Local force constants of transition metal dopants in a nickel host: Comparison to Mossbauer studies

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Abstract: We have used the x-ray absorption fine-structure technique to obtain temperature-dependent mean-squared relative displacements for a series of dopant atoms in a nickel host. We have studied the series Ti, V, Mn, Fe, Nb, Mo, Ru, Rh, and Pd doped into Ni, and have also obtained such data for pure Ni. The data, if interpreted in terms of the correlated Einstein model of Hung and Rehr, yield a ratio of a (host-host) to (host-impurity) effective force constant, where the effective force constant is due to a cluster of atoms. We have modified the method of Hung and Rehr so that we obtain a ratio of near-neighbor single spring constants, rather than effective spring constants. We find that the host to the 4d impurity force constant ratio decreases monotonically as one increases the dopant atomic number for the series Nb, Mo, Ru, and Rh, but after a minimum at Rh the ratio increases sharply for Pd. We have compared our data to Mossbauer results for Fe dopants in Ni, and find qualitative disagreement. In Mossbauer studies, the ratio of the Ni-Ni to Fe-Ni force constant is found to be extremely temperature dependent and less than one. We find the corresponding ratio, as interpreted in terms of x-ray absorption spectra and the correlated Einstein model, to be greater than one, a result that is supported by elastic constant measurements on $Ni_xFe_{(1-x)}$ alloys.

Index Keywords: iron; manganese; molybdenum; neodymium; nickel; rhodium; ruthenium; titanium; transition element; vanadium; absorption spectrophotometry; article; chemical structure; comparative study; elasticity; force; mathematical analysis; measurement; model; Mossbauer spectroscopy; structure analysis; temperature dependence; X ray analysis

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