Half-metallic Mn_2RuAl/MgO (001) heterojunctions: An *ab intio* study

◦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

In spintronics applications, materials possessing high spin polarization and high Curie temperature (T_C) are highly desired. Many Co-based Heusler alloys are known to have these features. Recently we extended our research to exploration of Co-free Heusler alloys with high T_C and high spin polarization at the Fermi level [1]. Based on first-principles calculations, we studied Mn_2RuAl full Heusler alloy in its bulk form and its heterojunctions with MgO. Mn_2RuAl crystallizes in cubic Hg_2CuTi-type inverse Heusler structure. The magnetic ground state is ferrimagnetic with net magnetic moment of 1.0 μ_B, which is consistent with the previous report [2]. The Curie temperature is predicted to be 670 K within a mean-field approximation. The electronic structure is nearly half-metallic in its bulk phase as shown in Fig. 1(a).

Thereafter, we studied Mn_2RuAl/MgO (001) heterojunctions for both the MnAl and MnRu terminations, in which Mn atoms are located on top of O atoms. It turns out that the MnAl-terminated interface is energetically more favorable than the MnRu-terminated one. We observed that the heterojunction remains perfectly half-metallic for the MnAl terminated case, whereas in the MnRu termination, it preserves relatively high spin polarization (82%) at the Fermi level (see Figs. 1(b) and 1(c)). Note that the lattice mismatch between MgO and Mn_2RuAl is only 0.25%. All these features could make Mn_2RuAl a potential candidate for electrodes of MgO-based magnetic tunnel junctions (MTJs). We discuss the temperature dependence of tunneling magnetoresistance in Mn_2RuAl/MgO/Mn_2RuAl MTJs on the basis of the magnetic stiffness of Mn_2RuAl beneath the interface with MgO.

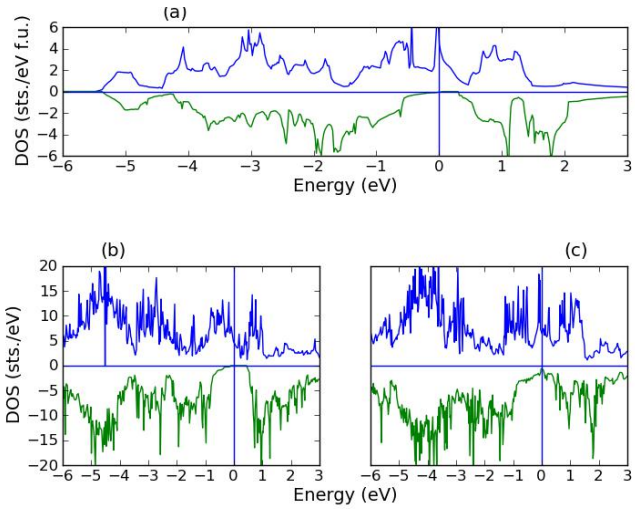

Fig. 1. Density of states calculated for (a) bulk Mn_2RuAl and Mn_2RuAl/MgO (001) heterojunctions with (b) MnAl- and (c) MnRu-terminated interfaces.

This work was in part supported by JST CREST (No. JPMJCR17J5) and CSRN, Tohoku University.

[1] Y. Onodera *et al.*, Jpn. J. Appl. Phys., in press (https://doi.org/10.35848/1347-4065/ab9c75).

[2] S. Ghosh *et al.*, Phys. Scr. **94**, 125001 (2019).