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Presentation Title

Spin-dependent transport phenomena in heterostructures based on half-metallic Heusler alloys: A theoretical study

Abstract

Half-metallic ferromagnets are promising materials for improving the performance of various spintronics devices. The efficiency of spin injection from half-metallic ferromagnets into semiconductors observed so far is, however, much lower than that expected. The low efficiency can be attributed to interfacial states which appear in the minority-spin band gap and degrade half-metallic characteristics. Therefore, high spin polarization at the ferromagnet/semiconductor interface is crucial for improving the efficiency of spin injection into semiconductors. We have carried out theoretical design of highly spin-polarized junctions between half-metallic Heusler alloys and semiconductors or insulators on the basis of first-principles density-functional calculations.

The half-metallic features are degraded by the interfacial states for all Heusler-alloy/semiconductor (001) junctions studied so far. The interfacial states are originated from the symmetry lowering at each atomic site as well as reunited dangling-bond orbitals at the hetero-junction. On the other hand, high spin polarization is almost preserved at specific (110) junctions between Heusler alloys and semiconductors, e.g. Co_2CrAl/GaAs (110), Co_2MnSi/GaAs (110) [1], and Co_2FeSi/Si (110) [2]. The high spin polarization at the (110) interfaces owe a lot to the local coordinate around each atomic site as well as the bonding characteristics at the hetero-junction. Indeed, the optimization of atomic positions forces the interfacial states away from the Fermi level, leading to the minority-spin band gap retained.

In order to improve spin-injection efficiency via MgO barrier into semiconductors, we have succeeded to design highly spin-polarized interfaces at CrAl-terminated Co_2CrAl/MgO (001) junctions [3]. We

confirmed that the CrAl-terminated interface is energetically favorable compared to the Co-terminated interface. The eminent property is originated from the significant enhancement of the Cr magnetic moment at the interface compared to the bulk value.

We investigated the effect of non-collinear magnetic structures at the interface of $Co_2MnSi/MgO/Co_2MnSi$ MTJs to elucidate the origin of the temperature dependence of the TMR ratio [4]. The tunneling conductance for antiparallel magnetization increases with increasing the tilting angle θ of magnetic moments on a certain atomic layer near the interface, while that for parallel magnetization decreases due to the spin-flip scattering of tunneling electrons caused by the non-collinear magnetic structure. As a result, the TMR ratio decreases significantly with increasing θ. The exchange stiffness of the interfacial or sub-interfacial Co-layer is much smaller than that of bulk Co_2MnSi and also that of the interfacial MnSi-layer. The reduction of the exchange stiffness of the interfacial Co moment is related to the reduction of the Co moment itself compared to that of the bulk. In conclusion, the thermal fluctuation of the interfacial Co moments can be responsible for the remarkable reduction of the TMR ratio observed in the MgO-based MTJs with half-metallic Co-based Heusler alloys at room temperature. In particular, the spin-flip scattering caused by the non-collinear magnetic structures in the interfacial region plays a crucial role in the reduction of the TMR ratio. Higher TMR ratio at room temperature can be achieved, for an example, by inserting a few atomic layers of Fe between the Heusler-alloy electrode and the MgO barrier, since the inserting Fe layers prevent thermal fluctuation of interfacial magnetic moments due to an enhancement of the interfacial exchange stiffness as well as that of the interfacial magnetic anisotropy.

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[4] Y. Miura, K. Abe, and M. Shirai, *Phys. Rev. B* **83** (2011) 214411.