BEYOND RARE EARTH: INVESTIGATING FECO ALLOYS UNDER STRAIN FOR PERMANENT MAGNETS

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In modern technology, permanent magnets play a crucial role. Today ś strongest permanent magnets use rare earth elements, such as samarium and neodymium. However, these magnets have serious limitations, including a relatively low Curie temperature (T_C), restricting their application. Furthermore, the rare earth metals market experienced a significant price increase around 2011, prompting intensified research into alternative materials without these elements. Currently, rare earth element prices have risen again, so the quest for alternative permanent magnets remains relevant. FeCo alloys, particularly the $Fe_{0.4}Co_{0.6}$ body centered tetragonal alloy with lattice parameters c/a ratio close to 1.22, show promise, as indicated by Burkert *et al.*[1]. However, subsequent studies revealed structural relaxation in thin films with tetragonal deformation, leading to a body centered cubic structure for films thicker than about 15 monolayers.

Our research aims to broaden the understanding of magnetism in uniaxially deformed $Fe_{1-x}Co_x$ by investigating magnetic moments, magnetocrystalline anisotropy energy (MAE), and T_C of the alloys with Co content x in 0-1 range and c/a ratio ranging from 0.64 to 1.4. Density functional theory calculations using the full-potential local-orbital (FPLO)[2] and spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR)[3] codes provide magnetic moments and MAE. We approximate disordered alloys using two effective medium methods: the virtual crystal approximation (in FPLO) and the coherent potential approximation (in SPR-KKR). T_C is also determined with two methods: a qualitatively approximate disordered local moment method[4] and a quantitative method utilizing the intersection of Binder cumulants for two differently sized supercells to incorporate finite-size scaling in Monte Carlo calculations, which were conducted with UppASD code[5,6]. The approach reveals an additional high MAE region for squeezed structures with x higher than 0.7 and c/a lower than 0.85. Notably, the bct system with $c/a \approx 0.82$ lies along the fcc $\rightarrow$ hcp transition; so, we also investigated bct(0.82) $\rightarrow$ fcc and bct(0.82) $\rightarrow$ hcp transitions.

W.M., J.M., and M.W. acknowledge the financial support of the National Science Centre Poland under the decision DEC-2018/30/E/ST3/00267. Part of the computations were performed on resources provided by the Poznan Supercomputing and Networking Center (PSNC).

J.Á.C-R acknowledges the support of Olle Engkvist ś Foundation and Knut and Alice Wallenberg Foundation for financial support. The UppASD simulations were enabled by resources provided by the National Academic Infrastructure for Supercomputing in Sweden (NAISS) at the NSC Centre, partially funded by the Swedish Research Council through grant agreement no. 2022-06725.

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