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Electric-field control and effect of Pd capping on interface magnetocrystaline anisotropy of FePd-based thin films PHUONG-VU ONG, NICHOLAS KIOUSSIS, Department of Physics and Astronomy, California State University Northridge, Northridge, California 91330, USA, P. KHALILI AMIRI, K.L. WANG, Department of Electrical Engineering, University of California, Los Angeles, California 90095, USA, GREGORY P. CARMAN, Department of Mechanical and Aerospace Engineering, University of California, Los Angeles, California 90095, USA, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, California 92697-4575, USA — Using *ab initio* electronic structure calculations, we investigate effects of electric field and heavy metal cap of Pd on magnetocrystalline anisotropy (MCA) of FePd ultrathin film. It is revealed that while Pd ions favor in-plan MCA, perpendicular MCA of the thin film is mainly due to the spin-orbit coupling between unoccupied Fe d_{xy} and occupied Fe $d_{x^2-y^2}$ states. The sensitivity of the surface anisotropy energy to applied electric field is 18 fJ.V^{-1}.m^{-1}. By mapping distributions of d-orbital characters over electronic states, mechanism of the field control of anisotropy is elucidated. Furthermore, MCA of the thin film is shown to be strongly affected by Pd capping and a switching from perpendicular to in-plane anisotropy can be obtained by tuning the capping thickness. The effect is explained by spin-orbit couplings of the spin-polarized quantum well states induced by the Pd cap. These results are of practical importance since in magnetic junctions the ferromagnetic layer is mostly capped by a heavy metal electrode.

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