

Composition Dependence of Ni 2p Core Level Shift in Fe_{1-x}Ni_x Alloys

Authors : Shakti S. Acharya, V. R. R. Medicherla, Rajeev Rawat, Komal Bapna, Deepnarayan Biswas, Khadija Ali, K. Maiti

Abstract : The discovery of invar effect in 35% Ni concentration Fe_{1-x}Ni_x alloy has stimulated enormous experimental and theoretical research. Elemental Fe and low Ni concentration Fe_{1-x}Ni_x alloys which possess body centred cubic (bcc) crystal structure at ambient temperature and pressure transform to hexagonally close packed (hcp) phase at around 13 GPa. Magnetic order was found to be absent at 11K for Fe₉₂Ni₈ alloy when subjected to a high pressure of 26 GPa. The density functional theoretical calculations predicted substantial hyperfine magnetic fields, but were not observed in Mossbauer spectroscopy. The bulk modulus of fcc Fe_{1-x}Ni_x alloys with Ni concentration more than 35%, is found to be independent of pressure. The magnetic moment of Fe is also found to be almost same in these alloys from 4 to 10 GPa pressure. Fe_{1-x}Ni_x alloys exhibit a complex microstructure which is formed by a series of complex phase transformations like martensitic transformation, spinodal decomposition, ordering, mono-tectoid reaction, eutectoid reaction at temperatures below 400°C. Despite the existence of several theoretical models the field is still in its infancy lacking full knowledge about the anomalous properties exhibited by these alloys. Fe_{1-x}Ni_x alloys have been prepared by arc melting the high purity constituent metals in argon ambient. These alloys have annealed at around 3000C in vacuum sealed quartz tube for two days to make the samples homogeneous. These alloys have been structurally characterized by x-ray diffraction and were found to exhibit a transition from bcc to fcc for $x > 0.3$. Ni 2p core levels of the alloys have been measured using high resolution (0.45 eV) x-ray photoelectron spectroscopy. Ni 2p core level shifts to lower binding energy with respect to that of pure Ni metal giving rise to negative core level shifts (CLSs). Measured CLSs exhibit a linear dependence in fcc region ($x > 0.3$) and were found to deviate slightly in bcc region ($x < 0.3$). ESCA potential model fails to correlate CLSs with site potentials or charges in metallic alloys. CLSs in these alloys occur mainly due to shift in valence bands with composition due to intra atomic charge redistribution.

Keywords : arc melting, core level shift, ESCA potential model, valence band

Conference Title : ICMSCMP 2015 : International Conference on Material Science and Condensed Matter Physics

Conference Location : Berlin, Germany

Conference Dates : May 21-22, 2015