

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Strain effect on magnetocrystalline anisotropy of 5d TM/Fe and TM/Fe/MgO(001) (TM=Ta, Ir, Pt, Au): A first principles study¹ PUREV TAIVANSAIKHAN, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Ulsan 680-749, Republic of Korea, DORJ ODKHUU, Department of Physics, Incheon National University, Incheon 406-772, Republic of Korea, SUNG-HYON RHIM, SOON CHEOL HONG, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Ulsan 680-749, Republic of Korea — Strain effect on magnetization and magnetocrystalline anisotropy (MCA) of TM/Fe(001) [TM=Ta, Ir, Pt and Au] with and without MgO(001) substrate has been investigated using first-principles calculations. It is found that perpendicular MCA of Pt/Fe(001) changes to in-plane MCA in the presence of MgO substrate, where lattice is extended by 3.8% with respect to that without MgO. For Ta/Fe(001) and Au/Fe(001), PMCA is significantly enhanced by the MgO substrate, whereas MCA of Ir/Fe(001) remains in-plane. Furthermore, thickness dependence of MCA on both the TM and Fe layers will be also discussed.

¹Supported by Basic Research Program (2010-0008842) and Research Centers Program (2009-0093818) through National Research Foundation of Korea.

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Date submitted: 14 Nov 2014

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