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Interface States due to Intrinsic Defects in Si(100)/SiO_2

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1. Introduction

Interface states or traps are exceedingly harmful to the performance and the reliability of the MOS (metal-oxide-semiconductor) devices. The Si dangling-bond (SDB) defects, the typical intrinsic defects at the Si/SiO_2 interface, have been considered to be one of the the origin of the interface states or traps. They have been called P_b centers, a generic name for different SDB defects. In the Si(100)/SiO_2 interface, P_{b0} and P_{b1} centers have been known as this type of defects [1]. The P_{b0} is modeled as a $\bullet Si{\equiv}Si_3$ defect. The P_{b1} had been tentatively assigned to $\bullet Si{\equiv}Si_2O$, but recent findings suggest that it exists on a Si-Si dimer and contains no O atoms [2]. To understand the electronic properties of various types of the P_b centers is important for the Si/SiO_2 interface engineering.

We investigate the interface states due to the two prototypes of SDB defects at the Si(100)/SiO_2. We also show the passivation of the interface states by the H atom.

2. Methodology

The atomic configurations of SDB defects at the Si(100)/SiO_2 interface and their electronic structures are investigated using the first-principles method [3] based on the density functional theory. The unit cells containing about 70 atoms are employed for our calculation. Only valence electrons are explicitly considered. To account for the core-valence interactions, we use a norm-conserving pseudopotential for silicon atom, and ultrasoft pseudopotentials [4] for oxygen and hydrogen atoms, respectively. The generalized gradient correction [5] is added to the local density approximation for the exchange-correlation potential. Spin polarization is taken into account to deal with the SDBs correctly

3. Modeling of Si/SiO_2 Interface and the Defects

In spite of a great number of investigations, the basic structural model of the Si/SiO_2 interface is not well-established. In our previous calculation [6] , we proposed the type-T interface shown in Fig. 1(a), which consists of tridymite-type SiO_2[7] on Si, as a likely stable interface structures when the layer is thin (about 7 Å) . Here, we employ the type-T interface as a model of the interface with no SDBs.

SDB defects are introduced at the type-T interface. An oxygen atom is removed to make a SDB at the interface. The other SDB formed at the same time in the SiO_2 layer is pointed to the opposite direction and terminated with OH. The SDB defect at the interface contains an O atom in its neighboring site. Here, we call this defect SDB1. The SDB0 defect is made by removing the O atom in the SDB1. It has basically the same structure as the recently proposed model for the P_{b1} center.

4. Interface States and Hydrogen Passivation

We optimized the atomic configurations around the defects at the interface. The stable configurations for SDB1 and SDB0 are shown in Fig. 1(b) and (c), respectively. The changes of the position of the atoms around the SDBs are small.

We calculated the electron densities of states for these systems to investigate the interface state. The results for SDB1 and SDB0 are shown in Fig. 2(a) and (b), respectively. For SDB0, two defect states appear in the band gap range from 1.6 to 2.9 eV. (In our calculation, the band gap and the position of the interface states can be discussed only qualitatively.) This corresponds to the results by DLTS measurements [8]. By examining the contribution of these states to the charge density distribution, we found that the states are strongly localized on the SDB0 at the interface. The lower state is occupied and the upper one is unoccupied in the neutral charge state. Thus, these states can contribute to the hole and electron trapping, respectively. The SDB1 also generate two defect states around the gap. But in this case, both of the states exist near the band edges. The interpretation of this result is somewhat delicate. But, from the comparison with the result of H terminated SDB1 shown in Fig. 2(c), we consider the lower level is in the band gap, and the upper level is in the conduction band. Thus, the SDB1 can contribute only to the hole trapping.

We introduced H atom into the interface to terminate the SDB1 and SDB0. The atomic configurations involving H atom were optimized again. The change of the atomic configuration are very small in each system. From the calculated electron densities of states, it is found that the interface states have been completely disappeared by the H atoms (Fig. 2(c) and (d)).

5. Summary

We investigated the interface states due to the SDB defects in Si(100)/SiO_2 using the first-principles method. It has found that

the SDB0 generate the interface states which can contribute to the hole and electron trapping. On the other hand, the interface states due to the SDB1 can contribute only to the hole trapping. These defects are completely passivated by introducing H atoms without changing the atomic configurations at the interface.

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References

[1] E. H. Poindexter, P. J. Caplan B. E. Deal, and R. R. Razouk, J. Appl. Phys., **52**, 879 (1981).
[2] A. Stesmans, B. Nowen, and V. V. Afanas'ev : Phys. Rev. **B58**, 15801 (1998).
[3] R. Car and M. Parrinello, Phys. Rev. Lett., **55**, 2471 (1985).
[4] D. Vanderbilt, Phys. Rev. **B41**, 7892(1990).
[5] J. P. Perdew, in Electronic Structure of Solids '91, edited by P. Ziesche and H Eschring (Academie Verlag, Berlin, 1991).
[6] T. Yamasaki, C. Kaneta, T. Uchiyama, T. Uda and K. Terakura, Ext. Abs. 1998 Int. Conf. on Solid State Devices and Materials, 118 (1998).
[7] A. Ourmazd, D. W. Taylor, and A. Rentshler, Phys. Rev. Lett., **59**, 213 (1987).
[8] G. J. Gerardi, E. H. Poindexter, P. J. Caplan and N. M. Johnson, Appl. Phys. Lett., **49**, 348 (1986).

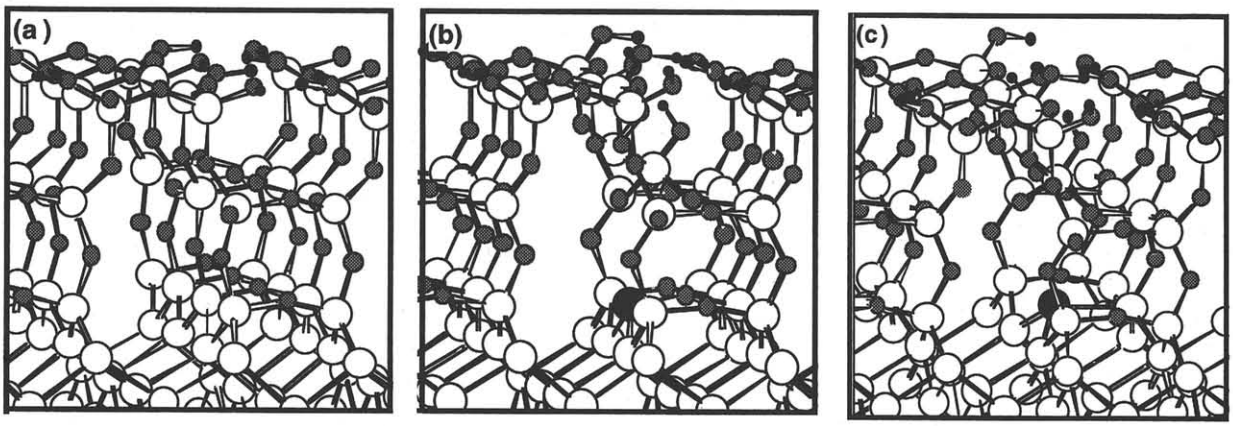

Fig. 1 Optimized structures of (a) type-T interface, (b) SDB1, and (c) SDB0 defects at the interface. Large circles are Si atoms. Defect Si atoms with dandling bond are black. Gray intermediate circles are O atoms and the black smallest are H atoms used to terminate the dangling bonds at the SiO_2 surface.

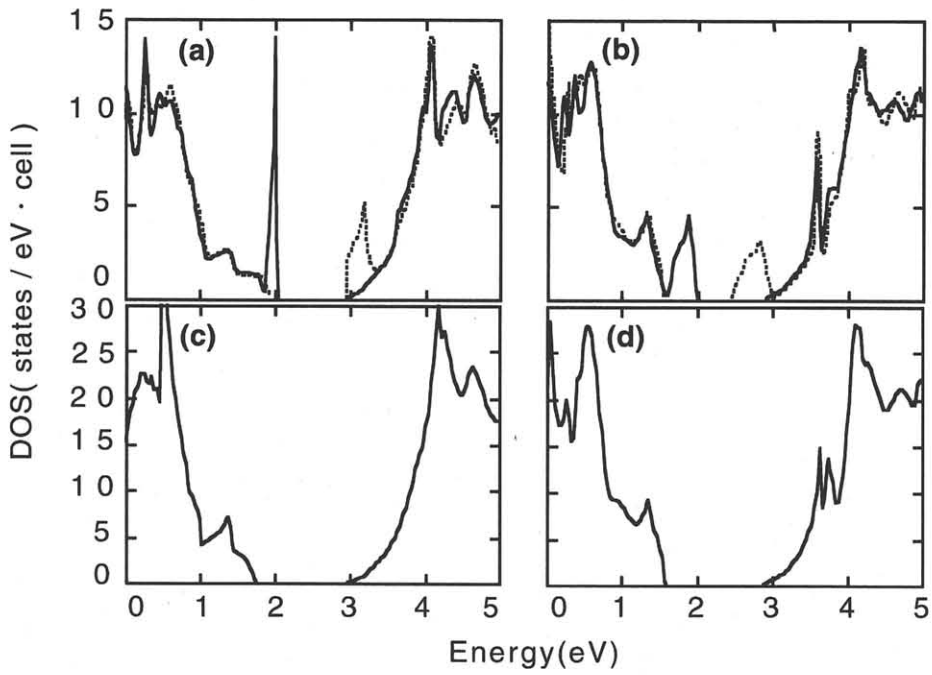

Fig. 2 Densities of states for the interface containing (a) SDB1, (b) SDB0, (c) H terminated SDB1, and (d) H terminated SDB0 defects. In (a) and (b), the densities of states for up and down spin ststes are shown separately with solid and dotted lines, respectively. In (c) and (d), total densities of states are shown with solid lines.