Study on structural elementary excitations at semiconductor surfaces and interfaces

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In this project, we have been focused on physical properties of structural elementary excitations of semiconductor surfaces and interfaces. In this year, we have focused on the physical properties of defects in SiO_2. The calculations were performed based on the first-principles calculation. Program package PHASE/0 was employed. [1]

Defects in SiO_2 have been widely studied because they are the source of device performance degradation for MOS field-effect transistors (MOSFETs), which is widely used for the integrated circuits. The gate insulator of MOSFET is made of silicon oxide SiO_2. Those studies revealed that O vacancies, one of typical defects, can trap charges, assist gate leak current, and also lead to the formation of eternal gate leakage paths. They also revealed the role of post oxidation annealing. However, recent progress of integrated circuit technology have forced the MOSFET device structure from planar to three dimensional. If we consider the vertical body-channel-MOSFET with silicon oxide gate insulator, the oxide can be strained because of the device formation process. The interface oxide might be compressed and the surface oxide be expanded due to the thermal oxidation of silicon for the gate formation process. The compressive and expanded strain are expected as much as 3% in the worst case. Such strain should affect on the physical properties of defects in silicon oxide gate insulator

Therefore, we first focused on the O vacancy and studied strain dependence of its formation energy and diffusion barrier. Based on these results, in this year, we have studied stability of various defects including the O vacancy, the charging effects on them, and their strain dependences. Some of the vacancies we have studies are fully terminated by H atom or OH group, and other are partially terminated. We modeled the host SiO_2 by alpha-quartz crystal with supercell containing 24 Si and 48 O atoms.

First, we have found a novel O vacancy defect which has only two -OSi bonds. This defect is unique because the widely known O vacancy defect has three -OSi bonds. This new O vacancy defect is stable because it accompanies a three-Si-member ring within the model, while ordinary alpha-quartz just contains only six-Si-member rings. Next, we have found that a dangling bond of Si can surely assist the gate leakage current because they show charging levels in the middle of band gap. Then, we have found that the compressive strain makes it easier to release the terminators H or OH, while it does not significally change the charging level positions. From these results, we have confirmed that strain in the gate insulator silicon oxide surely enhances the device performance degradation. Careful device formation process must be necessary.

References

[1] https://azuma.nims.go.jp