First-principles study on electronic structure of Si/SiO₂ interface—Effect of interface defects on local charge density

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Abstract
We present theoretical study on the electronic structures of the interfaces between Si substrate and SiO₂ under zero bias and when a bias of 1.0 V is applied to the substrate by the first-principle calculation based on real-space finite-difference approach. By comparing the density of states at the interfaces, we study the effect of the defects around the interface on the channel and leakage currents. In addition, the leakage current through the interfaces are examined. Our results indicate that the defects around the interface lead drastic change of the electronic structure of the interface under the electric field and enhance the leakage current through the SiO₂ films.

Keywords: First-principles calculation; Leakage current; SiO₂

1. Introduction
Today’s very large-scale integration (VLSI) technology is in need of an atomic scale understanding of issues arising from the miniaturization of silicon devices. Among these, the understanding and control of structural and electronic properties of Si/SiO₂ interfaces is a key subject; therefore, intensive studies have been made both experimentally and theoretically. From lots of experiments, it is expected that the defects at the Si/SiO₂ interface have an important consequence on electronic properties, and annealing of SiO₂ films in hydrogen ambient is very effective in reducing the defects within SiO₂ films and at the interface. In addition, when the SiO₂ layer is very thin (∼15 Å), there is concern that these defects drastically increase the leakage current through such thin films. In the interpretation of these phenomena, however, the effect of the interface defects is hardly revealed only through experiments because of problems with reproducibility. Thus, the theoretical approach is also important and efficient. In this paper, we present theoretical studies, using first-principles calculations, on the electronic structures of the interfaces between a Si substrate and a SiO₂ dielectric and also present information on the effect of defects on the leakage current under the electric field.

2. Computational method
Our first-principles calculations are based on the real-space finite-difference method [1–5], which enables us to determine the self-consistent electronic structure and the optimized atomic geometry with a high degree of accuracy, by making use of the timesaving double-grid technique [3,5] and the direct minimization of the energy functional [6]. We examine the Si/SiO₂ model proposed by Buczko et al. [7] using a crystalline SiO₂ layer stacked on a Si(001) surface. The computational model is shown in Fig. 1(a). The structure of the SiO₂ layers is α-quartz within a thickness of 14 Å and the Si substrate thickness is chosen to be 7.7 Å. The vertical length of the supercell is chosen to be 31.7 Å. In addition to the reference Si/SiO₂ interface model without any defects, we set up our target models such that after the oxygen around the interface is extracted, one dangling bond of a Si is terminated with a H atom, and the other bond is just as it is. These models are illustrated in Figs. 1(b) and (c). Eventually, 38 Si atoms, 33(32) oxygen atoms, and 12(13) hydrogen atoms are contained in the model without (with) the defects. The norm-conserving
Fig. 1. Optimized atomic geometry of SiO\textsubscript{2}/Si interfaces. (a) The interface without defects. (b) The oxygen atom at the interface is replaced by hydrogen atom. (c) The oxygen atom at first atom layer of SiO\textsubscript{2} is replaced by hydrogen atom. The vertical dotted line represents the boundaries of supercell.
pseudopotentials of Troullier and Martens [8,9] are adopted and exchange-correlation effects are treated by local-density approximation [10] of the density-functional theory [11,12]. We take a cutoff energy of 96 Ry, which corresponds to a grid spacing of 0.17 Å, and a higher cutoff energy of 867 Ry in the vicinity of nuclei with the augmentation of double-grid points. The $k$-space integrations, in this time, are performed with the discrete grid that corresponds to $25k$ points in the irreducible wedge of the two-dimensional Brillouin zone of the interface. Structural optimization is implemented until the remaining forces acting on atoms are smaller than 82.4 pN. After the optimization, the electronic structures of the substrate under zero bias and an external electric field of 0.27 V/Å [13], which corresponds to an external bias of −1.0 V, are examined with the atomic positions are kept frozen. From these calculations, the effect of the defects on the electronic structures of the interfaces is estimated. Next, the vacuum region of the reference Si/SiO$_2$ models is removed and the jellium electrodes are directly attached to each model to investigate their electron conduction properties at zero bias limit. In the case of the conduction calculation, the $k$-space integrations are performed with the discrete grid that corresponds to $2k$ points in the irreducible wedge of the two-dimensional Brillouin zone of the interface. We calculate the current charge distributions by attaching the Al jellium electrode to the substrate directly (see Fig. 2) in order to explore how the defects contribute to the leakage current through the SiO$_2$ layers.

3. Result and discussion

We find that electrons under the zero bias localize around the interface almost uniformly regardless of whether or not the defects exist, whereas the charge distributions are very different among the models when a bias of −1.0 V is applied to the substrate. Fig. 3 shows charge densities around the interface with the energy between the Fermi energy and +1 eV. In addition, we find that the existence of defects disrupts the electronic structures in the interface and the localization of electrons not only in the interface but also in the oxide layers. These results indicate that the defects around interface make the charge distribution inhomogeneous in the channel region of metal oxide semiconductor field effect transistors.

![Fig. 2. Schematic description of model attached Al jellium electrodes in the case of the interface without defects.](image)

![Fig. 3. Charge densities around interface with energy between Fermi energy and +1 eV when vacuum region of Si/SiO$_2$ models is set at about 5 Å. (a) The interface without defects. (b) The defect located at interface. (c) The defect located at first atom layer of SiO$_2$.](image)
Such a distribution would have considerable effect on the source–drain current which is one of the most important issues for MOS devices. Moreover, due to the defects around the interface, the average effective oxide thickness gets thinner, which may give rise to the local pass of the leakage current through ultra-thin SiO$_2$ layers. Finally, in order to examine how electrons incident from the electrode is trapped by the defects around the interface, the vacuum region is removed and the electrodes are attached to them directly. The results of the charge distributions of the respective models are shown in Fig. 4. Note that electrons are trapped by the defects in the Si/SiO$_2$ models with defects. This result indicates that the defects around the interface certainly make the average effective oxide thickness thinner, and that the defects at the interface enhance the leakage current through the oxide layers. These features of the charge distributions at the interface should be taken into account when designing MOS devices.

4. Conclusion

We have studied the effect of the defects at the Si/SiO$_2$ interface on their electronic structures under zero bias and a finite bias of $-1.0$ V. Our findings indicate that the defects around the interface lead to a drastic change in the electronic structure of the interface under the electric field. Furthermore, by calculating the current charge distributions of the electrons indicating from the electrode, we confirmed that the defects around the interface largely contribute the leakage current through the oxide layers. In a future study, it is necessary to investigate more elaborately the effect of defects at the interface on the leakage and channel current both experimentally and theoretically.

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