Effect of magnetism on the vibrational properties of the Ni-Cu alloy: a first-principles study\textsuperscript{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\textsubscript{1-x}Cu\textsubscript{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 ≤ x ≤ 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 ≈ 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.

\textsuperscript{1}This research was supported by PROMEP/103.5/12/4367 under project BUAP-PTC-299