AB INITIO STUDY OF ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF $Gd(Ni_{1-x}Fe_x)_3$ ALLOYS

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9.7 cm

The electronic structure and magnetic properties of $Gd(Ni_{1-x}Fe_x)_3$ alloys were measured recently by means of different methods. The measurements indicated several intriguing properties of the alloy. In the Ni-rich region the alloys display magnetocaloric properties but with relatively low Curie temperature. Increasing the Fe contents results in a linear decrease of the saturation magnetization while the Curie temperature reach the maximum at $x \simeq 0.5$. The XPS valence band measurements reveal the presence of correlation between the magnetic properties and electronic structure near the Fermi level.

In this paper we present the theoretical investigations of the electronic and magnetic properties of $Gd(Ni_{1-x}Fe_x)_3$ alloys. The electronic structure calculations were carried out with the use of *ab initio* FP-LAPW method. The GGA-LSDA form of exchange-correlation potential was applied with addition of the enhanced Coulomb correlation term for Gd-4f states. To simulate fractional concentrations the supercell approach was implemented. Using the results of *ab-initio* calculations the many particle, generalized s-f model for disordered alloy with strongly correlated band electrons was parametrized. Applying the Coherent Potential formalism the concentration dependence of Curie temperature and electrical conductivity was determined. The theoretical results are compared with experimental data.

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