Study on physical properties of structural elementary excitations of semiconductor surfaces and interfaces

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Our project has been focused on physical properties of structural elementary excitations of semiconductor surface and interfaces. We have performed three topics in this year. One is the physical properties of SiO interstitials in SiO_2 at interface with Si [1, 2]. The second is the physical properties of oxygen vacancies (V_O) in SiO_2 at interface with Si. And the third is the physical properties of vacancies in a two-dimensional material $MoSe_2$. The calculations were performed based on the first-principles calculation. Program package VASP was employed for the first and the third topics, while program package PHASE0 was employed for the second topic.

In the first topic, we focus on the role of SiO interstitials for the selfdiffusions in SiO_2 under compressive pressure. It is known that SiO interstitials are injected into the oxide when Si is thermally oxidized. In addition, for Si pillar oxidation, it is known that a large compressive pressure as high as 5 GPa is induced in the oxide. We have calculated the pressure effect for temperatures 3000, 4000, 5000, and 6000 K, and derived activation volumes as well as activation energies. We found that the SiO really acts as a unit for the diffusion mechanism. As the result, the pressure dependence of Si diffusion is largely affected by the SiO incorporation, while that of O diffusion is not much affected. [1, 2]

In the second topic, we focus on the strain effect on V_O diffusion in SiO_2. As described before, for the Si pillar oxidation, a large compressive pressure is accumulated in SiO_2. We have calculated activation barriers as the function of modulated lattice constants. We have also checked crystal polymorph dependence for Quartz, Cristobalite, or Tridymite. As the results, we found that the barrier height increases with the Si density almost being independent of the polymorph type. The reason comes from the fact that the initial Si-Si distance at V_O controls the barrier height.

In the third topic, we focus on the supporting effect on vacancy formation in monolayer $MoSe_2$. The results are similar to our previous study on MoS_2. We found that the supporting effect makes the charging more difficult because the reduced quantum confinement shrinks the band gap. The hetero-stacking also makes the charging more difficult because the type II band alignment also shrinks the band gap. These lead to the reduction of charging effect on the vacancy formation.

References

[1] H. Kageshima, Y. Yajima, K. Shiraishi, and T. Endoh, Jpn. J. Appl. Phys. **58** (2019) 111004 (11pages).

[2] Y. Yajima, H. Kageshima, K. Shiraishi, and T. Endoh, 2019 International Workshop on Dielectric Thin Films for Future Electron Devices – Science and Technology – (2019 IWDTF), Tokyo, Japan, p-7 (Nov. 18, 2019).