Theoretical study of the SiO_2/Si interface and its effect on energy band profile and MOSFET gate tunneling current

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Abstract: Two SiO_2/Si interface structures, which are described by the double bonded model (DBM) and the bridge oxygen model (BOM), have been theoretically studied via first-principle calculations. First-principle simulations demonstrate that the width of the transition region for the interface structure described by DBM is larger than that for the interface structure described by BOM. Such a difference will result in a difference in the gate leakage current. Tunneling current calculation demonstrates that the SiO_2/Si interface structure described by DBM leads to a larger gate leakage current.

Key words: interface; MOSFETs; gate tunneling current
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1. Introduction

The continuing growth of circuit density needs the dimensional scaling of MOSFETs, thus reducing the equivalent oxide thickness (EOT) of gate dielectric, which reaches values as small as several angstroms[1]. As a consequence, the interfacial transition layer between Si and its oxide has become a significant fraction of the total thickness, and its detailed physical properties have a strong impact on the device performance such as channel mobility, leakage current, time dependent dielectric breakdown, and hot-electron induced effects. Understanding the atomic scale structural and electronic properties of this interface is, therefore, of paramount importance for the progress of Si-based microelectronics. Despite decades of study, and the availability of a great deal of experimental information about the interface[2, 3], the precise bonding arrangement in the interface region remains unknown, partially because the oxide network is amorphous. Atomistic simulation treatment of the SiO_2/Si interface is a technically challenging problem attempted by many groups using a variety of techniques. Several structural models of the SiO_2/Si interface have been proposed[4–7]. However, there have been rather few theoretical studies on the effect of SiO_2/Si interfaces on devices performance based on first principles calculations. In order to understand it, two interface models, the bridge-oxygen model (BOM)[8] and the double-bonded model (DBM)[9], were chosen and calculated via first principles, and based on the calculations, their impact on the energy band profile and gate tunneling current was evaluated.

2. Calculation method

2.1. Model structures

It is well-known that SiO_2 is amorphous for the thermal oxidation grown gate dielectric in MOSFETs; however, the electronic properties of bulk SiO_2 crystals are still important in tunneling current analysis in the nanoscale oxide thickness according to Yamada *et al.*'s work[10]. The structural and electronic properties of many different crystalline forms of silicon dioxide such as amorphous SiO_2, α-quartz and β-cristobalite[11] have been studied by applying different theoretical and experimental methods[12–15]. However, there are no models which can precisely describe the overall atomic-scale properties of SiO_2. A realistic model of SiO_2 is of primary importance when studying the SiO_2/Si(100) interface. In the present work, β-cristobalite is a natural choice due to its structural simplicity[8, 16–18]. The Si(100) surface was considered in this work because it is the most favored surface in MOSFET devices due to its low interface state density and correspondingly superior electrical characteristics.

Two simple-model structures for SiO_2/Si interfaces, DBM (see Fig. 1(a)) and BOM (see Fig. 1(b)), were considered in this work. The modeled SiO_2/Si supercell structures were constructed from 2 layers of crystalline diamond Si(100) and 2 layers of crystalline SiO_2 in the ideal β-cristobalite structure. The experimental lattice constants are 5.43 and 7.16 Å, respectively, and the lattice mismatch is 32%. The mismatch can be reduced by rotating the two SiO_2 unit cells by an angle of $\pi/4$ so that the diagonal of the Si diamond structure approximately fits the cubic edge of the β-cristobalite unit cell. The superposition of the Si and SiO_2 layers produces dangling bonds on some of the interface Si atoms. These dangling bonds can be satisfied by adding a single O atom onto one of the Si atoms in the DBM. The resulting supercell has 73 atoms and dimensions 5.43 Å in the x–y plane and 25.18 Å in the z direction. In the BOM, an O atom saturates two dangling bonds of two different Si atoms; this supercell contains 72 atoms. The Si–O–Si angle is 144° and the length of the interface Si–O bonds is 2.02 Å. No cell optimization of the models has been carried out.

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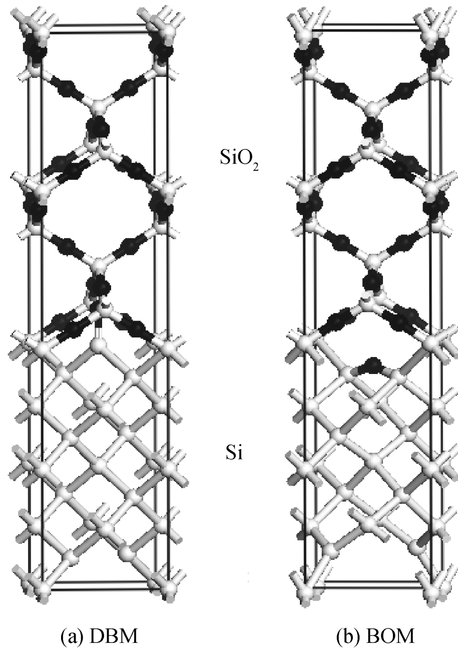

Fig. 1. Two SiO_2/Si supercell models. (a) DBM, which contains 73 atoms (48 Si and 25 O). (b) BOM, which contains 72 atoms (47 Si and 25 O atoms). O: balls in black, and Si: balls in gray. Both unit cells are rectangular and of size 5.43 × 5.43 × 25.18 Å.

2.2. Macroscopic averaging potentials via first principles

The geometrical optimization and energy calculations were performed using the CASTEP program (Cambridge serial total energy package)[19], which employs the plane pseudopotential method to calculate the total energy within the framework of the Kohn–Sham DFT. The calculations of electron-exchange associated items were carried out using the PW91 form of the GGA correction method. The Vanderbilt ultrasoft pseudopotentials were used, which allow numerically converged calculations at relatively low kinetic energy cutoffs of the plane wave basis. The Broyden, Fletcher, Goldfarb and Shanno (BFGS) algorithm was applied to optimize the model structures. Four k-points were taken in the Brillouin area, and the ground state energy was calculated with the Pulay density mixed method under the following conditions: the precision is 2.0×10^{-5} eV per atom, the cutoff energy of the plane wave is 290 eV, 300 eV for BOM and DBM respectively.

Further, the valence band profiles were calculated using the average potential method[20]. The electrostatic potentials for the supercell were averaged in the xy plane; then, macroscopic averaging potentials were calculated in the z direction:

$$\overline{V(z)} = \frac{1}{t}\int_{z-t/2}^{z+t/2} V(z')\mathrm{d}z', \tag{1}$$

where $V(z)$ is the plane-averaged electrostatic potential, and t is the lattice periodicity along z.

2.3. Gate tunneling current calculation

As dielectric film thickness decreases, electrical transport due to direct and FN conduction dominates device characterization, and the transition region between SiO_2 and Si influences the Fowler–Nordheim (FN) tunneling and direct tunneling (DT) currents through the ultrathin oxide.

FN tunneling current through a triangular barrier can be written as[21, 22]

$$J_{\mathrm{FN}} = BF^2 \exp(-C/F), \tag{2}$$

where F is the electric field across the oxide, and B and C are constants and are given respectively by[23]

$$B = \frac{q^3 m}{16\pi^2 \hbar m_{0x}^* \phi_0}, \tag{3}$$

$$C = \frac{4}{3}\frac{(2m_{0x}^*)^{1/2}}{q\hbar}\phi_0^{3/2}, \tag{4}$$

where m is the free electron mass, m_{ox}^* is the effective mass of electron on the conduction band of SiO_2, $\hbar$ is the reduced Planck's constant, and ϕ_0 is the barrier height (eV) between Si and SiO_2.

The above FN equation for the tunneling current was derived using the Wentzel–Kramers–Brillouin (WKB)[24] approximation that the electron wave interference effect is neglected, the oxide layer is flat, and the barrier lowering by image force as well as the temperature were neglected.

Taking the transition region (width d) into account, the FN tunneling current through a triangular barrier can be rewritten as[25]

$$J = J_{\mathrm{FN}} \exp\frac{2d\sqrt{2m_{\mathrm{ox}}^*\phi_0}}{3\hbar} = B_1 F^2 \exp\left(-\frac{C}{F}\right), \tag{5}$$

where

$$B_1 = B\exp\frac{2d\sqrt{2m_{\mathrm{ox}}^*\phi_0}}{3\hbar}. \tag{6}$$

The actual potential barrier deviates from the ideal triangular barrier because a transition region between Si and SiO_2 exists, and gradually changes from Si to SiO_2. This actual barrier shape makes the FN tunneling current much higher compared with that of the ideal one. The transition region width has an exponential impact on the FN tunneling current from Eq. (5).

However, when the oxide layer becomes ultra-thin and the applied voltage is below the potential barrier height, the classical FN formula is not applicable. In this case, the direct tunneling current must be considered and it can be described as[26]

$$J_{\mathrm{DT}} = \frac{B}{\left[1-\left(1-\dfrac{qV_{\mathrm{ox}}}{\phi_0}\right)^{1/2}\right]^2}F^2 \times \exp\left(-\frac{C}{\dfrac{\phi_0^{3/2}-(\phi_0-qV_{\mathrm{ox}})^{3/2}}{\phi_0^{3/2}}F}\right). \tag{7}$$

Again, the band structure variations influence the direct tunneling current similar to that of FN tunneling current. The direct tunneling current will increase exponentially if the transition region extends more widely.

3. Results and discussion

3.1. Energy band profile

At the SiO_2/Si interface, the band changes continuously from Si to SiO_2 (Fig. 2). From Fig. 2 the interface region is roughly 5 Å for both models. Other groups have reported similar results for different SiO_2/Si structures[27, 28]. The calculated interface region width is comparable with the experimental result[29].

However, it is important to define the transition region in atomistic detail. A definition of the transition region has been provided by suboxide or partially oxidized Si atoms[30]. In the present study, another way was chosen. The coordinates in the z direction, corresponding to the band profile changes in a trend away from the averages and vice versa, were set as the interface region boundaries. For example, the band goes down away from its average at point a in Fig. 2, so the coordinate z_1 corresponding to point a can be set to a boundary for BOM interface structure. Similarly, the other boundary can be set at z_2. This enabled us to easily evaluate the device performance such as calculating the gate FN tunneling current.

In the transition region, the band profiles behave differently for the two interface models. Firstly, the band of DBM is mostly higher than that of BOM. This can be easily understood by analyzing the charges of atoms in the transition region. All atoms distributed in the transition for DBM have more positive charges than those for BOM from the CASTEP calculations. Secondly, there is an obvious peak in the band of DBM, while there are no such peaks for BOM. The peak corresponds to the interface O atom double-bonded to Si. Due to a more positive chemical environment such as Si and O charges, it stands out from the band trend. The band profile is influenced by the interface structure[27]. Lastly, the band of BOM is closer to the average of the SiO_2 band than that of DBM. In other words, the transition region for BOM is thinner than that of DBM. This is because the BOM structure is less influenced by the interface O bridging two Si atoms, while the DBM structure is more influenced by the interface O double bonded to one atom; moreover, this interface O atom is near the SiO_2 layers from Fig. 1 and thus the band profile is closer to the SiO_2 band.

This transition region feature is supposed to influence the performance of devices consisting of SiO_2/Si structures, e.g., gate FN tunneling current in MOSFETs.

3.2. Gate tunneling current

As stated above, the band profile in the interface transition region varies mainly due to atomic scale interface structures. The band profiles deviate from the ideal abrupt barrier between Si and SiO_2, and thus increase the FN tunneling current. Next, the FN tunneling currents through SiO_2 on Si with different interface structures were calculated and compared.

The transition region width was calculated according to the method discussed above. It is 3.2 and 5.6 nm respectively from Fig. 2. Other parameters used in this work are m^*_{ox} = 0.5 m, α = 1.4, $\phi_0 = 3.15$ eV and the thickness of SiO_2 is 1.62 nm. As mentioned earlier, the thickness of SiO_2 is larger than that of two layers of SiO_2 because the band profiles go deep in Si.

According to Eq. (6), B_1/B varies greatly with the two SiO_2/Si interface models (Fig. 3), and it is 2.8 times larger for DBM. This means that the B_1 factors are greatly increased for

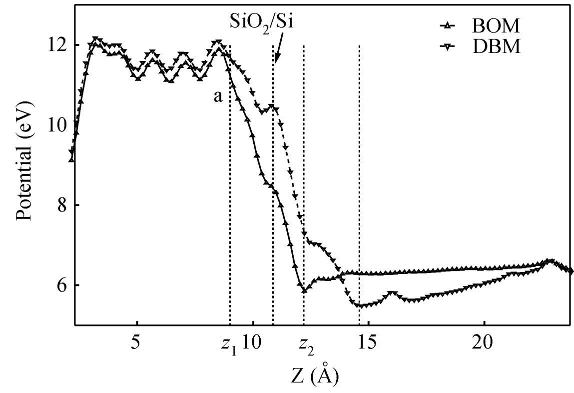

Fig. 2. Band profiles along the z direction for the SiO_2/Si interface models DBM and BOM. Coordinates z_1, z_2 correspond to transition region boundaries for BOM, the dotted line labeled with SiO_2/Si means the original SiO_2/Si interface as the models set.

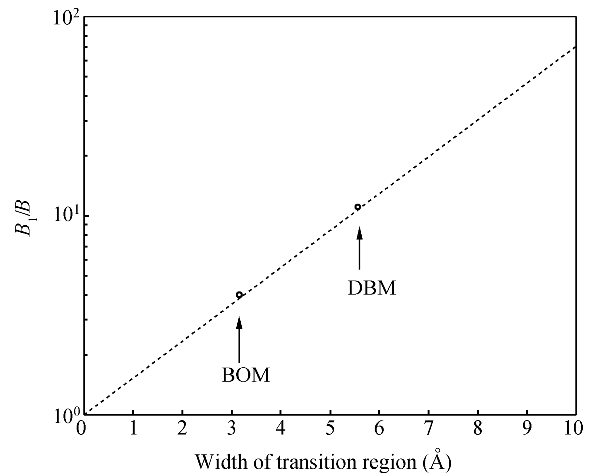

Fig. 3. B_1/B comparison for SiO_2/Si interface structures: DBM and BOM.

Table 1. FN tunneling current (A/cm^{-2}) versus interface structures under applied voltages.

Voltage (Interface)	1	2
Ideal barrier	4.3×10^{-12}	2.0×10^{-5}
BOM	1.7×10^{-11}	7.9×10^{-5}
DBM	2.9×10^{-11}	1.4×10^{-4}

both DBM and BOM SiO_2/Si structures, compared with that of the ideal SiO_2/Si structure because there are transition regions for the two models, and the barrier is changed.

The FN tunneling currents for ideal, BOM and DBM interface structures were calculated (Fig. 4). For the DBM and BOM SiO_2/Si interface structures, the tunneling currents are larger than that of the ideal barrier SiO_2/Si interface structure. One can have a rough image from Table 1. Obviously the DBM interface structure has the most impact on the gate FN tunneling current.

Furthermore, the calculated direct tunneling current for the BOM interface structure is roughly 3 times larger than that of the ideal barrier interface structure, while the direct tunneling current for the DBM interface structure is roughly one order

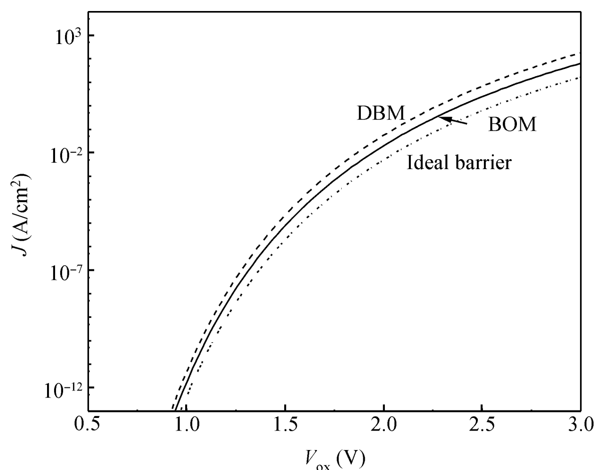

Fig. 4. Effect of SiO_2/Si interfaces on FN tunneling current under different applied voltages across the oxide.

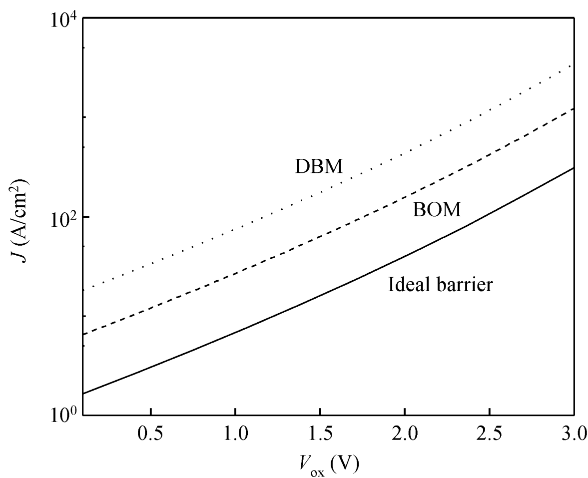

Fig. 5. Effect of SiO_2/Si interfaces on direct tunneling current under different applied voltages across the oxide.

larger (Fig. 5). The energy band for the DBM interface structure extends more widely in the transition region, and it thus greatly increases the direct tunneling current. Compared with the calculated FN tunneling currents, the direct tunneling currents are larger and are strongly affected by the SiO_2/Si interface structures.

The gate tunneling current depends on the SiO_2/Si interface structure because the barrier varies with SiO_2/Si interfaces. This tunneling current affects the device performance, and increases the power dissipation of the circuits. As high dielectric constant dielectrics are integrated into the devices, it is observed that an interfacial oxide layer exists between the high dielectric constant material and Si substrate[31], and the interface issue between Si and its oxides is still a primary challenge for Si-based technology.

4. Conclusion

The SiO_2/Si interface is of primary importance for Si-based semiconductor devices. By considering two interface models, the present work has investigated the interface band profile and its impact on gate tunneling current via first principle calculations. The results show how the band profile varies with interface structures for the chemical environment variation in the transition region. The band profile of the DBM SiO_2/Si interface is higher and extends more widely than that of the BOM SiO_2/Si interface. Furthermore, the gate FN and direct tunneling current are exponentially increased because a transition region exists between SiO_2/Si, and it is increased more for the DBM SiO_2/Si interface. The SiO_2/Si interface greatly impacts the MOSFET performance, which needs to be extensively evaluated[32].

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