Orissa Journal of Physics
ISSN 0974-8202

Vol. 23, No.2
August 2016
pp. 179-186

Structural Analysis of the Cu-Mn Alloys using XRD Technique

S K PARIDA

Department of Physics, Institute of Technical Education and Research,
Siksha 'O' Anusandhan University, Khandagiri Square, Bhubaneswar 751030, Odisha, India
*e.mail: skparidaphysics@gmail.com

Received: 5.6.2016 ; Revised : 9.7.2016 ; Accepted : 31.7.2016

Abstract : Co-melting technique is used to prepare $Cu_{0.5}Mn_{0.5}$ alloys. The products were synthesized by the fusion of high pure copper (99.99%) and manganese (99.99%) metals in presence of inert atmosphere. The lattice constant, unit cell volume, structure and inter-planar spacing between two given plane are evaluated by XRD analysis. The average crystallite size is calculated using the Scherrer's equation. Due to intermixing of Cu atoms in the matrix of Mn, a lattice strain is produced in the alloys. Williamson-Hall (W-H) analysis is used to study the individual contributions of crystallite sizes and lattice strain on the peak broadening of the $Cu_{0.5}Mn_{0.5}$ alloys.

Keywords: Co-melting, Crystallite size, W-H analysis, lattice strain & peak broadening.

1. Introduction

The structural behavior of a material from its composition and microstructure is the real dream for a materials scientist. Till today we are far away from a complete understanding of the mechanical behavior of metals. An alloy is a metallic solid solution or a mixture of two or more elements. Complete solid solution alloys give single phase microstructure, while partial solutions give two or more phases that may or may not be homogeneous in distribution, depending on thermal treatment. Alloys usually have shown different properties from those of the constituent elements [1-5]. One of the vital issues in condensed matter physics is the role played by disorder on electronic properties of solids. Materials are never perfectly ordered and some amount of disorder is always present. Due to disorder, local environment around different atomic sites exhibits small changes [6-14]. Microscopic properties like electron binding energy and

magnetic moment are different from perfectly periodic lattice. Many of the challenging problems within solid state physics today are in some way or other connected to disorder. Weak disorder may be defined as a perturbation of the perfect crystalline order. To this category belong defects, vacancies and dislocations which are frequently observed in real materials. Strong disorder signifies a marked departure from crystalline order. The degree of deviation of physical properties from perfectly periodic lattice measures the amount of disorder present. CuMn alloys have been extensively studied recently due to their potential applications [15-17] in different areas like engraving industry, graphic plates, commentators and bridge bearing plates, specialized anti-corrosive applications etc. This fact encourages us to study the mechanical and structural properties of CuMn alloys with 50% at. wt.

In this paper, structural behaviors of $Cu_{0.5}Mn_{0.5}$ alloys have been discussed. The physical quantities such as lattice constant and unit cell volume are evaluated. The mechanical strain that produced due to interaction of Cu atoms in Mn matrix during the alloy formation is calculated using the Williamson-Hall relation.

2. Experiment

High pure Cu (99.99%) and Mn (99.99%) metal powder were taken in a stoichiometry weight ratio of 1:1 in a recrystallized alumina crucible. The crucible was placed in the hot zone of a high temperature furnace for co-melting at a temperature of 1373K with a variation of ± 1° C. As the melting point of Cu (1085 °C) is less than melting point of Mn (1246 °C), it is necessary to fuse both the metals simultaneously; the temperature of the furnace was raised to 1373 K with a heating rate of 600 °C per hour in presence of inert atmosphere. The materials were kept at the same temperature for five hours for uniform mixing of Cu and Mn with each other and then it was rapidly cooled by switching off the furnace at the high temperature. The fused samples were now considered for various characterizations. The phase and structural analysis of the samples were carried out using X-ray diffraction (XRD), where CuKα (λ=1.540 Å) is taken as the X-ray irradiation source. The strain produced in $Cu_{0.5}Mn_{0.5}$ alloys due to introduction of Cu atoms into the Mn matrix is calculated using the Williamson-Hall relation.

3. Results and Discussion

3.1 *XRD Analysis*

The XRD pattern of $Cu_{0.5}Mn_{0.5}$ alloys are shown in Fig. 1. The lattice parameter, volume and space group of pure Cu and Mn metals from literature have mentioned in Table 1.

Table: 1 Lattice parameter, volume and space group of pure Cu and Mn elements.

Sample	**Structure**	**Lattice parameter (Å)**	**Volume $(Å)^3$**	**Space group**
Cu	Cubic	a = 3.65	47.24	$Fm\bar{3}m$ (JCPDF #040836)
Mn	FCC Cubic	a = 8.85	68.23	$I-43m$ (JCPDF #040783)

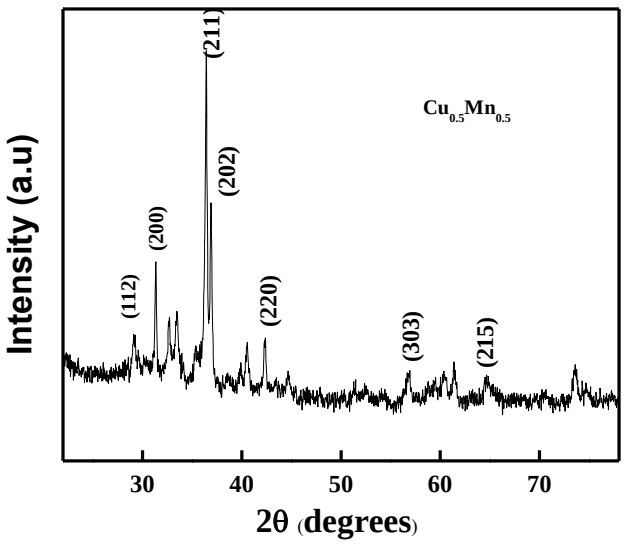

Fig. 1: The XRD patterns of $Cu_{0.5}Mn_{0.5}$ alloys recorded using CuKα radiation source.

Table: 2 Lattice parameters, volume and space group of $Cu_{0.5}Mn_{0.5}$ alloys

Sample	Structure	Lattice parameter (Å)	Volume $(Å)^3$
$\mathbf{Cu_{0.5}Mn_{0.5}}$	FCC Cubic	a = 8.658	67.22

The XRD analysis indicates that CuMn system has the cubic structure. The lattice parameters and volume of the unit cell for the system have been calculated using Unit-Cell-Win software which is presented in Table 2. From Table 1 and Table 2, it is confirmed that during preparation CuMn alloy system, Cu atoms incorporate into Mn matrix.

3.2 *Scherrer Method*

The XRD technique can be used to estimate the peak broadening with crystallite size and lattice strain due to crystal imperfections, dislocation and defect [18]. The crystallite size of the $Cu_{0.5}Mn_{0.5}$ alloys were determined by the X-ray line broadening method using the Scherrer equation: $= \frac{k\lambda}{\beta cos\theta}$, where λ is the wavelength of the used X-ray source (λ = 1.54056 Å), k is anisotropic constant (~ 0.89), θ is the peak position and β is the full width at half maximum measured in radians [19]. Therefore, on the simplification of the Scherrer formula $D = \frac{k\lambda}{\beta cos\theta} \Rightarrow cos\theta = \left(\frac{k\lambda}{D}\right)\frac{1}{\beta}$ .The plots were drawn taking $\frac{1}{\beta}$ on the *x*-axis and $cos\theta$ along *y*-axis for $Cu_{0.5}Mn_{0.5}$ alloys as shown in fig.2. A linear fit line to the experimental data can be used to calibrate the slope $\frac{k\lambda}{D}$ and ultimately the average particle size for $Cu_{0.5}Mn_{0.5}$ alloy is 34.6 nm.

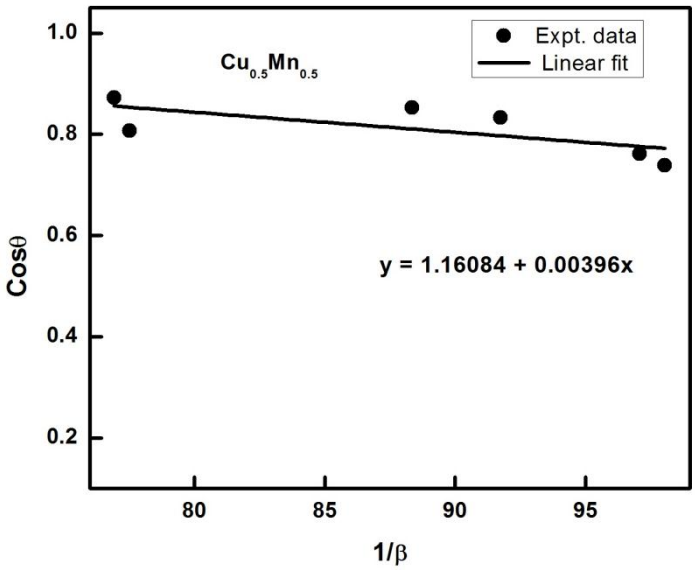

Fig. 2: Scherrer plot of $Cu_{0.5}Mn_{0.5}$ alloys. Fit to the data, the crystalline size *D* is extracted from the slope of the fit line.

3.3 *Williamson-Hall Method*

The crystal imperfections and distortions introduce the strain-induced broadening in the alloys and which is related by $\varepsilon \approx \beta/tan\theta$. This implies that there will be a new method called Williamson-Hall (W-H) method in which the strain varies with $tan\theta$ instead of $\frac{1}{cos\theta}$ mentioned in Scherrer method. The W-H method includes the idea of additive property of the total broadening produced in the alloys. They assumed the total broadening in breadth of Bragg's peak is the sum of the broadening due to crystallite size and strain [20]. The distinct role of the θ induced size and strain broadening and can be evaluated by using Williamson-Hall method of analysis [21].

Therefore,

$$\beta = \beta_{size} + \beta_{strain} ,\Rightarrow \beta = \frac{k\lambda}{Dcos\theta} + 4\varepsilon tan\theta \Rightarrow \beta cos\theta = \frac{k\lambda}{D} + 4\varepsilon sin\theta$$

The above equation is true only when the material is isotropic nature; it means the material properties are independent of the direction along which they are measured. The model is developed using the concept that the strain assumed to be uniform in all crystallographic direction called Uniform Deformation model (UDM). Under the UDM calculation; the term $4sin\theta$ was plotted along *x*-axis and $\beta cos\theta$ plotted along *y*- axis. The slope and *y*-intercept of the fitted line

represents the strain and particle size. In my experiment, during the formation of $Cu_{0.5}Mn_{0.5}$ alloy, Cu atoms enter into the Mn matrix. Due to strong interaction of Cu and Mn atoms in alloys, a mechanical strain is produced and can be calculated using the Williamson-Hall relation $\beta cos\theta = \frac{k\lambda}{D} + 4\varepsilon sin\theta$, where ε is the strain produced in alloys. The particle size and strain in the sample are 33.9 nm and 0.0027 respectively.

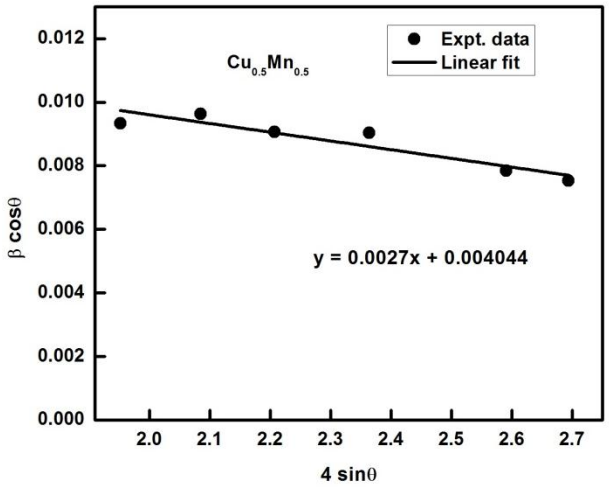

Fig. 3. The Williamson-Hall analysis of $Cu_{0.5}Mn_{0.5}$ alloys assuming Uniform Deformation Model (UDM). Fit to the data, the strain is extracted from the slope and crystalline size *D* is extracted from the *y*-intercept of the fit.

The particle size and lattice strain of the $Cu_{0.5}Mn_{0.5}$ alloys system have been calculated by Scherrer and Williamson-Hall method. A comparative study of these alloys system is mentioned in Table 3.

Table:3 Comparative studies of particle size and strain by Scherrer and Williamson-Hall method

Sample	**Scherrer method**	**Williamson-Hall method**	
	Particle size (*D*) in *nm*	**Particle size (*D*) in *nm***	**Strain (ε)**
$Cu_{0.5}Mn_{0.5}$	34.6	33.9	0.0027

The average particle size estimated through Scherrer method and W-H method are very close to each other whereas the lattice strain produced in the $Cu_{0.5}Mn_{0.5}$ alloys is 0.0027.

4. Conclusion

$Cu_{0.5}Mn_{0.5}$ alloys were prepared by co-melting technique. The structural properties were investigated using X-ray diffraction technique. The CuMn system has the cubic structure. The average crystallite size calculated using the Scherrer equation for $Cu_{0.5}Mn_{0.5}$ alloys is 34.6 nm and the result is in good agreement with Williamson-Hall method. W-H analysis and size-strain plot method were used to study the individual contributions of crystallite sizes and lattice strain on the peak broadening of the $Cu_{0.5}Mn_{0.5}$ alloys. The lattice strain of the $Cu_{0.5}Mn_{0.5}$ alloys is 2.7×10^{-3}.

References

[1] K Siegbahn, *Rev.Mod. Physics* 54, 709 **(1982)**

[2] C Norris and HP. Myers, *J. Phys. F: Metal Phys*. **1**, 62 (1971)

[3] AD McLachlan, J G Jenkin, RCG Leckey and J Liesegang, *J. Phys. F: Metal Phys*. **5** , 2415 (1975)

[4] K Berndt, U Marx and O Brummer, *Phys. Stat. Sol*. **B 94**, 541 (1979)

[5] KC. Prince and V Chab, *J. Electron Spec. and Relat. Phen.* **52**, 61-66 (1990)

[6] Tsuneaki Miyahara et. al, *J. Phys. Soc. of Japan* **58**, 2160-2166 (1989)

[7] Z. W. Lu, S.-H. Wei and Alex Zunger, *Phys. Rev*. **B 44**, 10470 (1991)

[8] S.-J. Oh and Tschang-Uh Nahm, *J. Elec. Spec. and Relat. Phen*. **78**, 43 (1996)

[9] G G. Kleiman, R Landers, S G C. de Castro and P A P. Nascente, *Surface Science* **287**/**288**, 749 (1993)

[10] K Kokko et.al, *Phys. Rev*. **B 60**, 4659 (1999)

[11] A K Santra and C N R Rao, *Applied Surface Science* **84**, 347 (1995)

[12] I Coulthard and T. K. Sham, *Phys. Rev. Lett*. **77**, 4824 (1996)

[13] J S Faulkner et.al, *Phys. Rev. Lett*. **81**, 1905 (1998)

[14] W Olovsson, IA Abrikosov and B Johansson, *J. Elect. Spec. and Relat. Phen*. **127**, 65 (2002)

[15] B Mouffok, H Feraoun and H Aourag, *Material Letters* **60**, 1344 (2006)

[16] L L Chang, S Wen, SL. Li, XD. Zhu, and XJ Shang, *Materials Characterization* **108**, 145 (2015)

[17] Y Z Tian, JJ. Li, P Zharg, SD. Wu, ZF Zhang, M Kwasaki, and TG. Langdon, *Acta Materialia* **60**, 269 (2012)

[18] KD. Rogers and P Daniels, *Biomaterials* **23**, 2577 (2002)

[19] BD Cullity and SR Stock, Elements of X-ray Diffraction 3rd edn. (Upper Saddle River, NJ: Prentice Hall) (2001).

[20] M Birkholz, Thin Film Analysis by X-ray Scattering. Wiley-VCH Verlag GmbH and Co. KGaA, Weinheim, (2006).

[21] A Khorsand Zak, WH. Abd. Majid, ME Abrishami, Ramin Yousefi, *Solid State Sciences* **13**, 254 (2011)