A first-principles study on tunneling magnetoresistance of magnetic tunnel junctions with D022-type Mn3Ga and Mn3Ge
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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, D022-Mn–Ga alloys have attractive features of experimentally demonstrated the high perpendicular MCA ($K_u > 1.0 \text{ MJ/m}^3$), the high Curie temperature ($T_c=730\text{K}$) and the small saturation magnetization ($M_S=0.25\mu_B/\text{atom}$) due to the antiferromagnetic behavior [1,2]. Furthermore, a recent experiment succeeded to fabricate thin films of D022-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 D022-Mn3Ga or Mn3Ge by using the first-principles electronic and ballistic-transport calculations. First, we calculated the band-structures of bulk D022-Mn3Ga and Mn3Ge. We found that Mn3Ga has the totally symmetric $\Delta_1$ 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 Mn3Ge has the $\Delta_1$ band around the Fermi level only in the majority-spin state. Since the Fermi level of Mn3Ga in the minority-spin state is located at the valence band edge of the $\Delta_1$ state, an additional valence electron due to replacement of Ga by Ge causes the half-metallic electronic structure on the $\Delta_1$ state. Note that the Fermi level of Mn3Ga and Mn3Ge in the majority-spin state is located in the middle of the $\Delta_1$ band. This means that Mn3Ge has a possibility to show large TMR effects in MgO-based MTJs.

Then, we calculated TMR ratios of Mn3Ga/MgO(1nm)/Mn3Ga(001) and Mn3Ge/MgO(1nm)/Mn3Ge(001) MTJs with the MnMn- and MnGa(Ge) terminations. We found that TMR ratios of Mn3Ga-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 $\Delta_1$ 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 Mn3Ge-based MTJs due to the half-metallic electronic structure on the $\Delta_1$ state of Mn3Ge. Thus, we conclude that D022-Mn3Ge is a promising material providing large TMR effects as well as high $K_u$ and small saturation magnetization.

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