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Theoretical analysis of atomic process on the growth surface

KAWANO, Jun[1*], KANGAWA Yoshihiro[2]

[1]CRIS, Hokkaido Univ., [2]RIAM, Kyushu Univ.

In order to understand formation process of minerals, it is important to analyze the atomic process on the growth surface. First-principles calculation of the growth surfaces is useful for this purpose, and is often used for semi-conducting materials. Recent progress of computer technology would make it applicable for more complex system such as minerals, which will provide more realistic information for the mineral growth in the atomic scale.

Here, as an example of this kind of approach, incorporation process of nitrogen (N) into GaAsN grown under a hydrogen atmosphere was analyzed. GaAsN with small N content has the zinc blende structure, and in this system it is difficult for nitrogen (N) to be incorporated into the solid owing to the large difference in the bond lengths of Ga-N and Ga-As. Therefore, we first determined the stability of reconstructed GaAs(001) surfaces absorbed by hydrogen (H) in dependence on chemical potentials of the constituent elements, and we found that two hydrogenized structures appear when the partial pressure of hydrogen is high. Then energies needed for N substitution to the As site were calculated. The results suggest that N is more easily substituted to surface sites bonded with H, which could be the origin of H-related defects. We are planning to apply this approach to actual mineral system.

Keywords: First-principles calculation, growth surface, surface reconstruction