Ab-initio study on IrCrMnZ/MgO heterojunctions (Z= Al, Ga, Si, Ge)

T. Roy[1], M. Tsujikawa[1,2], M. Shirai[1,2,3]

RIEC, Tohoku Univ.[1], CSRN, Tohoku Univ.[2], CSIS (CRC), Tohoku Univ.[3]

E-mail: tufan@riec.tohoku.ac.jp

Spin-polarized conduction electrons and high Curie temperature (T_C) of Co-based Heusler alloys have made these systems attractive in spintronics applications. Co_2MnSi/MgO/Co_2MnSi(001) is the most studied MTJ based on Heusler alloys [1]. However, the lattice mismatch between Co_2MnSi and MgO is about 5% [1]. Recently, we successfully predicted and fabricated CoIrMnAl, which has excellent lattice matching with MgO, but its T_C is in the moderate range (~ 400 K) [2,3]. Recently, we extended our research activity to Co-free Heusler alloys [4]. In the pursuit of predicting new promising Heusler alloys, we investigate IrCrMnZ (Z= Al, Ga, Si and Ge) systems and their heterojunction with MgO along (001) directions. We found that IrCrMnZ have ferrimagnetic ground state, with highly spin-polarized Δ_1 state. The electronic structure of the bulk phases is presented in Fig. 1. Within mean-field-approximation, we obtained T_C higher than 1,000 K for IrCrMnZ except IrCrMnSi ($T_C \approx$ 800 K), because of a strong exchange coupling between nearest neighboring Mn and Cr spins.

Furthermore, we studied IrCrMnZ/MgO (001) heterojunctions for both IrCr- and MnZ-terminated interfaces, in which Ir and Cr or Mn and Z atoms are located on the top of O atoms of MgO depending on the termination. For every junction, the MnZ-terminated interface is energetically favorable. Interfacial lattice mismatch is about 1%, which could minimize misfit dislocation. Apart from the IrCrMnSi/MgO junction, the high spin polarization at the interface is maintained. We further discuss the spin-dependent transport properties of IrCrMnZ/ MgO/IrCrMnZ (001) MTJs.

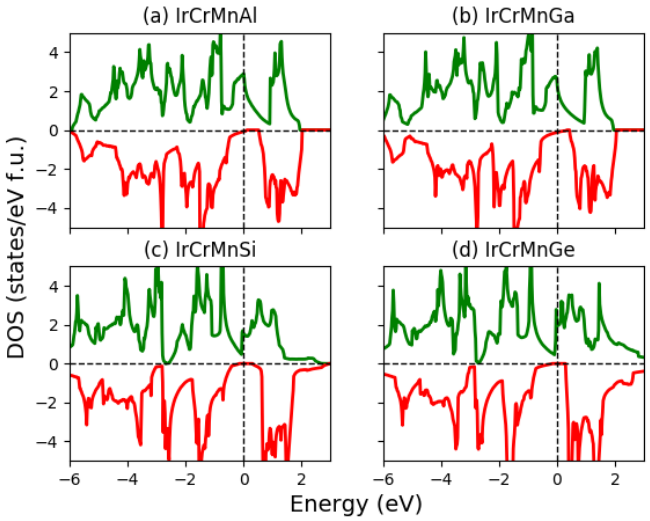

Fig. 1. Density of states calculated for (a) IrCrMnAl, (b) IrCrMnGa, (c) IrCrMnSi, (d) IrCrMnGe. The Fermi level is set at 0 eV.

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