Orissa Journal of Physics
ISSN 0974-8202

Vol. 22, No.2
August 2015
pp. 237-239

XRD Peak Shift in $Fe_{1-x}Ni_x$ binary alloys

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Received : *5.6.2015* ; *Accepted : 20.07.2015*

Abstract : Polycrystalline alloys viz. $Fe_{0.5}Ni_{0.5}$ and $Fe_{0.3}Ni_{0.7}$ have been prepared using arc melting method and were investigated structurally using X-ray Diffraction Technique (XRD). XRD of both the above samples confirms that they are in fcc phase. A peak shift is observed towards higher angles with increase in Ni concentration. Such rigid shift in the reflections to higher angles could be due to the lattice contraction upon Ni substitution.

Keywords: Arc Melting, X-ray Ray Diffraction, fcc, alloys

PACS Numbers : 61.10.Nz, 61.66.Dk

1. Introduction

FeNi binary alloys have wide range of application viz. laser cavity construction, dimensional stabilizers, super-tanker construction, etc. Scientists and physicists are more excited about some anomalies like invar effect [1] and elinvar effect [2] observed in some compositions. Changing the Ni concentration the coefficient of thermal expansion (CTE) of $Fe_{1-x}Ni_x$ can be tuneable[3]. Elemental Fe and low Ni concentration $Fe_{1-x}Ni_x$ alloys possess body centred cubic (*bcc*) crystal structure whereas increase in Ni concentration form 40% to 90% in $Fe_{1-x}Ni_x$ alloys result face centered cubic (fcc) crystal structure for all the alloys.[4] A hexagonally close packed (*hcp*) phase is observed at a pressure around 13 GPa. Magnetism was found to be absent at 11K for $Fe_{92}Ni_8$ alloy when subjected to a high pressure of 26 GPa.[5] The properties of FeNi alloys are important for understanding the geophysics of the core of the Earth and also for understanding the propagation of high-pressure shock waves through engineering materials. A martensitic transformations (*fcc* to *bcc*) is observed for FeNi alloys with Ni content between 30-34% at around 250K while cooling down the specimen.

2. Sample Preparation

$Fe_{1-x}Ni_x$ (x=0.5, 0.7) alloys were prepared by co-melting the stoichiometric amounts of high purity (99.99%) metals under argon atmosphere in a water cooled copper hearth in a mini arc furnace. The stoichiometric amounts of pure Fe and Ni had been loaded onto a copper hearth which was sucked into the vacuum chamber from bottom against gravity while evacuating the chamber using a rotary pump. Gas line and the vacuum chamber had been purged three times with argon gas using a rotary pump connected to the vacuum chamber. A vacuum of 10^{-3} Torr was obtained and then argon gas was injected through a leak valve up to a pressure of few Torr. A titanium ball kept on the edge of the hearth was melted to remove oxygen impurities present in the chamber. Titanium sublimed when heated. Titanium possesses multiple valence states and thus forms various oxide compounds during sublimation and gets adsorbed on the walls of the chamber in solid form and thus the pressure in the chamber improves. The constituent metals of the alloys had been co melted keeping the high melting point metal on top so that it receives more heat and gradually heat is transferred to the metal at the bottom. This helps in maintaining the stoichiometric ratio of the constituents of supplying differential heating to the metals and melting them simultaneously. Melting was repeated several times by reorienting the obtained chunk each time. All the compositions of FeNi alloys as mentioned above were prepared by melting stoichiometric amounts of required metals. Both the samples under study had been verified for single phase formation using XRD technique [6]. XRD pattern was indexed using powderX software.

3. Results and Discussion

Figure 1 shows the XRD patterns of $Fe_{0.5}Ni_{0.5}$ and $Fe_{0.3}Ni_{0.7}$ alloys. Clean XRD patterns with no impurity phases have been observed for both the alloys. XRD patterns have been indexed using POWDERX software assuming fcc structure. All the reflections are indexed. Observed reflections <111>, <200>, <220> and <311> have non zero structure factor and give rise to sharp reflections in

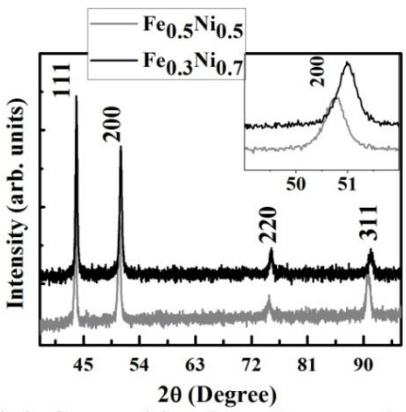

Fig1: Composition dependence peak shift

XRD. As the observed intensity id proportional to the magnitude of structure factor, the structure factor of <111> set of planes is the maximum for fcc structure. When Ni concentration is increased from 50% to 70 % then shift in peaks is observed. We have considered the peak shift for 200 lattice plane which is found to be 0.2^0 towards right. So a positive shift is observed in high Ni content alloy for all the peaks indexed in figure1. The positive shift indicates that when Ni is introduced into Fe matrix in fcc region, lattice contracts and the lattice parameter decreases. We have also observed that peak shift is more for reflections at higher angles.

4. Conclusion

FeNi alloys have been prepared by arc melting method using hugh purity Fe and Ni metals. Alloys produced are of high purity with no impurity phases. Alloys prepared in this study ar of fcc structure. Positive shift is observed for all the peaks with the increase in Ni content.

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