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Anisotropy of Iron-Series Permanent Magnets[1] RALPH SKOMSKI, Dept. Phys. & Astr. and NCMN, University of Nebraska, G. C. HADJIPANAYIS, Dept. Phys. and Astr., University of Delaware, D. J. SELLMYER, Dept. Phys. & Astr. and NCMN, University of Nebraska — Element-strategic considerations have sparked renewed interest in rare-earth-free permanent magnets, but the prediction of the magnetocrystalline anisotropy from the atomic structure is still in its infancy, and there are no rules predicting the d anisotropy as function of the atomic structure. We have obtained tight-binding estimates for a variety of clusters and etxtended structures of different symmetry and d-band filling. A expected, the anisotropy strongly oscillates as a function of the d-band filling. Our calculations indicate that nearly filled d bands tend to yield anisotropy parallel to the pair axis. Sites with trigonal symmetry support bigger anisotropies than cubic and tetragonal environments, but this is a crystal- field effect similar to that in $BaFe_{12}O_{19}$ rather than a band-structure effect. Shape anisotropy is important in alnico- type nanostructured permanent magnets. We find a maximum of the energy product as a function of packing fraction, namely a maximum value of $\mu_o M_s^2/12$ realized at a volume fraction of 2/3. For $Fe_{65}Co_{35}$, this yields an upper limit of 390 kJ/m^3 [49 MGOe].

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