First-principles study of atomic and electronic structures of intermetallic compound catalysts

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This fiscal year, we carried out the following studies using the VASP code with the PAW method and the PBE exchange-correlation functional.

Quasicrystals (QCs) are long-range ordered materials with no translational symmetry. Partly because the atomic structure of most QCs have not been solved completely, DFT studies have usually been carried out using the surface of a crystalline phase having a close composition and common structural building unit to the quasicrystalline phase. Recently, however, single-element quasiperiodic ultra-thin films have been obtained using the Ag-In-Yb QC as a template. The Ag-In-Yb QC belongs to the only QC family whose atomic structure has been solved unambiguously. Thus, DFT studies using the actual quasiperiodic surface atomic arrangement are required to elucidate the atomic structure of the ultra-thin films. Although a straightforward way to approximate the QC surface is to use an atomic cluster extracted from the structural data of the QC, the cluster size dependence of the adsorption energy for the aperiodic surfaces has not been well studied. Therefore, this time we studied the convergence behavior of the adsorption energy of a single Bi atom concerning the cluster size [1]. Two types of clusters, the cylindrical and hemispherical clusters, are tested. Unnaturally rippled potential energy surfaces were obtained for clusters with smaller radius regardless of the cluster thickness. It was revealed that the ripples are disappeared when clusters with a sufficient cluster radius of 1.4 nm or larger are used. This trend is also confirmed in their root mean square errors. Consequently, it was concluded that both cluster models tested with a specific size are expected to give relative adsorption energy within an error of 0.15 eV. It was also pointed out that the cylindrical cluster model is relatively economical in terms of the calculation cost than the hemispherical cluster model.

We also investigated the surface atomic structure of the antiferromagnetic 1/1 Au-Al Tb approximant crystal using DFT calculation[2]. Experimentally observed stable surface atomic structure showing a linear row structure of Au/Al atoms, which is an example of a surface reconstruction in this family of QC-related systems, was found stable by the calculation.

We studied the influence of the adsorbed oxygen atoms on the surface atomic structure and electronic structure of PdZn(111) surface using DFT calculation[3].

References

[1] M. Sato, T. Hiroto, Y. Matsushita, and K. Nozawa, Mat. Trans. **62** (2021) 350.

[2] S. Coates, K. Nozawa, M. Fukami, K. Inagaki, M. Shimoda, R. McGrath, H. R. Sharma, and R. Tamura, Phys. Rev. B **102** (2020) 235419.

[3] Y. Otani, Master Thesis (Kagoshima University, 2021).