First principles calculations on magnetic transport properties of Fe/MgO superlattices

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Tunneling magnetoresistance (TMR) effect in magnetic tunnel junctions (MTJs) has found applications in spintronic devices such as magnetic read heads, magnetic random access memories, and magnetic sensors. The high TMR ratio is the key to spintronic devices and efforts to search promising materials of the MTJs with a crystalline barrier such as MgO are strongly desired. Moreover, developments of voltage-based magnetic tunnel junctions (VMTJs) to improve an energy-power consumption in spintronic devices, e.g. by insertions of heavy metals such as 4d or 5d transition-metals at Fe/MgO interface, have recently started. Here, in order to systematically investigate the magnetic transport properties as well as the effect of the geometrical and magnetic structures, we have developed magnetic transport calculation method by using full-potential linearized augmented plane-wave (FLAPW) method within a model of superlattices, and applied this approach to the TMR of Fe/MgO/Fe-based MTJs and that with heavy-metal insertions. Self-consistent calculations were carried out based on the generalized gradient approximation, and the transport coefficients were evaluated based on Kubo and Boltzmann formulations. To treat different spin states, namely parallel and antiparallel magnetization alignments between the neighbor’s Fe layers in the superlattice, we introduced the generalized Bloch theorem. For the Fe/MgO (assumed several atomic-layers of MgO), we confirmed that the TMR oscillates with the thickness of the Fe films and the magnitude of the TMRs is close to the literature values, showing the validity of the present approach. We furthermore considered the TMR in spin spiral structures with spirals propagating along the plane normal and found that the TMR ratio increases as the spiral wave vector increases. Results of Fe/MgO with heavy-metal insertions at the interface will be further presented.

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