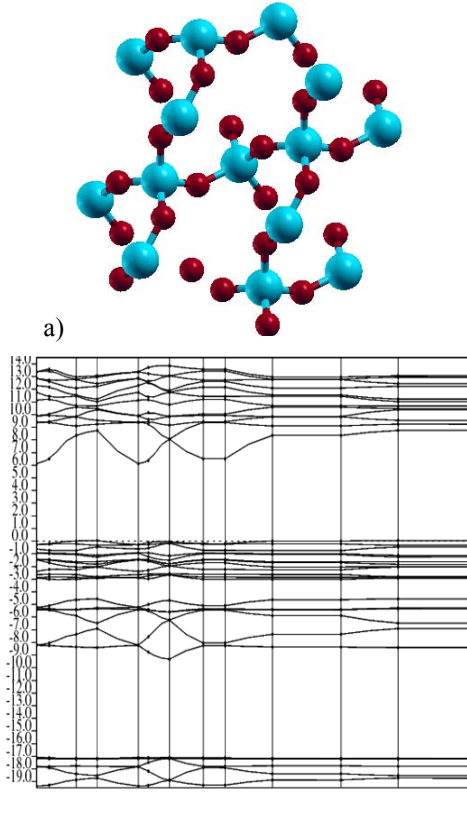

a)

b)

Figure 2. a) Example of alpha quartz unit cell we use for SiO$_2$ DFT simulations along with b) its calculated dispersion curves plotted for high symmetry k points.

II. DENSITY FUNCTIONAL THEORY CALCULATIONS

We use density functional theory to calculate dispersion relations and densities of states in bulk silicon carbide and SiC-SiO$_2$ interfaces. These simulations are based on the approximate many body solution of the Schrodinger equation. The solution takes into account electron kinetic energy, attractive energy between electrons and nuclei, repulsive energy between nuclei, kinetic energy of nuclei, and attractive energy of nuclei. To calculate an approximate solution to the above problem (or to obtain the bandstructure for various physical arrangements), we use the Quantum Espresso simulator [1]. We also note that the structures input into the DFT simulator (physical locations of the atoms) are relaxed before the corresponding bandstructures and densities of states are calculated. This is especially important for investigating possible SiC-SiO$_2$ interfaces since the details of the interface are not known and hence there is an uncertainty about the locations of the defects, types of defects, and atoms at the interface. As we arrange different atoms in suspected configurations, we let the system relax before we calculate further details. This avoids energy levels that might emerge due to the stress on the individual atoms in the system, which otherwise may correspond to unstable configurations.

Figure 1 and 2, respectively, show silicon carbide and silicon dioxide cells used in our DFT calculations. We also show the density of states curve calculated for bulk silicon carbide as well as electron dispersion relations obtained for the α-quartz, which is used as the silicon dioxide layer in SiC-SiO$_2$ interface studies.
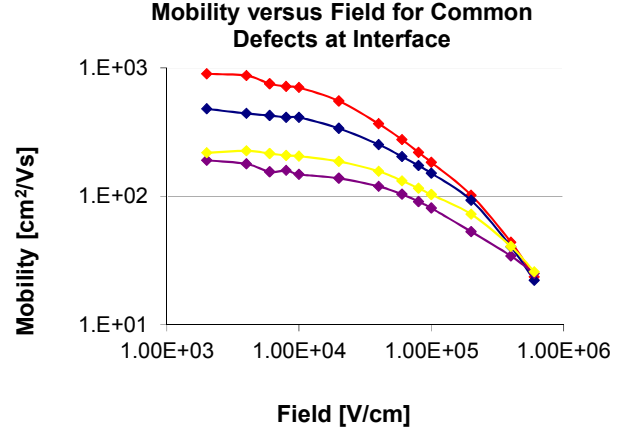
Mobility versus Field for Common Defects at Interface

Figure 3. Electron-phonon limited mobility for bulk SiC (red curve - top), abrupt SiC-SiO$_2$ interface (blue curve –second from top), SiC-SiO$_2$ interface with an oxygen interstitial (yellow curve –second from bottom), and SiC-SiO$_2$ interface with a carbon interstitial (purple curve –bottom).

III. SILICON CARBIDE MONTE CARLO TRANPORT

To determine mobilities and carrier velocities in bulk silicon carbide and at various SiC-SiO$_2$ interfaces, we develop a Monte Carlo transport simulator [2] that uses the deformation potential approximation, Fermi's golden rule, and the densities of states calculated by DFT to calculate carrier scattering rates.

$$\Gamma_{ac}(E) = \frac{D_{ac}^2 k_B T}{\rho \hbar v^2 \pi} DOS(E) \qquad (1)$$

$$\Gamma_{op}^{ab}(E) = \frac{D_{op}^2 \hbar}{2\rho E_{op}\pi} N(E_{op}) DOS(E + E_{op}) \qquad (2)$$

$$\Gamma_{op}^{em}(E) = \frac{D_{op}^2 \hbar}{2\rho E_{op}\pi} [N(E_{op}) + 1] DOS(E + E_{op}) \qquad (3)$$

$$\Gamma_{imp}(E) = \frac{N_{imp} e^3}{16\hbar k^4 \epsilon^2 \pi} \left(\frac{\gamma^4}{1 + \gamma^2}\right) DOS(E) \qquad (4)$$

Equations (1)-(4) show the scattering rates as a function of density of states. Here (1) is the acoustic phonon scattering rate that is calculated using acoustic deformation potential, D_{ac}, Boltzmann constant, k_B, temperature, T, density, ρ, reduced Planck's constant, $\hbar$, and sound velocity, v, in addition to the density of states. Equation (2) represents the optical phonon absorption rate, and (3) is for optical phonon emission rate. Above, E_{op} is the optical phonon energy, and $N(E_{op})$ is the Bose-Einstein phonon occupation number at this phonon energy. Additionally, (4) shows the ionized impurity scattering rate based on the Brooks-Herring formalism. In the last equation, the newly introduced variables are impurity concentration, N_{imp}, dielectric constant, ϵ, momentum, k, and
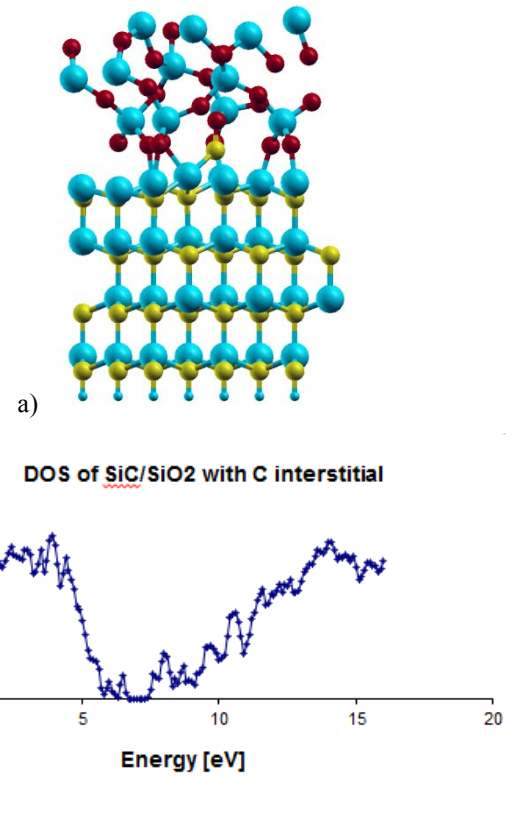
DOS of SiC/SiO2
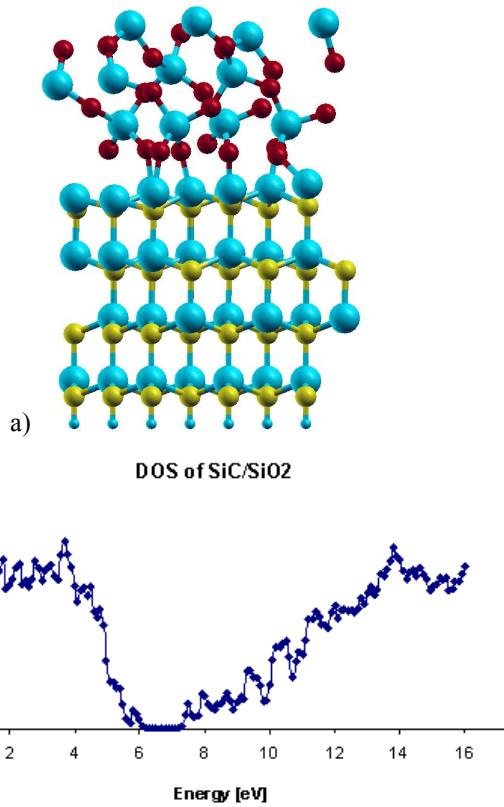
Figure 4. a) Unit cell used in DFT calculations for abrupt SiC-SiO₂ interface b) The DFT calculated densities of states curves for the above structure.

DOS of SiC/SiO2 with C interstitial

Figure 5. a) Unit cell used in DFT calculations for SiC-SiO₂ interface with a carbon interstitial b) The DFT calculated densities of states curves for the structure in a).

screening parameter, γ. Furthermore, we also include the polar optical emission and absorption scattering rates into our transport calculations. (The constants used in these equations along with details of transport calculations can be found in [2].) In addition, we note that the above equations for scattering rates are obtained by eliminating the effective mass in standard scattering rate formulas, and adding the DFT calculated densities of states into the equations.

We also use the densities of states (DOS) curves to calculate an average dispersion relation for electrons. More specifically, we integrate the DFT DOS curves in energy. The resulting integral is proportional to the cube of the momentum. Therefore we relate momentum to a unique energy solving for the energy that satisfies the aforementioned integral (integral of DOS(E) from the conduction band minimum to E equals to k^3 times a constant factor).

Using the averaged dispersion relation along with the scattering rates, we determine the low field mobility for the system. The red curve in Figure 3 shows our simulated mobility versus field curves for intrinsic bulk silicon carbide. In this figure, the low field mobility shown for bulk silicon carbide is approximately 900 cm²/Vs, and it rolls off, as expected, for rising applied fields.

IV. SiC-SiO2 INTERFACE: DENSITY FUNCTIONAL THEORY AND MONTE CARLO PREDICTIONS

To investigate physical origins of traps and defects at the SiC-SiO₂ interface, and to examine effects of different interface configurations on mobilities, we use the vast data (possible defects, traps, structures as well as dispersion relations and densities of states curves) that can be extracted from DFT calculations along with our Monte Carlo transport simulations. DFT results of possible defects such as vacancies, interstitials, silicon-oxycarbide bridges [3], and substitutions provide effects of each type of defect on the bandstructure and densities of states. We then compare the calculated trap distributions and total concentrations with those of measured to decide on most likely defects at the SiC-SiO₂ interface. In addition to using the total interface trap density and its distribution within the bandgap for finding configurations that govern operation of modern SiC devices, we also use Monte Carlo calculated mobilities to further narrow the possibilities for the interface.

Figures 4 and 5 show two of our SiC-SiO₂ interface configurations: Figure 4 depicts an abrupt SiC-SiO₂ interface and Figure 5 shows the same interface with a carbon interstitial. Here blue, yellow and red spheres represent silicon, carbon and oxygen, respectively. The SiC bottom layer is composed of 36 carbon and 36 silicon atoms, and the top layer is a matching α-quartz. The unit cells used in DFT calculations are those shown in Figures 4(a) and 5(a) along with vacuum

layers at the bottom and top of each structure. Due to the thickness of this vacuum layer, one can think of the structure as a quasi-two-dimensional interface layer. Further, we passivate the dangling carbon atoms at the bottom with hydrogen, represented by small blue spheres. Figures 4(b) and 5(b) show the calculated densities of states for the abrupt interface, and the interface with carbon interstitial, respectively. In both DOS plots, the valence band starts from roughly 6eV (=Ev) and corresponds to energies lower than Ev. The conduction band roughly starts from 7.5eV (=Ec), and includes energies larger than Ec. We note that DFT calculations may give rise to smaller bandgaps (which may be corrected using hybrid functional calculations); however, the DFT provides reasonable values for DOS. The calculated DOS within the conduction and valence bands can be used to obtain carrier transport characteristics. The simulated DOS within the bandgap can be used in conjunction with a reference experimental value to determine the total trap densities that may arise due to different physical structures.

To obtain mobilities in different SiC-SiO$_2$ transition regions and Coulomb limited channel mobilities, we use our aforementioned Monte Carlo simulator. There are two inputs to the MC simulator. The first is the volume of the unit cell to calculate DOS per volume. The second is the DFT-DOS curve or values starting from the conduction band edge of a given structure. As can be noticed in the plotted DFT-DOS curves, the determination of the conduction band edge for a given structure is nontrivial, since there are states within the bandgap and DOS does not show a jump in values where the Ec starts. Thus we use the following algorithm: The first energy larger than the DFT calculated Fermi level where DOS approaches 10 states/eV is used as the edge of the conduction band or Ec. We further assume that the quasi two-dimensional interface layer simulated enables us to use a three-dimensional transport simulator provided that the DFT-DOS has correct units. Additionally, we assume that the DOS bumps corresponding to silicon dioxide states are high in energy and do not significantly affect the simulated transport curves. Likewise, the effect of bulk SiC on the transport is minimal as pure SiC gives rise to larger mobilities, and the subtleties arising in the bandgap and near Ec are observed to be directly correlated with defects, traps, vacancies, etc. introduced at the interface. Therefore, MC calculations provide bulk and Coulomb limited mobilities in SiC-SiO$_2$ transition regions.

Our previous study that corroborates with experiments performed on differently doped SiC MOSFETs [4], along with spectroscopy measurements [5], indicate that there can be a transition region between SiC and SiO$_2$, and therefore it may exhibit mobilities varying from that of SiC. To investigate this, we simulated transport in structures shown in Figures 4 (abrupt SiC-SiO$_2$ interface) and 5 (SiC-SiO$_2$ interface with a carbon interstitial) along with bulk SiC and SiC-SiO$_2$ interface with an oxygen interstitial. Our calculated electron-phonon limited transition region mobilities, which are lower than that of bulk SiC, are plotted in Figure 3. These calculated results corroborate well with mobilities calculated using different techniques [4,6].
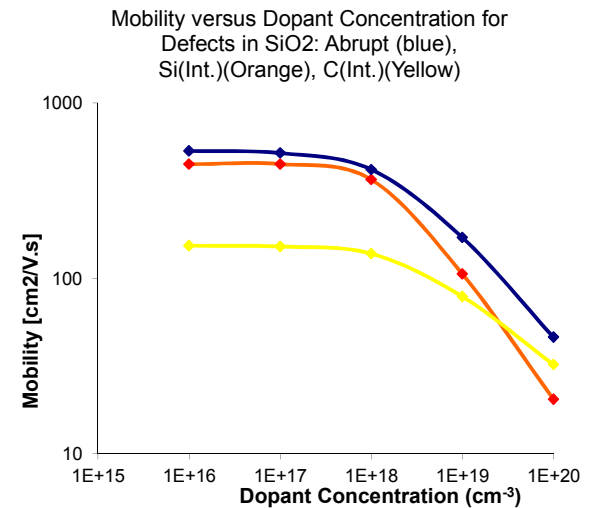

Figure 6. Electron-phonon and coulombic scatterer limited mobility as a function of ionized impurity (coulombic scatter) for abrupt SiC-SiO2 interface (blue curve –top), SiC-SiO2 interface with an oxygen interstitial (orange curve –middle), and SiC-SiO2 interface with a carbon interstitial (yellow curve –bottom).

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 Vth) are usually less than 50 cm^2/Vs. This is thought to be due to Coulomb scattering from trapped interface charges [4,6]. To examine effects of different amounts of interface traps on the aforementioned transport calculations, we calculate the low field mobility as a function of different levels of coulombic scatterers in these structures. The results plotted in Figure 6 show mobilities in lower double digits as the coulombic scatterer concentration approaches 10^{20} cm^{-3}. Assuming a transition region thickness of 1nm, the above-mentioned coulombic scatterer concentration can be translated into an aerial concentration of 10^{13} cm^{-2}, which is consistent with total acceptor type trap levels measured for SiC-SiO$_2$ interfaces [4,6].

In summary, we investigate possible SiC-SiO$_2$ interface layers using DFT, and calculate bandgap traps and dispersion relations arising from these structures. We then input DFT-DOS values into our MC simulator to calculate transition layer bulk mobilities and Coulombic scatterings. The calculated mobilites corroborate well with experiments, and the simulations provide in-depth insight into the physical and electrical properties of SiC-SiO$_2$ interfaces.

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