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On the origin of the magnetic susceptibility anomaly in nearly ferromagnetic alloys ROMEO DE COSS, Cinvestav, Department of Applied Physics, Cordemex 97310, Mérida, Mexico, AARÓN AGUAYO, Universidad Autónoma de Yucatán, Mérida, Yucatán, México, FILIBERTO ORTIZ-CHI, Cinvestav, Department of Applied Physics, Cordemex 97310, Mérida, Mexico — The magnetic susceptibility of the Ni-Rh and Ni-Cu alloys shows an anomaly near the transition from ferromagnetism to paramagnetism. In order to contribute to understand this phenomenon, we have studied the electronic and magnetic properties of the $Ni_{1-x}Cu_x$ alloy by means of first principles calculations. The ground state properties were obtained using the Full-Potential Linear Augmented Plane Waves method. The alloying was modeled using the self-consistent virtual crystal approximation. The spin magnetic susceptibility is calculated from the total energy as a function of the spin moment, obtained using the Fixed Spin Moment methodology. We found that the calculations predict correctly the reduction of the magnetic moment with the Cu concentration and that the critical concentration where the magnetic moment goes to zero is $x_c = 0.5$, in excellent agreement with the experimental data. The calculated magnetic susceptibility is in good agreement with the experimental data in the whole range of concentrations for the $Ni_{1-x}Cu_x$ alloy, in particular the anomaly present at $x \approx 0.4$ is reproduced by the calculations. This research was supported by Conacyt-México under Grant No. 83604.

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