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A first-principles study on tunneling magnetoresistance of magnetic tunnel junctions with $D0_{22}$-type Mn_3Ga and Mn_3Ge

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Magnetic materials with high perpendicular magneto-crystalline anisotropy (MCA) have great advantage in the reduction of the switching current and the enhancement of the thermal stability of spin-transfer torque-switching(STT)-type magnetoresistive random access memories (so-called Spin-RAMs). Among the magnetic materials with perpendicular MCA, $D0_{22}$-Mn–Ga alloys have attractive features of experimentally demonstrated the high perpendicular MCA (K_u > 1.0 MJ/m^3), the high Curie temperature (T_C=730K) and the small saturation magnetization (M_S=0.25μ_B/atom) due to the antiferromagnetic behavior [1,2]. Furthermore, a recent experiment succeeded to fabricate thin films of $D0_{22}$-MnGe and to obtain the high uniaxial anisotropy and small saturation magnetization[3].

In this study, we have investigated the spin dependent transport properties of MgO-based MTJs with $D0_{22}$-Mn_3Ga or Mn_3Ge by using the first-principles electronic and ballistic-transport calculations. First, we calculated the band-structures of bulk $D0_{22}$-Mn_3Ga and Mn_3Ge. We found that Mn_3Ga has the totally symmetric Δ_1 band crossing the Fermi level both in the majority- and minority-spin state in contrast to ferromagnetic transition metals such as bcc-Fe[2]. On the other hand, the Mn_3Ge has the Δ_1 band around the Fermi level only in the majority-spin state. Since the Fermi level of Mn_3Ga in the minority-spin state is located at the valence band edge of the Δ_1 state, an additional valence electron due to replacement of Ga by Ge causes the half-metallic electronic structure on the Δ_1 state. Note that the Fermi level of Mn_3Ga and Mn_3Ge in the majority-spin state is located in the middle of the Δ_1 band. This means that Mn_3Ge has a possibility to show large TMR effects in MgO-based MTJs.

Then, we calculated TMR ratios of Mn_3Ga/MgO(1nm)/Mn_3Ga(001) and Mn_3Ge/MgO(1nm)/Mn_3Ge(001) MTJs with the MnMn- and MnGa(Ge) terminations. We found that TMR ratios of Mn_3Ga-based MTJs depend strongly on the interfacial structures, which are about 600% for the MnMn termination [2] and 35% for the MnGa termination. The relatively small TMR ratio of the MnGa termination can be attributed to the presence of the Δ_1 state around the Fermi level in both spin channels. On the other hand, we obtained over 4000% TMR ratios for both the MnMn and MnGe terminations of Mn_3Ge-based MTJs due to the half-metallic electronic structure on the Δ_1 state of Mn_3Ge. Thus, we conclude that $D0_{22}$-Mn_3Ge is a promising material providing large TMR effects as well as high K_u and small saturation magnetization.

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