Structural Behaviour of $Cu_{100-X}Zr_X$ Alloy on Various Temperature Range

Shrivastava Anik[1], Choudhary Sana[1], Khan Misbah[1], Ansari Ilma[1]

[1] Department of Physics, G M Momin Women's College, Bhiwandi, Maharashtra, 421308

Abstract: Molecular dynamics simulations were carried out on system $Cu_{100-X}Zr_X$ (X=50, 55, 60) by employing the embedded atom method (EAM) based potentials. In this work is the structural behaviour of $Cu_{100-X}Zr_X$ (X=50, 55, 60) were studied by calculating radial distribution functions at various temperature range.

Keywords: Molecular dynamics, Radial distribution function, Metallic glass.

Introduction

The excellent properties of metallic Cu-Zr alloy over their counterparts have attracted the attention of the scientific and industrial communities [1–4]. The challenge lies in predicting the internal structure of alloys in order to predict glass forming compositions and thus, has been an active area of research [5–10].Several empirical rules and criteria have been proposed to predict the structure of alloy system to predict glass forming ability (GFA) followed by rigorous experimentation [11–14]. Certainly, these rules have played an important role in providing enough information to synthesize bulk metallic glasses (BMGs), but experiments have also suggested that a minor change in composition can effectively change GFA [15]. Hence, it is essential to employ simulations and modelling methods for the study of structure of alloy to reduce the associated time, energy and costs associated with these studies. Binary alloys are basically simple to model and as a result of the possibility of wide glass forming compositions in Cu–Zr binary systems. Additionally, Cu–Zr systems have experimental data availability [13, 14] for the comparison, and accessibility of EAM potentials for Cu and Zr elements for simulation. One such simulation method which can be used to understand the behaviour of metallic glasses at the atomic level and to predict GFA is Molecular dynamics (MD).

In the present work, MD simulations have been applied to binary $Cu_{100-X}Zr_X$ (X=50, 55, 60) alloys in order to study the structural behaviour of alloy system by calculating radial distribution functions at various temperature range.

Method

The molecular dynamics simulation (MD) of the copper-zirconium alloy was carried out using constant number of particles-pressure-temperature (NPT) ensemble. To model the atomic interactions, EAM potentials provided with in Large-scale atomic/molecular massively parallel simulator software (LAMMPS) [16,17] was used to simulate the Cu 100-x Zr x (x = 50, 55, 60) alloy systems. The simulated system consisted of 5000 atoms in a cubic unit cell of B2 structure with in periodic boundary conditions. First, the model system was heated at 300 K to relax the system, then temperature was raised up to 3000 K and held there for 400 picoseconds (ps) in order to allow atoms to forget their initial structure. After that, the system was rapidly cooled to 2100 K and then slowly cooled from liquid state to 300 K at a cooling rate of 1 × 1011 K/s. At each temperature, the quantities of interest were obtained by taking averages over 80 ps. The MD time step selected for the simulation was 2 fs (1 fs = 1 × 10 −15 second).

Result

Structural features of a system, particularly for liquids and amorphous structures can be calculated using radial distribution function (RDF). The RDF can be calculated as

$$\int_{r=0}^{\infty} \rho g(r).4\pi r^2 dr = N - 1$$

Where N denotes the number of atoms in shell of thickness dr at distance r in the simulation cell

Figure (1) presents the RDF of the model structure $Cu_{100-X}Zr_X$ (X=50,55,60) at room temperatures 300 K. We started our simulation from the FCC structure, which can be observe from the RDF that the first- nearest-neighbour positions are occupied by dissimilar atoms only and the Second nearest neighbour positions are occupied by similar atoms only

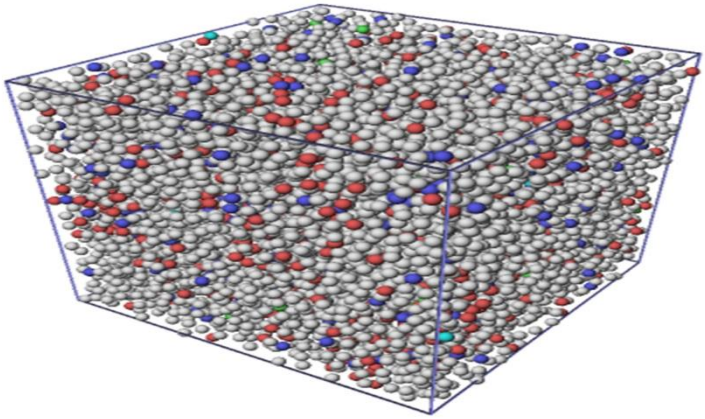

Figure (1) Supercell containing 5000 atoms after cooling

However, at 3000 K the emergence of wide peaks in the RDF Fig.2 shows that the model has melted and in a liquid state. For example, g(r) Cu-Zr indicates a peak at the first nearest-neighbour distance 2.44 Å, which is close to the value in liquid state of the pure element

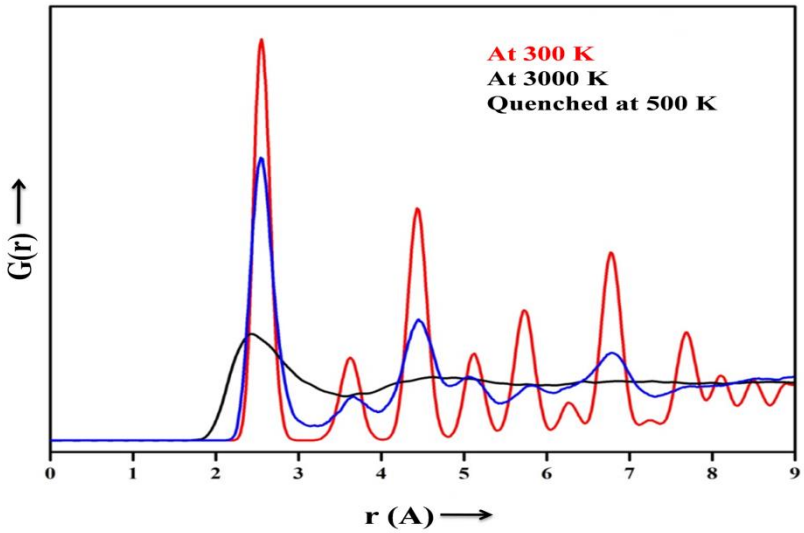

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Figure (2) RDF at 3000 K during equilibration state

Upon cooling to 300 K at the rate of 30 K/ ps, we can also see that the feature of long range disorder in the RDF Fig. (3) and the second peaks of g(r) Cu-Zr, g(r) Cu-Cu, and g(r) Zr-Zr are distinctly split as well, showing the formation of an amorphous phase. The first peak of unlike pairs is relatively sharp compared with those of like atom pairs, which qualitatively suggests a preferred interaction of unlike atom pair

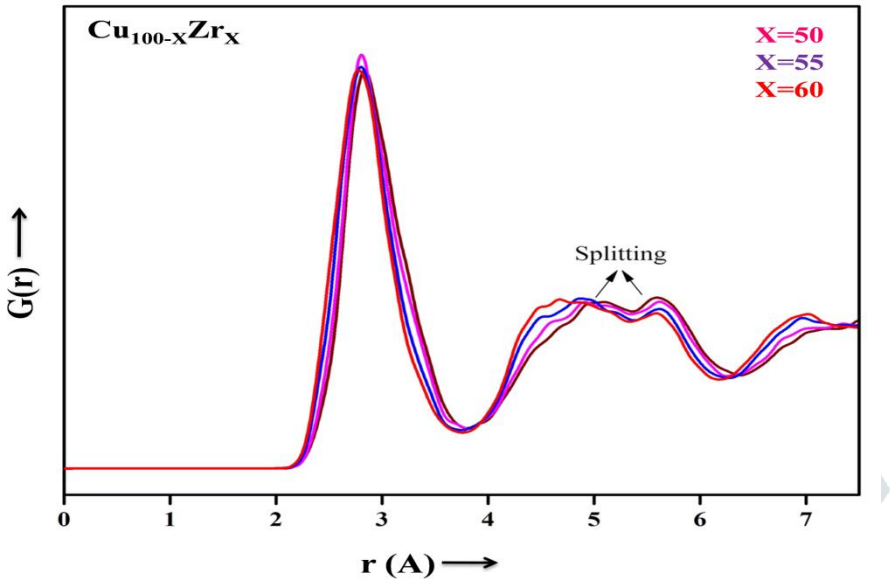

Figure (3) RDF after quenching at 300 K

However, the RDFs of $Cu_{100-X}Zr_X$ (X=50,55,60) show similar pattern with compositions, which is not fully clear, but this may happen due to the insignificant change in thermal entropy when compared to the configurational entropy of alloys, which play the important role in glass formation.

Conclusion

Radial Distribution functions (RDFs) were calculated from MD simulation, for binary $Cu_{100-X}Zr_X$ (X=50, 55, 60) to understand the structure at various temperature range. Distinct splitting of the second peaks has been observed in a Cu-Zr, which was due to randomness of atoms also an indication of glassy phase. Although RDFs are almost superimposed, irrespective of the composition variation; But they provide us a much useful information about the local structure of amorphous alloys.

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