First-principles investigation of spin-orbit coupling effects on the tunneling magnetoresistance in 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 4*d* or 5*d* 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[1] within a superlattice model, and discussed the effect of spin-orbit coupling (SOC) by insertions of heavy metals such as 4*d* and 5*d* transition-metals at a Fe/MgO interface. 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 systematically investigated the effect of SOC to the TMR ratio. The TMR ratios with one monolayer of 4*d* (Ru, Rh, Pd) and 5*d* (Os, Ir, Pt) metals inserted at the Fe/MgO interface were calculated. The TMR ratios for both 4*d* and 5*d* insertions decrease due to an introduction of the SOC. The trends in the TMR ratios for both the 4*d* and 5*d* metal insertions are similar, but the magnitude of reduction of the TMR ratios depends on the SOC strength where the Pt insertion has the largest reduction of the TMR ratio. An analysis of the electronic structures for the origin of the TMR reductions by the insertions is presented.

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