Heavy metal capping and strain effects on magnetocrystalline anisotropy of 5*d* transition metal/Fe/MgO: A-first principles study

P. Taivansaikhan*, S. H. Rhim and S. C. Hong†
Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Ulsan 680-749, Republic of Korea
†Corresponding author e-mail: schong@ulsan.ac.kr

Adding heavy metals to 3*d* TMs is one of ways to enhance MCA, utilizing the strong SOC of heavy metals. In this presentation, we report capping effect on magnetocrystalline anisotropy (MCA) of 5*d* transition metal (TM)/Fe/MgO (TMs= Hf, Ta, W, Re, Os, Ir, Pt, and Au) using a first-principles study. All TM/Fe/MgO except the cases of W and Pt retain the perpendicular MCA (PMCA) of Fe/MgO without the TM capping. In particular the late elements of Ir and Os show giant PMCA.

We will also report effect of lattice mismatch coming from different substrates by calculating MCA as a function of 2D lattice constant. The MCAs of TM/Fe/MgO are not so sensitive to compressive strain except W and Pt, as shown in Figure 1. However, compressive strain (up to 4 %) on W/Fe/MgO and Pt/Fe/MgO yields meaningful changes on their MCAs, even switching of in-plane MCA into PMCA for Pt/Fe/MgO. We will further elucidate physical origin of capping and strain effects on MCAs of TM/Fe/MgO.

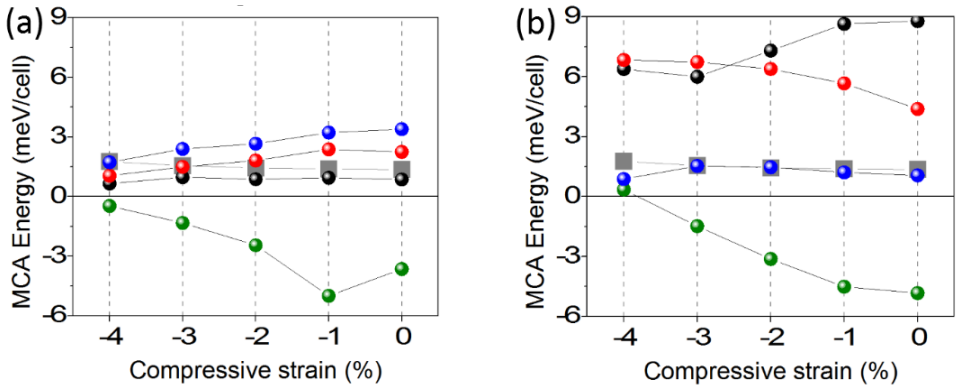

Fig. 1. MCA energy of 5d TM/Fe/MgO under strain. (a) The early TMs on Fe/MgO and (b) the late TMs on Fe/MgO. Black, red, green, and blue-balls denote Hf (Os), Ta (Ir), W (Pt), and Re (Au) on Fe/MgO, respectively, while grey-square represents Fe/MgO.