Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Electric field-driven magnetocrystalline anisotropy switching of Fe/MgO: Towards full understanding from first principles K. NAKAMURA, T. AKIYAMA, T. ITO, Mie University, M. WEINERT, University of Wisconsin-Milwaukee, A.J. FREEMAN, Northwestern University — Controlling magnetic properties by an external electric field (E-field) is a key challenge in modern magnetic physics. Here, we investigate the magnetocrystalline anisotropy (MCA) modification by an E-field for thin films of Fe on a MgO substrate from first principles. Calculations were carried out by using the film FLAPW method[1] with full optimization by atomic force calculations in which an E-field effect is incorporated.[2] Results predict that the Fe/MgO interface gives rise to a large out-of-plane MCA due to an Fe-O hybridization at the interface and a MCA modification is induced by a change in the d-band structures at the Fermi level when an E-field is introduced. Importantly, however, the existence of an interfacial iron- oxide layer between the Fe layer and the MgO substrate is found to play a key role in demonstrating an electric field-driven MCA switching, i.e., from out-of-plane MCA to in-plane MCA — as observed in experiments.[3]

[1]Wimmer, Krakauer, Weinert, and Freeman, PRB **24**, 864 (1981).
[2]Nakamura et al., PRL **102**, 18702 (2009); Weinert et al., J. Phys.: Condens. Matter **21**, 084201 (2009).
[3]Shiota et al., Appl. Phys. Express **2**, 063001 (2009).

Kohji Nakamura
Mie University

Date submitted: 18 Nov 2009 Electronic form version 1.4