Electric field effects to the anomalous and spin Hall conductivities in Fe thin films on MgO(001)

Mie University[1]

° Abdul-Muizz Pradipto[1], Toru Akiyama[1], Tomonori Ito[1] and Kohji Nakamura[1]

E-mail: a.m.t.pradipto@gmail.com

The application of gate voltage is known to modify various magnetic properties of materials which may be useful for spintronic applications [1]. Here the effects of applying external electric fields to the anomalous and spin Hall conductivities in Fe thin film models with different layer thicknesses on MgO(001) are investigated by using first principles calculations. These model systems have been chosen not only because of the importance of Fe/MgO interfaces for magnetic tunnel junction applications, but also in the study of gate voltage effects to the magnetism in metallic interfaces. Our calculations are based on the Density Functional Theory (DFT) formalism as implemented in the Full-Potential Linearized Augmented Plane Wave (FLAPW) code [2]. We consider the in-plane anomalous and spin Hall conductivities on the basis of the linear response theory by using the calculated eigenvectors and utilizing the Kubo-formula. We observe that, for the considered systems, the application of positive electric field associated to the accumulation of negative charges at the Fe side generally enhances the negative (positive) the anomalous (spin) Hall conductivities. The mapping of the Hall conductivities within the two-dimensional Brillouin zone shows that the electric-field-induced modifications are related to the modification of the band structures of the atoms at the interface with the MgO substrate. In particular, the external electric field affects the Hall conductivities via the modifications of the d_{xz},d_{yz} orbitals, in which the application of positive electric field pushes the minority spin states of the d_{xz},d_{yz} bands closer to the Fermi level. A better agreement with the anomalous Hall conductivity for bulk Fe and a more realistic scenario for the electric field modification of Hall conductivities are obtained on using the thicker layers of Fe on MgO (Fe_3/MgO and Fe_5/MgO) [3].

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