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The structure and thermal parameters of ordered $Cu_{65}Fe_{10}Pd_{25}$ ternary alloy

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ABSTRACT

Structural and thermal parameters have been studied in $Cu_{65}Fe_{10}Pd_{25}$ alloy during order–disorder (O–D) transformation using differential scanning calorimetry (DSC) and high temperature X-ray diffraction (HTXRD). The results reveal that the $Cu_{65}Fe_{10}Pd_{25}$ alloy undergoes an O–D transformation at T_c=797 K. The alloy shows $L1_2$ type ordering below T_c and has disordered face centered cubic (fcc) structure above T_c. The lattice parameter shows a positive deviation from Vegard's rule which may be related to the weakening of interatomic forces by the addition of Fe. The integrated intensity data obtained from the diffraction experiments was utilized to determine the coefficient of thermal expansion ($\alpha(T)$), mean square amplitude of vibration ($\overline{u^2}(T)$) and Debye temperatures (Θ_D) during the O–D transformation. The abrupt change in the value of lattice parameter and coefficient of thermal expansion at T_c shows that the nature of O–D transition is first order. These results have been discussed by comparing them to those for Cu_3Pd alloy.

1. Introduction

The formation of ordered structures and the development of long-range order (LRO) in the arrangement of atoms of different type is characteristic of many alloy systems. Atomically ordered alloys possess specific physical properties. The copper–palladium (Cu–Pd) alloys are of great interest with regard to their application as well as from the point of view of the scientific understanding. Structurally ordered Cu_3Pd alloys have a face centered cubic (fcc) lattice of the $L1_2$ type, which depends on temperature, composition and thermal treatment [1,2].

Ordered Cu–Pd and other transition metals alloys are extensively used in electronic industry as electro-contact materials. Therefore, it is necessary to know the role of the mechanisms of scattering of charge carriers and the peculiarities of the Fermi surface in the development of transport properties of such alloys [3]. These alloys have received a lot of attention from researchers because Cu–Pd alloys exhibit variety of ordered phases. It has been reported that disordered fcc Cu–Pd alloys, in the range of about 8–30 at% Pd, transform into a variety of ordered structures below 773 K [4].

Thermal expansion is one of the fundamental physical properties in materials science and engineering. INVAR alloys are one of the examples which are being used in precise mechanical machines [5]. The mechanical properties of alloys are also directly linked to their characteristic Debye temperature (Θ_D). Determination of Debye temperature is given of great importance in crystallography because of its use in structural refinement and explanation of various properties. The scientific understanding and technological importance of thermal expansion of the alloys has lead to its measurement for various materials [6,8,17].

The structural properties of alloys can be modified by the addition of ternary alloying elements. The addition of Fe in Cu–Pd alloys is expected to improve the order–disorder transformation temperature (T_c) and magnetic properties of these alloys. In the present study, structure and thermal properties of $Cu_{65}Fe_{10}Pd_{25}$ alloy are investigated by using high temperature X-ray diffraction (HTXRD). Thermal parameters were determined by using the Bragg line displacement method [6]. Thermal parameters of $Cu_{65}Fe_{10}Pd_{25}$ alloy in both ordered and disordered states have been determined and compared.

2. Experimental method

The sample of $Cu_{65}Fe_{10}Pd_{25}$ alloy (5 g) was prepared from spectroscopically pure Cu, Fe and Pd metals by using arc-melting furnace with water cooled copper hearth under an atmosphere of purified argon. The samples were remelted six times to ensure the

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homogeneity of the alloy constituents. The ingot was sealed in quartz tubes under a vacuum of 2.0×10^{-3} Pa and annealed for 20 h at 1273 K in order to homogenize them. Thin slices were cut from the ingot, one of which was annealed at 723 K for one week and subsequently furnace cooled to room temperature to avoid the accumulation of surplus vacancies.

The composition of $Cu_{65}Fe_{10}Pd_{25}$ alloy was determined by using electron probe microanalyzer (EPMA, JXA-8100, JEOL). The composition was measured at ten different points and the average composition was taken as the true composition of the alloy. The homogeneity variation of the alloy was found to be less than 1 at%.

The sample was then grinded and polished to produce a smooth surface suitable for HTXRD experiments. The HTXRD experiments were performed on a Bruker D8 AXS diffractometer fitted with an evacuated chamber having a Pt–Rh heater and precise temperature measurement arrangement. Diffraction patterns were taken in the scattering angle range of 15–135° under θ–θ geometry with divergence and receiving slits of 0.5° using Ni-filtered CuKα radiation. The tube parameters were 45 kV and 40 mA. The HTXRD experiments were performed in the range of 300–1173 K with an increment of 50 K in general but 10 K near the order–disorder (O–D) transition temperature (T_c). The data was corrected for instrumental errors by using a highly pure silicon powder as external standard.

The thermal analysis of the sample was performed on a differential scanning calorimeter (DSC, model SBT-Q600) under nitrogen atmosphere at a heating rate of 20 K/min up to a temperature of 1500 K.

3. Results and evaluation

3.1. Differential scanning calorimetry

Fig. 1 shows the DSC thermograms of $Cu_{65}Fe_{10}Pd_{25}$ alloy. The change in heat flow beyond 1395 K reflects the on-set of melting of the alloys. A small endothermic peak at 797 K was observed which shows change of phase from ordered to disordered. These results are consistent with those obtained from HTXRD explained later.

3.2. Structural study by X-ray diffraction

Fig. 2 shows the X-ray diffraction patterns of $Cu_{65}Fe_{10}Pd_{25}$ alloy taken at various temperatures. The prominent feature of all

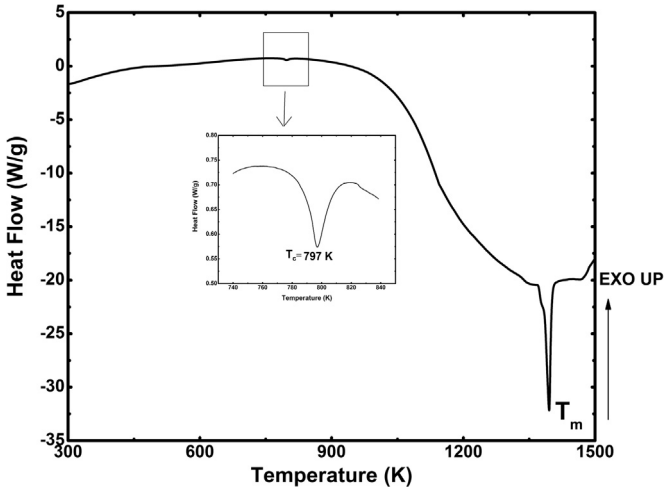

Fig. 1. Thermogram of $Cu_{65}Fe_{10}Pd_{25}$ alloy recorded on a differential scanning calorimeter at a heating rate of 20 K/min.

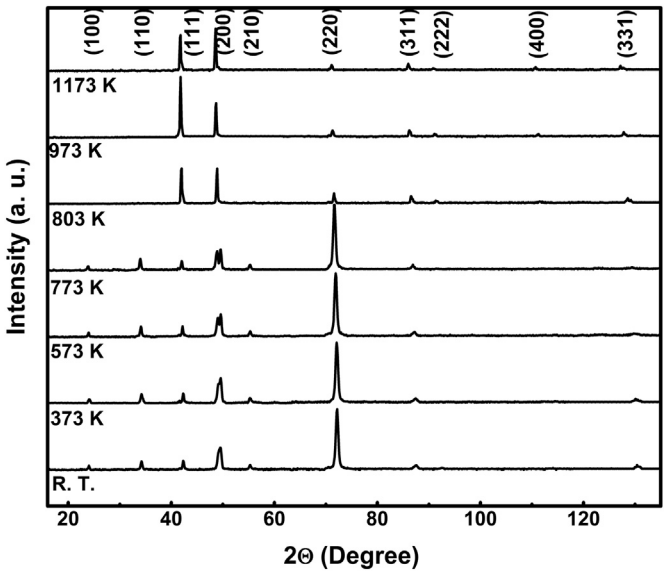

Fig. 2. X-ray diffraction patterns of $Cu_{65}Fe_{10}Pd_{25}$ alloy taken at various temperatures during in-situ diffraction experiments.

patterns is the presence of sharp (100)-, (110)-, and (210)-superlattice reflections and (111)-, (200)-, (220)-, (311)-, (222)-, (400)- and (331)-fundamental reflections. The small peak adjacent to (200) originated from the Pt–Rh heater used in the HTXRD experiments. The superlattice reflections disappear above 797 K, which indicate the O–D transformation.

The structure factor for $Cu_{65}Fe_{10}Pd_{25}$ alloy with $L1_2$ type ordered structure is:

$$F_{Fundamental} = c_{Pd}f_{Pd} + 3\left(c_{Cu}f_{Cu} + c_{Fe}f_{Fe}\right) \quad (1)$$

$$F_{Superlattice} = c_{Pd}f_{Pd} - \left(cC_{Cu}f_{Cu} + c_{Fe}f_{Fe}\right) \quad (2)$$

The observed superlattice and fundamental reflections obey Eqs. (1) and (2), respectively, which confirm that the alloy has $L1_2$ type ordered structure.

The true value of lattice parameter at room temperature was obtained by the extrapolation of lattice parameters for each reflection against Nelson–Riley function and was found to be 3.697 ± 0.002 Å. The value of lattice parameter shows a positive deviation from Vegard's rule (3.673 Å). This result is consistent with the Cu_3Pd alloy [4]. The data obtained from HTXRD experiments was utilized to obtain the temperature dependence of lattice parameter (Fig. 3(a)) and the thermal parameters (Figs. 3 (b) and 4(a and b)).

The O–D transition observed in diffraction patterns at $T_c = 797$ K is also reflected in Fig. 3(a). The sudden change in lattice parameter at T_c indicates that this transition is a first order transition [16]. A change $\Delta a = 0.010$ Å was observed in the value of lattice parameter at T_c.

Two methods have been reported for the determination of thermal parameters from the X-ray diffraction data. One is the use of integrated intensity data of all Bragg reflections in the pattern at a fixed temperature (usually referred to as Wilson-plot method [18]). The second method employs the temperature dependence of integrated intensity of a high angle Bragg reflection (usually referred to a Bragg-line displacement method) and is used to eliminate the effects of preferred orientation. The later method has been used in the present study and results are given in the following sections.