First-principles study of anomalous and spin Hall conductivities in Fe/MgO superlattices with transition-metal insertions

Mie University,

○S. Ando, A.-M. Pradipto, T. Akiyama, T. Ito and K. Nakamura

E-mail: 417M601@m.mie-u.ac.jp

Hall effects have found applications in spintronic devices. In ferromagnetic material the Hall resistivity is proportional to the magnetization. This phenomenon is the anomalous Hall effect (AHE) which has important roles in the investigation and characterization of ferromagnetic materials. The spin Hall effect (SHE) and its inverse have been used to generate and detect the spin current in non-magnetic materials. Additionally, the SHE tunneling spectra have been considered to provide guidelines for engineering high-SHE materials. It is important to elucidate the magnetic transport properties such as AHE and SHE in the tunnel junctions. Here, in order to systematically investigate the magnetic transport properties as well as the effect of the geometrical and magnetic structures, we have performed magnetic transport calculation method by using full-potential linearized augmented plane-wave (FLAPW) method[1] within a superlattice model, and discussed the effect of the insertions of heavy metals such as 4d and 5d transition-metal at the Fe/MgO interface to the magnetic transport properties. Self-consistent calculations were carried out based on the generalized gradient approximation, and the transport coefficients were evaluated using the Kubo formulations. For the Fe/MgO (assuming several atomic-layers of MgO) with one monolayer of 4*d* (Ru, Rh, Pd) and 5*d* (Os, Ir, Pt) metals inserted at the Fe/MgO interface, we systematically investigated the anomalous and spin Hall conductivities along the film normal. Our results show that the anomalous Hall conductivity (AHC) is enhanced due to the insertion. The spin Hall conductivity (SHC) is also enhanced, and the magnitudes of SHC become large when 5*d* transition-metal elements are inserted. An analysis of the electronic structures for the origin of the AHC and SHC enhancement by the insertions will be presented.

[1] K. Nakamuara et al., Phys. Rev. B 67, 014420 (2003); Phys. Rev. Lett. 102, 187201 (2009).