World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:9, No:05, 2015

Composition Dependence of Ni 2p Core Level Shift in Fe1-xNix 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 Fe1-xNix alloy has stimulated enormous experimental and theoretical research. Elemental Fe and low Ni concentration Fe1-xNix 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 Mossbaur spectroscopy. The bulk modulus of fcc Fe1-xNix alloys with Ni concentration more than 35%, is found to be independent of pressure. The magnetic moment of Fe is also found be almost same in these alloys from 4 to 10 GPa pressure. Fe1-xNix 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. Fe1-xNix 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 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

Open Science Index, Materials and Metallurgical Engineering Vol:9, No:05, 2015 publications.waset.org/abstracts/23324.pdf