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

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Our project has been focused on the physical properties of structural elementary excitations of semiconductor surface and interfaces. We have performed two topics in this year. One is physical properties of vacancies in two-dimensional material MoS_2 [1]. The other is physical properties of SiO interstitials in SiO_2 at the interface with Si [2, 3, 4]. The calculations were performed based on the first-principles calculation. Program package VASP was employed.

In the first topic, we focus on the supporting effect on vacancy formation in monolayer MoS_2. Vacancy formation is generally more suppressed for the supported cases than the freestanding case in non-negatively-charged conditions. These are the results of difference in charging of vacancies. We can thus propose that MoS_2 should be processed in the S-rich and non-negatively-charged conditions to prevent the formation of vacancies. We can also propose that the choice of supporting substrate is important to process MoS_2 to obtain better quality electronic devices.

In the second topic, we focus on the pressure effect on SiO_2 with SiO interstitials. It is know that the SiO interstitials are injected into the oxide when the Si is thermally oxidized. In addition, for the Si pillar oxidation, it is known that a large compressive pressure as high as 5 GPa is induced in oxide. We therefore study the pressure effect on the dynamical property of SiO_2 with SiO interstitials. Analyzing calculated results, we found that the Si dynamical property is enhanced by the pressure at 3000 K, while it is slightly diminished at 6000 K. This indicates that Si dynamical property is more enhanced by the pressure at the experimental oxidation temperature such as 1000 K. We also fit the pressure dependence of Si diffusion coefficients by the Lorentz type function of pressure (at 3000 K) or parabolic function (at 6000 K). Then we evaluate the activation volume as the function of SiO density. The results show that the activation volume is negative in low SiO density, but its absolute value decreases with the SiO density. This suggests that the SiO interstitials suppress the pressure effects on Si dynamical property.

References

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