Study on structural elementary excitations at semiconductor surfaces and interfaces

Hiroyuki KAGESHIMA
Graduate School of Natural Science and Technology, Shimane University
1060 Nishi-Kawatsucho, Matsue, Shimane 690-8504

Our project has been focused on physical properties of structural elementary excitations of semiconductor surfaces and interfaces. We have performed one topic in this year. It is the physical properties of oxygen vacancies (V_O) in SiO_2 at interface with Si. [1] The calculations were performed based on the first-principles calculation. Program package PHASE/0 was employed.

Because of recent progress of integrated circuits, three-dimensional metal-oxide-semiconductor field-effect transistors (MOSFETs) have been attracting attention. The vertical body-channel-MOSFET has a gate insulating thermally oxide Si film around a Si pillar with a diameter of several tens of nm, but it is considered that a large stress distributes in the oxide film. When a Si nanowire with a width of 50 nm and a thickness of 30 nm is processed by dry oxidation at 1000°C for 80 min, it is known that a compressive strain of about 3% is accumulated near the interface and a tensile strain of about 3% is accumulated near the outer surface.

The strain induced in the oxide film must have an unconventional effect on the film reliability such as dielectric breakdown. It is known that the dielectric breakdown of the oxide film is triggered by V_O-related defects in the film. The V_O-related defects trap holes, and transform into 3-coordinated Si's with +1 charge. These 3-coordinated Si's diffuse and aggregate under a gate-channel electric field of MOSFET operation to create a one-dimensional conductive chain from the Si interface to the gate interface in the oxide film. Then, a gate leak current flows through this chain, and leads to the dielectric breakdown. Since the oxide film of the three-dimensional MOSFETs is subjected by the strain, it is considered that these processes are also affected by the strain.

We focused on the fundamental properties of V_O in the oxide film, and investigated the effect of strain on them using the first-principles calculation. We found that the stability of V_O increases under compression. We also found that the height of the diffusion barrier increases under compression. In addition, we found that the diffusion barrier height is determined by the Si-Si bond length of the V_O. Considering the gate oxide film in the vertical body-channel-MOSFET, the V_O density increases because the interfacial oxide film is subjected to compressive strain. This suggests that interfacial traps are more likely to occur and performance may be slightly degraded. On the other hand, tensile strain is applied to the surface oxide film to reduce the density of V_O, but diffusion of V_O is promoted. This means that the reliability of the oxide film is affected by the stain because V_O can diffuse from the interface of the oxide film to the surface.

References

[1] K. Yata and H. Kageshima, Jpn. J. Appl. Phys. **60** (2020) 035504 (6 pages).