Extended Abstracts of the 1998 International Conference on Solid State Devices and Materials, Hiroshima, 1998, pp. 500-501

First-Principles Investigation of Imperfect Structures in SiO_2: Origins of Charge Traps Inducing Leakage Currents

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1. Introduction

Stress induced leakage current (SILC) is known to be due to the electrons tunneling through the gap states generated in SiO_2 under electrical stresses [1]. Because SILC increases as hole injection increases [2], the electron tunneling sites (ETS) inducing SILC are expected to be generated by hole-assisted reactions in SiO_2. Our previous work demonstrated that hole-trapped oxygen vacancy is a possible origins of the ETS [3]. In this work, we employed the first-principles total-energy and band structure calculations to examine the possibility of the ETS being generated as a result of hole or electron capturing by 'imperfect' structures in SiO_2, such as the Si--H, Si--OH, and Si--O--O--Si structures. The results show that the hole-trapped Si--H bond will generate the ETS , but the Si--OH and Si--O--O--Si structures will not.

2. Methods of Calculation

In the present calculation, we employed a unit cell with the structure of α-cristobalite, and the cell consists of eight Si atoms and sixteen O atoms. The Si--H, Si--OH and Si--O--O--Si structures were mimicked by terminating Si atoms at an O vacancy site (see Fig. 1(a)) with H, OH, and O-O molecules, and the optimized structures were calculated as seen in Figs. 1(b)-(e). To examine hole and electron capturing by these structures, we compared the total energies of the different charged states by performing the first-principles total-energy calculations within a framework of local density approximation. The total energies of the charged states depend on the location of the Fermi level (Ef) determined by the applied bias. A high Ef corresponds to electron injection, while a low Ef corresponds to hole injection (see Fig. 2). When the total energy of the structure in the positively charged state is lowest at low Ef, the structure will be a hole trap, and if the negatively charged state is most stable at high Ef, an electron trap is generated. When the structures were found to capture holes or electrons, we examined whether the structures generate gap states. And if the generated gap state was located near the offset between the conduction bands of Si and SiO_2, the gap state was considered an origin of the ETS (Fig. 3).

3. Results and Discussion

The total energies for the different charged states are shown in Fig. 4 as functions of Ef. Under hole injection (low Ef), the SiO_2 system having the Si--H bond (Figs. 1(b) and (c)) becomes a hole trap because the total energy of the system becomes lowest in the positively charged states (see Figs. 4(a) and (b)). When holes are trapped, the Si--H bonds are elongated and a H_2 molecule or a H atom tends to dissociate from the Si atoms, as seen in Figs. 5(a) and (b). The H-dissociated structures generated by hole-trapping have the gap states (Figs. 6(a-1) and (b-1)), and the gap states can capture electrons when the Ef is raised because the H-dissociated structures are found to become most stable in the negatively charged state. The electron traps originating from the hole-trapped structures have the gap states near the offset between the conduction bands of Si and SiO_2 (see Figs. 6(a-2) and (b-2)), and thus the Si--H bonds will be the ETS inducing SILC. The Si--OH structure, on the other hand, will be neither a hole trap nor an electron trap because, as shown in Fig. 4(c), the structure is most stable in the neutral state. Although the Si--O--O--Si structure is not stable in the positively charged state as seen in Fig. 4(d), it is most stable in the negatively charged state under electron injection. This indicates that the Si--O--O--Si structure will be an electron trap. However, because the gap state of the electron-trapped Si--O--O--Si structure is located near the top of the SiO_2 valence band (Fig.7), the electron trap originating from the Si--O--O--Si structure in SiO_2 will not be an ETS.

4. Conclusion

Our first-principles calculations demonstrate that the Si--H bond will be a hole trap accompanied by H dissociation and that the dissociation generates a gap state which will be a tunneling path for electrons through SiO_2 films. The Si--O--O--Si structure is found to generate an electron trap under electron injection, but the electron-trapped state will not be a tunneling path for electrons. The Si--OH bond will generate neither hole nor electron traps.

References
[1] R. Mozzami and C. Hu, Tech. Dig. of IEDM92 139 (1992).
[2] N.Masukawa et al, IEEE Trans. Electron Devices 43,1924 (1996).
[3] A.Yokozawa et al, Tech. Dig. of IEDM97 703 (1997).

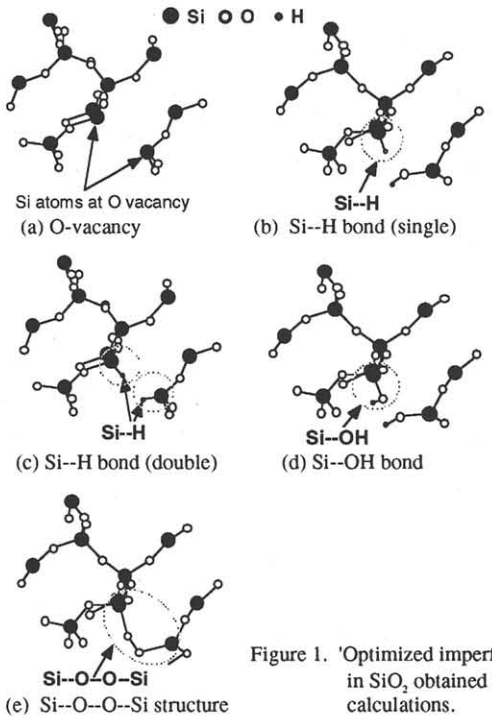

Figure 1. 'Optimized imperfect' structures in SiO_2 obtained by the present calculations.

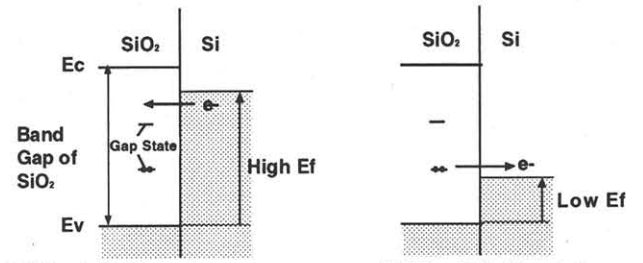

Figure 2. Schematic explanation of Fermi level Ef.

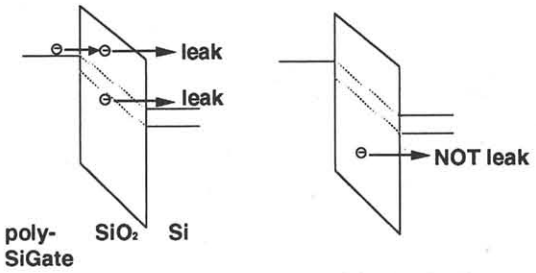

Figure 3. Schematic representation of gap states which (a) will and (b) will not generate the ETS.

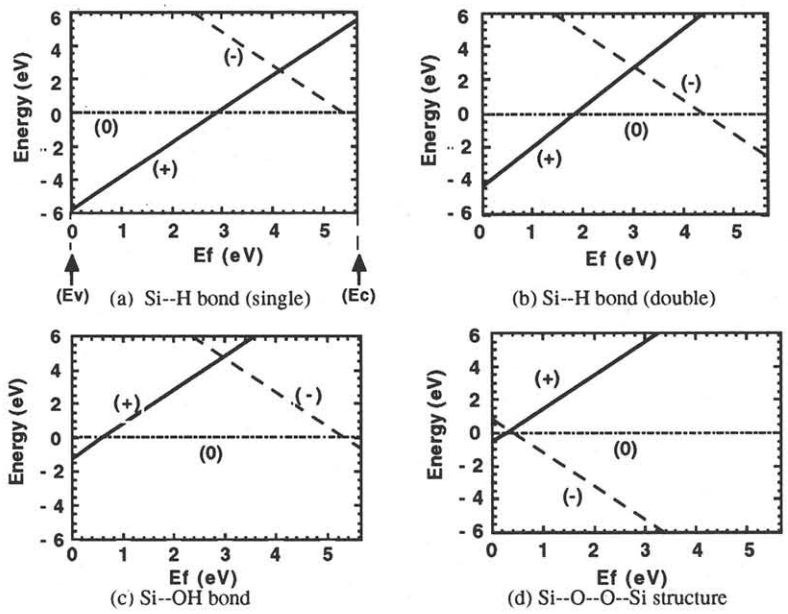

Figure 4. Comparison of the total energies of the different charged states. Ev and Ec correspond to the valence band top and conduction band bottom of SiO_2 obtained by the present calculation, respectively.

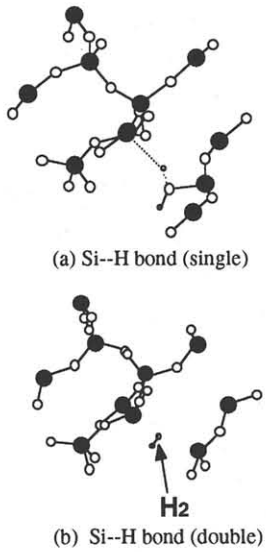

Figure 5. The H-dissociation from Si--H bonds after trapping holes.

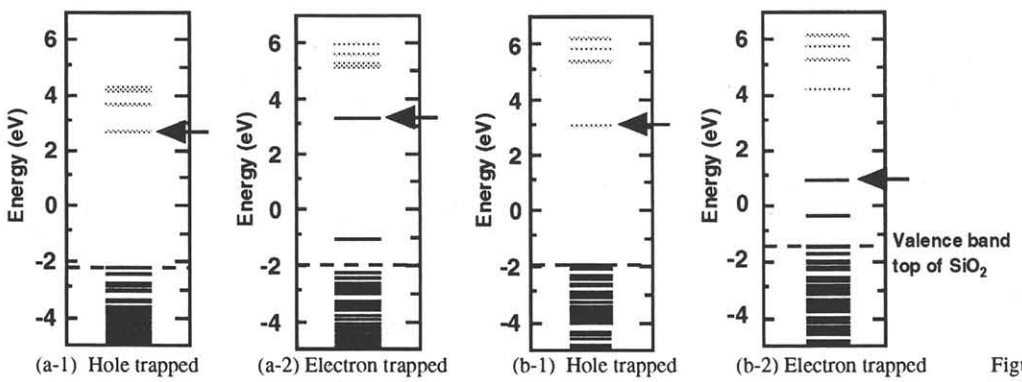

Figure 6. The energy level structures of the Si--H bonds when they (a-1)(b-1) trap holes and then (a-2)(b-2) trap electrons. The bottom of the Si conduction band is located at 4.5eV above the top of SiO_2 valence band(-----). ◀ indicate the gap states. (——:occupied, ...: unoccupied)

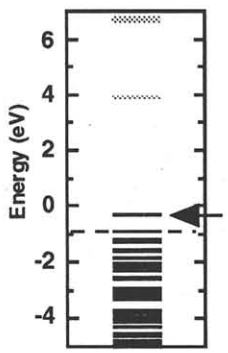

Figure 7. The energy level structures of the electron trapped Si--O--O--Si structure. ◀ indicates the electron trapped state. (——:occupied, ...: unoccupied)