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MECHANISM OF HIGH MAGNETIC ANISOTROPY IN Fe_3Pt THIN FILMS

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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 Fe_3Pt alloys , modified m-DO_{19} 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-DO_{19} Fe_3Pt 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-DO_{19} Fe_3Pt grown on (111) MgO substrate K_{eff} is easy plane. We further find that ration of K_1 and K_2 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- DO_{19} 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:

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