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Effects of Co doping on the metamagnetic states in fcc $Fe_{1-x}Co_x$[1]

ROMEO DE COSS, FILIBERTO ORTIZ-CHI, Departamento de Física Aplicada, Cinvestav-Merida, Yucatán, Mexico — It is well known that fcc-Fe have shows metamagnetism, with a low-spin state (LS) at small volume and and a high-spin state (HS) at large volume in the total-energy vs volume curve. In this work, we have studied the evolution of the metamagnetic states in the $Fe_{1-x}Co_x$ alloy as a function of Co concentration by means of first principles calculations. The ground state properties were obtained using the Full-Potential Linear Augmented Plane Waves method and the Generalized Gradient Approximation for the exchange-correlation functional. The alloying was modeled using the self-consistent virtual crystal approximation. The magnetic states are obtained from the total-energy as a function of the spin moment calculations, obtained using the Fixed Spin Moment methodology. For fcc-Fe, we found that the ground state corresponds to the LS state. Increasing the Co concentration the HS state decrease in energy. Thus, for $x = 0.05$ the energy of the LS and HS states is practically the same, corresponding to a spin-glass state. The LS state is substituted by a paramagnetic state for $x > 0.3$ of Co concentration. Interestingly, for the alloy with $x \sim 0.35$ the total-energy vs volume curve shows "effective symmetry," which is expected to exhibit invar behavior.

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