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Iron d-band Occupancy in NiAl Intermetallics

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Iron when sitting at Al sites in intermetallic NiAl has been shown to expand the lattice and produce an unusual solid solution softening effect. First-principles calculations predict that an Fe atom develops a large magnetic moment and an expanded effective atomic size when it occupies a site on the Al-sublattice(1). In this study, electron energy loss spectroscopy was used to examine the magnetic characteristics of Fe substituted on the Ni and Al sites in the B2 ordered NiAl compound. We have found a higher L-edge branching ratio for Fe when on the Al site compared to Fe on the Ni site. This corresponds to an enhanced magnetic moment of Fe confirming the theoretical predication.

(1) C.T. Liu, C.L. Fu, L.M.Pike and D.S. Easton, *Acta Materialia* **50** 3203 (2002).