Capping and strain induced modification on magnetocrystalline anisotropy:5*d* transition metal/Fe/MgO

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Recently, magnetic tunnel junctions consist of transition metal capping/ferromagnetic metal/insulator (capping/metal/insulator) have triggered an overwhelming interest because of its strong PMCA as well as huge magnetoresistance. However, the origin of the PMCA is still poorly understood. Moreover, strain can be considered as one factor to engineer MCA, since lattice mismatch occurs quite often. In this talk, first-principles calculations of TM/Fe/MgO [TMs= Hf, Ta, W, Re, Os, Ir, Pt, and Au] reveal systematically that magnetocrystalline anisotropy (MCA) is tremendously affected by the 5*d*-TM capping as well as interfacial strain. All TM/Fe/MgO except the W and Pt show perpendicular MCA. In particular, the cappings by Re (+3.25 meV/cell), Ir (+4.48 meV/cell) and Os (+8.52 meV/cell) enhance MCA gigantically. On the other hand, the MCA is less affected by strain except for W and Pt. Interestingly, in W and Pt cappings, transition from in-plane to perpendicular MCA occur at 4% compressive strain.

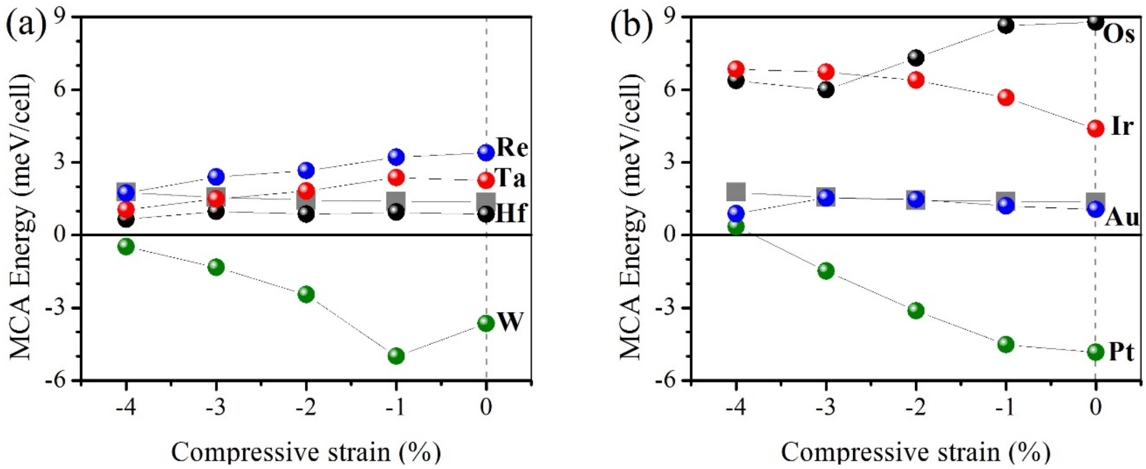

Fig. 1. MCA energy of 5d TM/Fe/MgO under different strain. (a) early TMs on Fe/MgO and (b) late TMs on Fe/MgO. Black, red, green, and blue-balls denote Hf (Os), Ta (Ir), W (Pt), and Re (Au) on Fe/MgO, respectively, while grey-square represents Fe/MgO.