MECHANISM OF HIGH MAGNETIC ANISOTROPY IN Fe₃Pt THIN FILMS

Oleg Mryasov¹,² and Takao Suzuki ¹

¹ University of Alabama, MINT Center, Tuscaloosa.
² University of Alabama, Department of Physics, Tuscaloosa.

Many applications of magnetic material application require large perpendicular magnetic anisotropy energy (MAE). These application include permanent magnets, magnetic recording MRAM media. Materials with improved MAE properties continue to be in high demand with goal of finding composition, phases, structures with large and controllable anisotropy. Here we summarize experimental [1,2] and computational results for unusual phase of Fe₃Pt alloys, modified m-DO₁₉ structure stabilized in this film form on MgO substrates. Understanding mechanism of observed magnetic anisotropy in this unusual phase is the main goal of present study. We investigate MAE of m-DO₁₉ Fe₃Pt using electronic structure calculations with spin orbit coupling included within self-consistent constrained density functional theory calculations [3,4]. We find in agreement with experimental results [3] and earlier calculations [4] that for m-DO₁₉ Fe₃Pt grown on (111) MgO substrate Kₐeff is easy plane. We further find that ratio of K₁ and K₂ can be varied in a broad range due to lattice constant variation relevant to the growth results for different MgO substrate orientations. We identify m-DO₁₉ as important factor for unusual MAE of this phase. We argue that other hcp based phases for example for Co-W alloy could exhibit large magnetic anisotropy.

References: