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Local Forces of Transition Metal Dopants in a Nickel Host: Comparison to Local Magnetism and Mossbauer Results

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Beamline(s): X11A

Introduction: We have used the X-ray absorption edge 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, Cr, Mn, Fe, Nb, Mo, Ru, Rh, and Pd doped into Ni, and have 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 host-host to host-impurity effective force constant. For the case of Fe doped into Ni, there is qualitative disagreement between our results and the results for a force constant ratio using the Mossbauer effect. In the Mossbauer studies, the ratio of a Ni-Ni to Fe-Ni force constant is found to be extremely temperature dependent and less than one. We find the analogous ratio, as determined by X-ray absorption spectra and the correlated Einstein model, to be greater than one.

Methods and Materials: Random solid solution alloys were manufactured by arc melting and appropriate annealing under vacuum in sealed quartz tubes. The alloys were checked by x-ray diffraction and had the expected structures. Near neighbor distances agreed with previous results obtained by Scheuer and Lengeler¹, for those alloys studied by both experimental groups. Temperature dependent XAFS was obtained, and the dopant – near neighbor mean-squared relative displacement (MSRD) determined as a function of temperature, between about 40 degrees K and room temperature. Silicon (111) monochromator crystals were used at the X-11 A beam line of the NSLS. The plot of dopant – near neighbor MSRD versus temperature was fit to an Einstein model functional relationship and the slope of the MSRD versus temperature curve determined by extrapolating to the high temperature region where the curve is linear and the equipartition of energy theorem holds. In the correlated Einstein model of Hung and Rehr², the ratio of the slope for host-impurity MSRD versus T, divided by the corresponding slope for host – host (pure Ni) MSRD versus T, yields a ratio R_X of effective local near neighbor force constants K , where

$$1. R_X = (K_{\text{Host-Host}} / K_{\text{Host-Impurity}})$$

Results: Plots of R_X versus dopant atomic number Z were constructed for the 3d and 4d dopant series. For the 3d dopants the R_X value is about 1.2 except for a maximum for V dopants. For the V dopant case the R_X value is Greater than 1.5. We note that only for the V dopant case, for the systems studied here, is there a substantial local magnetic moment anti-aligned relative to that of the ferromagnetic Ni host³. For the 4d dopants the value of R_X dips to a minimum of about 0.9 for the case of Rh in Ni, the only case we find for which an R_X value exists that is less than unity. For the case of Fe in Ni, we disagree with the results of Mossbauer spectroscopy. In Mossbauer spectroscopy, ratios of force constants A_{100} have been measured for dopant – host relative to host – host near neighbors^{4,5}. The ratio R_M is determined where

$$2. R_M = [A_{100}(\text{host-host})] / [A_{100}(\text{impurity – host})]$$

In the literature, R_M is found to be extremely temperature dependent and always less than one^{4,6,7}. We find R_X to be greater than one for Fe in Ni.

Conclusions: The XAFS determined ratio R_X is not quite the same quantity in principle as the Mossbauer ratio R_M . The quantity R_X is a ratio of effective spring constants in which the host and near neighbor atoms are displaced from each other along the line between them, about their common center of mass, in a cluster including the absorber and back scatterer and all their near neighbors². The ratio R_M is a ratio of single spring constants for displacement of the central atom along the (100) direction, all other atoms being fixed in place. However, although we would expect a numerical difference may exist between R_M and R_X , we cannot account for the *qualitative* difference between the XAFS and Mossbauer results for Fe in Ni. In a nutshell, Mossbauer studies find the Fe – Ni single spring force constant to be greater than the host – host force constant of pure Ni. Our XAFS studies find the effective Fe – Ni force constant to be less than the corresponding host – host force constant of the pure Ni matrix. We feel it is important to resolve this discrepancy.

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