Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Effect of magnetism on the vibrational properties of the Ni-Cu alloy: a first-principles study[1] OMAR DE LA PENA-SEAMAN, IVAN BUSTAMANTE-ROMERO, Institute of Physics (IFUAP), Benemerita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BOHNEN, Institute of Solid State Physics (IFP), Karlsruher Institute of Technology (KIT) — We have studied the lattice dynamical properties of the $Ni_{1-x}Cu_x$ magnetic alloy within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation for modeling the alloy. The system has been investigated for both non-magnetic (NM) and ferromagnetic (FM) phases. The performance of LDA and GGA exchange-correlation functionals on the properties under study was analyzed. The structural optimization for each magnetic phase, NM and FM, in the full range of concentrations ($0 \leq x \leq 1$) was performed. By studying the electronic structure and its evolution as a function of x, we determined the FM-NM phase transition at $x \approx 0.45$. The calculated full phonon dispersion for NM and FM phases are compared between each other and with experimental data available in the literature at different concentrations. In addition, a detailed analysis of the force constants average coupling was performed, finding a clear signature of the magnetism effects on the vibrational properties for the Ni-Cu alloy.

[1]This research was supported by PROMEP/103.5/12/4367 under project BUAP-PTC-299

Omar De la Pena-Seaman
Institute of Physics (IFUAP),
Benemerita Universidad Autonoma de Puebla (BUAP)

Date submitted: 08 Nov 2012 Electronic form version 1.4