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The Role of Lattice Dynamics on The Thermal Properties of Cu-Ni Alloys BERK ONAT, Informatics Institute, Istanbul Technical University, Istanbul, Turkey, SONDAN DURUKANOGLU, Faculty of Engineering and Natural Sciences, Nanotechnology Research and Application Center, Sabanci University, Istanbul, Turkey — We have investigated Cu-Ni alloys with both disorder and order phases in fcc structures to analyze the effect of temperature dependent vibrational thermodynamical properties. The interactions between the atoms in the model systems are defined using an EAM type potential, specifically developed for Cu-Ni alloys. Vibrational thermodynamic functions are determined within the harmonic approximation of lattice dynamics and the vibrational densities of states are calculated using real space Green's function technique. In addition, through ab-initio calculations we have estimated the electronic contributions to set the ground for a comparative discussion. Our results show that the overall characteristics of thermodynamic functions of Cu-Ni alloys of varying concentrations are governed by the lattice vibrations. We will present our results for free energy, heat capacity and entropy of ordered/disordered Cu-Ni alloys with the experimental findings and discuss the electronic, anharmonic and lattice dynamic contributions.

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