

Abstract Submitted
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Ab-initio study of the structural and magnetic properties for the fcc Fe-Co alloy.¹ FILIBERTO ORTIZ-CHI, Cinvestav Unidad Mérida, AARÓN AGUAYO, Universidad Autónoma de Yucatán, ROMEO DE COSS, Cinvestav Unidad Mérida — We have studied the structural and magnetic properties of the fcc Fe-Co alloy by means of first-principles calculations. For modeling the alloy we have used the ab-initio self-consistent Virtual Crystal Approximation. The ground state properties was calculated with the Fixed Spin Moment methodology and the Full-Potential LAPW method. For the exchange-correlation potential we have used the Generalized Gradient Approximation. For ferromagnetic fcc-Fe we find an anti-invar behavior (ELS<EHS) with the co-existence of two ferromagnetic states (metamagnetism). For the fcc-FeCo alloy we find a progressive evolution of the metamagnetism with the Co concentration. Using the calculated total-energy vs the lattice parameter and the Boltzman distribution function, we have obtained the lattice parameter as function of the temperature, in order to determine the thermal expansion coefficient α as function of the Co-concentration. We find that Fe65Co35 show an invar behavior.

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