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Molecular dynamics study of the structural and dynamical properties of binary $Cu_{50}Zr_{50}$ bulk metallic glass

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ABSTRACT

Molecular dynamics simulations were carried out on $Cu_{50}Zr_{50}$ system by employing the embedded atom method (EAM) based potentials. The evolution of structure and dynamics with temperature was discussed using radial distribution functions, the volume temperature curve, icosahedral short range order, glass transition temperature and fragility parameter. The simulated results were found in agreement with the available experimental data.

Keyword: Metallic alloys, molecular dynamics, Voronoi tessellation, glass transition temperature.

INTRODUCTION

The strengthening of metallic alloys relative to its pure metal constituents is a subject of great technological and scientific interest, and in particular, bulk amorphous alloys can have excellent strength and corrosion resistance for structural applications. These metallic amorphous phases can be produced if a molten metallic alloy is cooled at rates (10^6 K/s) which are highly adequate to suppress crystallization in the melt, and liquid-like structural configuration can be frozen into the solid state. The vitrification of a liquid metal was first reported by Clement et al. [1] in 1959 for the Au–Si alloy, when the molten state of Au75Si25 was rapidly quenched. Later, in 1969 Chen and Turnbull [2] obtained the amorphous ternary alloy for Pd–M–Si (with M = Ag, Cu, or Au). Just until 1974, a critical casting thickness of 1mm was synthesized for the Pd–T–P (T = Ni, Co, Fe) alloy [3]. In the 1980s, Turnbull et al. [4] produced glassy Pd40Ni40P20 by processing it in a boron oxide flux, and the critical casting thickness was increased to 1cm, and the first ever bulk metallic glass came into picture. Johnson et al. [5] developed a pentanary alloy based on Zr–Ti–Cu–Ni–Be in 1992, with a critical casting thickness up to 10cm; the alloy became known as Vitreloy 1, the first commercial bulk metallic glass.

However, the origin of the high GFA in BMG alloys is still unresolved issue at present time; a comprehensive analysis of the thermodynamic, structural, and kinetic properties is required, especially in the under-cooled region where the nucleation and growth or glass transition takes place. From the thermodynamic point of view and particularly in classical nucleation theory, better glass former is expected to be characterized by a greater stability in its under-cooled state against crystallization. The aim of this work was tantamount to analyze the atomic structure and dynamics through computer simulation to understand the glass formation in $Cu_{50}Zr_{50}$. In present paper, structural and dynamical properties have been studied by means of radial distribution function G(r), Voronoi tessellation and fragility parameter calculations using molecular dynamics (MD) simulations to understand the glass formation in binary $Cu_{50}Zr_{50}$. This particular alloy was chosen using that fact that it can be used as the base system for other multi-component glass former composition, and it also has available experimental data for the comparison. Computer simulation using MD is able to provide detailed information about the said properties which the experiments have limited access

MATERIALS AND METHODS

We have performed molecular dynamics (MD) simulation based on the embedded atom method potential in the constant number of particles-pressure-temperature (NPT) ensemble by using the LAMMPS code [6,7]. The MD simulations were conducted in a supercell consisted of 5000 atoms under periodic boundary conditions. To simulate a random alloy with a given composition, we randomly substituted the proper amount of copper (zirconium) atoms with equal number of zirconium (copper) atoms in the initial B2 structure. The NPT MD simulations were performed in steps of 100 K, in a temperature range from 300 to 3000 K. The temperature was high up to 3000 K in order to allow atoms to disperse and fail to remember their initial sites. Simulation time step of 2 fs was used. At each temperature, the MD simulation time for determining the properties was 160 ps. The simulated melting temperature is greater than experimentally obtained melting temperature, since model system had a free surface and the high heating rate.

RESULTS AND DISCUSSION

3.1 Radial distribution function (RDF)

RDF is one of the most powerful techniques to analyze the inherent structure of liquids and amorphous alloys. It describes the spatial distribution of all other atoms with respect to the reference atom. For bulk materials it is given by,

$$G(r) = \frac{V}{N^2}\langle \sum_i \sum_{i \neq j} \delta(r - r_{ij})\rangle \quad (1)$$

Here N is the number of atoms and, g(r) is the probability of finding the atoms in the simulation box. For random distribution, it always goes to unity. MD simulations have been performed on cubic FCC structure of Pm3m symmetry at 300K, which is ordered in nature. The system was heated at a constant heating rate of K/ps up to 3000 K and then held at that temperature for 800 ps. Later it was quenched at a cooling rate of 1×1011 K/ps from 3000 K to 300 K. RDFs for a selected system, was generated by MD simulation.

Figure 1 show typical RDF patterns of close-packed $Cu_{50}Zr_{50}$ at 300K, depicting crystalline state with well-defined RDF peaks up to 7 Å. The same figure shows a molten liquid state at 3000 K characteristics of very broad RDF peaks and vanishing peak height to be nearly indistinguishable. The RDF patterns of melt-quenched alloy structure show subtle splitting in the second RDF peak representing an amorphous state is distinguishable. Comparison among RDFs manifest that the first nearest neighbour of the crystalline structure and the amorphous structure after melt-quenching is the same 2.80 Å a median value between atomic sizes of Cu 2.6 Å and Zr 3.2 Å. The results of RDF calculation are reasonable and close to those disclosed in literature [8], thus our MD calculation seems to be convincing for current work.

3.2 Melting and glass transition

Figure 2 exhibits the change in volume as a function of temperature for $Cu_{50}Zr_{50}$ alloy systems. As the temperature of the model system is raised from 300K to 3000K with a constant heating rate, volume increases linearly up to a certain temperature. Later, at this temperature a subtle shift starts appearing in volume temperature (V-T) curve. This shift is a sign of a phase transition and tells that our system has melted. The melting represents the liquidus temperature (T_l) of this composition.

WA parameter ($R_{WA}=g_{min}/g_{max}$), which emphasizes the local character of g(r) has been used to calculate Tg of $Cu_{50}Zr_{50}$, where g_{min} is the value of g(r) at the first minimum and g_{max} is the value of g(r)at the first maximum in RDF curve. Figure (3) represents the plot between R_{WA} versus temperature. The T_g value has been deduced from the intersection point shown in the plot.

3.3 Icosahedral ordering

To study the development of icosahedral ordering in Cu50Zr50, Voronoi tessellation analysis was done. The Voronoi index < n3, n4, n5, n6 > specifies the number of faces with subscript presenting edge on Voronoi polyhedra. We have calculated Cu and Zr centred Voronoi indices from 1200 K to 300K at a step of 100K and presented their variation with temperature for Cu50Zr50 as showed in figure 4a and figure 4b. From the figures it was observed that Cu centred truncated Voronoi polyhedra < 0,2,8,2 > and icosahedra < 0,0,12,0> played central role in glass formation and their population increased up to 18 % during super cooling, but the other polyhedra such as <0,2,8,0>, <0,3,6,1>, <0,3,6,3> and <0,1,10,2> almost remained constant with temperature. On the other hand the Zr centred polyhedra like <0,3,6,4>,< 0,3,6,5>, <0,2,8,4>, <0,2,8,5>, <0,2,8,6>, <0,1,10,4>,< 0,1,10,5> and <0,0,12,4> have shown gradual change in population with the temperature. Though some Cu and Zr centred

polyhedra evolve slowly during the cooling they play an active role in slowing down of dynamics and increases viscosity of the molten alloy system.

3.4 Fragility

To confirm the analysis, fragility parameter for the selected composition for which short range order is very important were calculated at temperatures above Tg in the temperature range of 1150 K – 770. The simulation data were produced during cooling using the Green-Kubo method [9, 10] in the form of

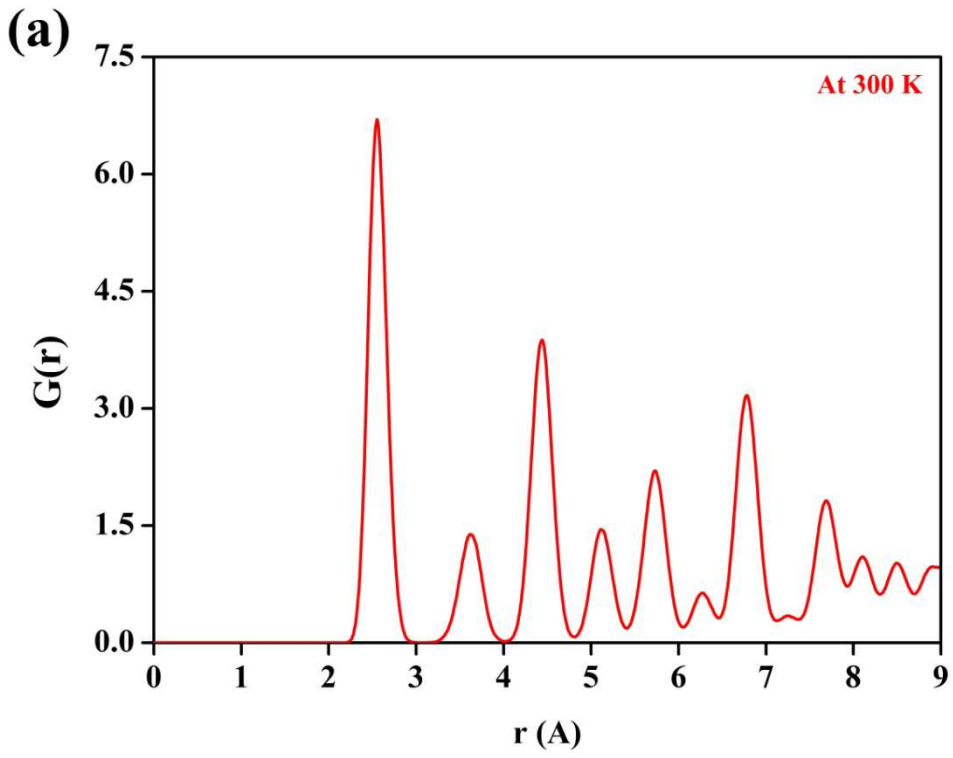
$$\eta = \frac{V}{K_B T}\int \langle p^{\alpha\beta}(t_0) p^{\alpha\beta}(t_0 + t)\rangle \, dt \qquad (2)$$

Where V is the volume of the simulation cell, KB is the Boltzmann constant, T is the temperature, denotes the ensemble average and $P_{\alpha\beta}$ are the shear component of the stress tensor. The slope of the logarithm of the viscosity with respect to the inverse temperature at viscosity 10 poise is defined as the fragility m. A strong liquid exhibits an Arrhenius type temperature dependency of the viscosity, whereas the temperature dependence of the viscosity for a fragile liquid deviates from the Arrhenius behaviour with a sudden change in the viscosity value at the glass transition temperature [11,12]. The evolution of the viscosity is represented by Vogel-Fulcher-Tammann (VFT) relation given by

$$\eta = Aexp\left(\frac{B}{T-T_0}\right) \qquad (3)$$

$$m = \frac{dlog(\eta)}{d\left(\frac{Tg}{T}\right)}|_{T=Tg} \qquad (4)$$

The viscosities obtained at different temperatures were fitted as shown in figure 5 using equation (3), since the MD simulations can determine viscosities only at temperatures considerably higher than the glass transition temperature due to time-step limitations, the slope of the fitted curve at 10 poise viscosity is defined as the measure of fragility.



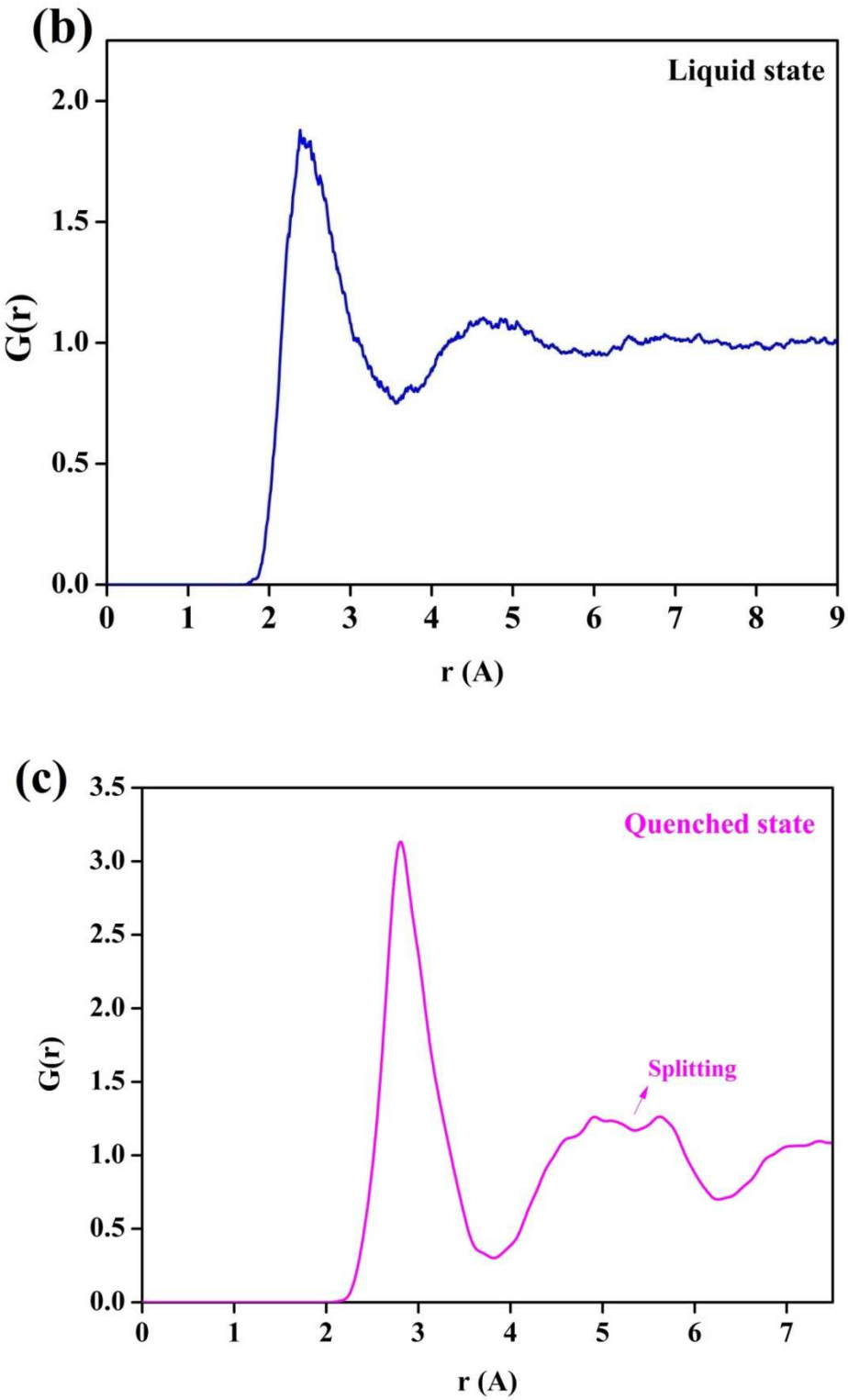


Figure 1 A typical RDF of $Cu_{50}Zr_{50}$ for (a) at 300 K (crystalline), (b) Liquid and (c) Quenched state

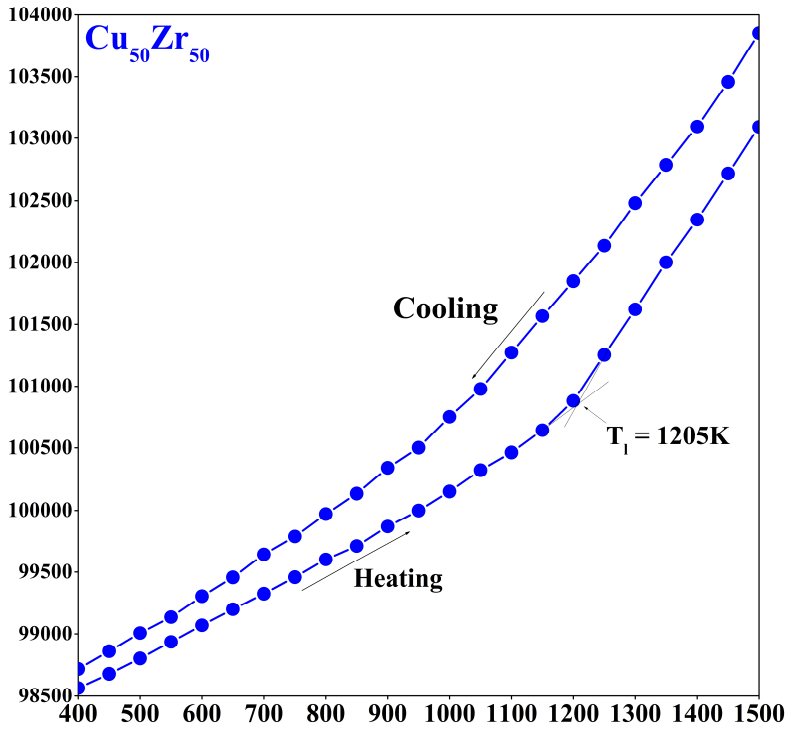


Figure 2 Variation in volume as a function of temperature for $Cu_{50}Zr_{50}$ system

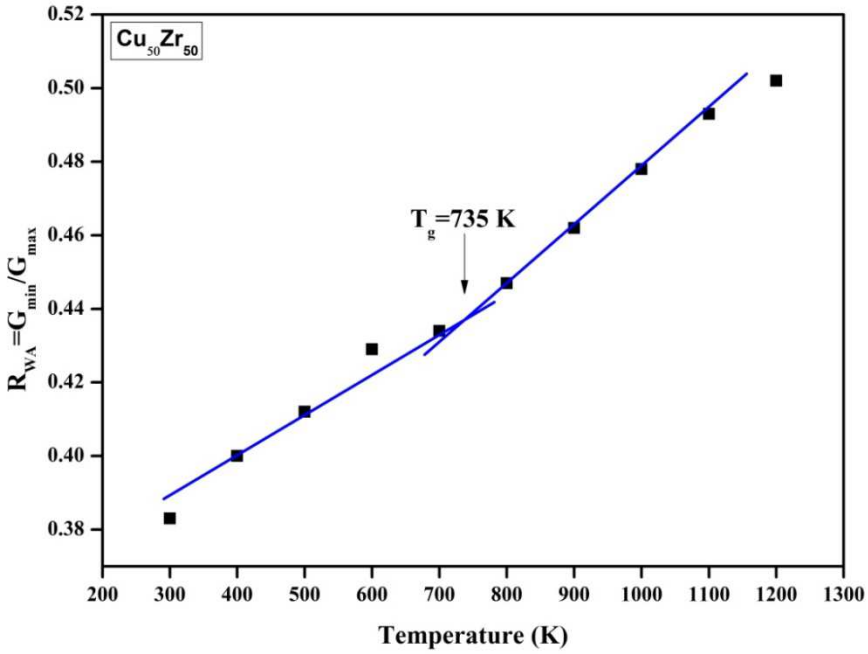


Figure 3 Glass transition temperature from Wendt-Abraham (RWA= Gmin/Gmax) for $Cu_{50}Zr_{50}$

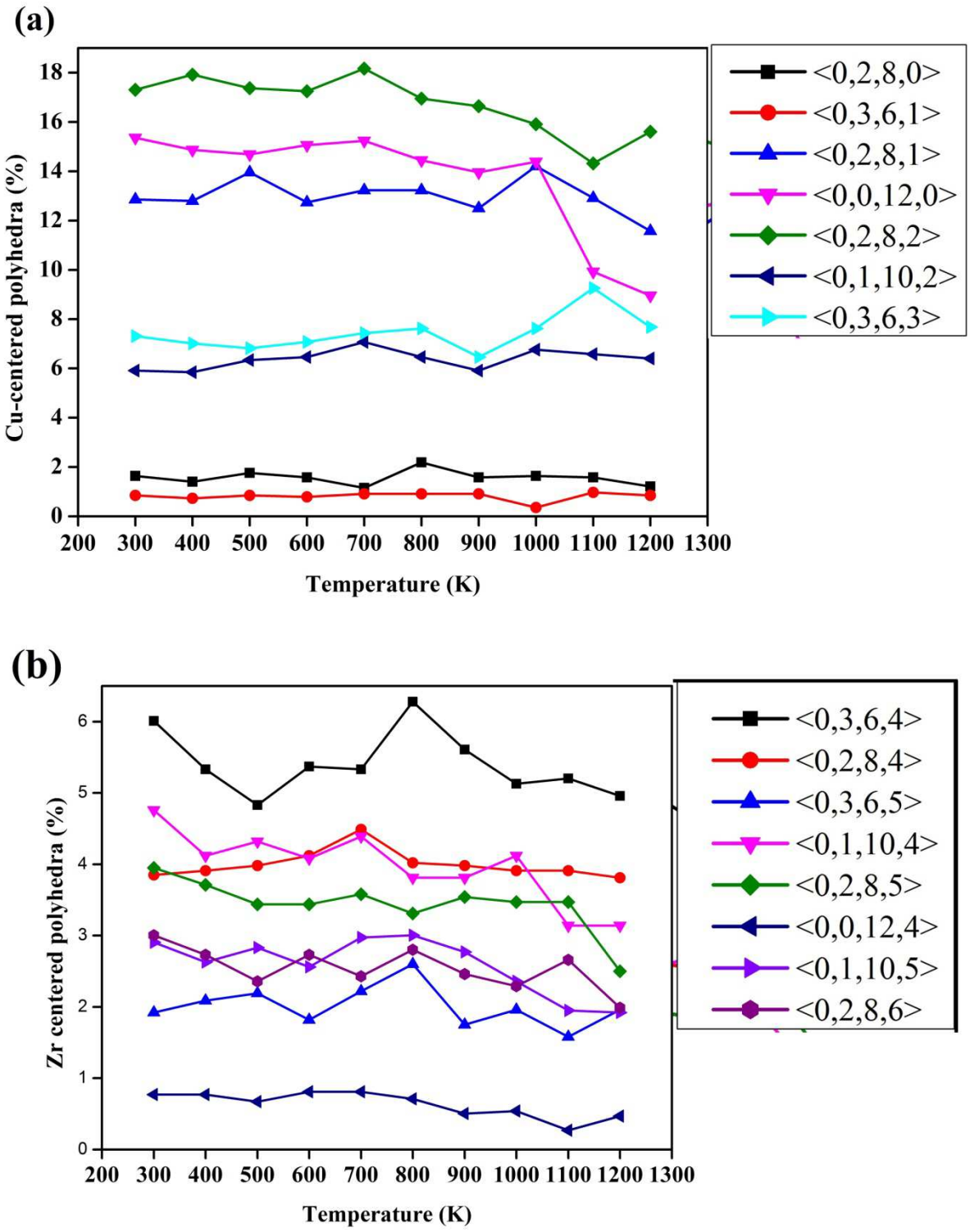


Figure 4 Average percentages of Voronoi polyhedra in $Cu_{50}Zr_{50}$ (a) Cu centred and (2) Zr centred polyhedra

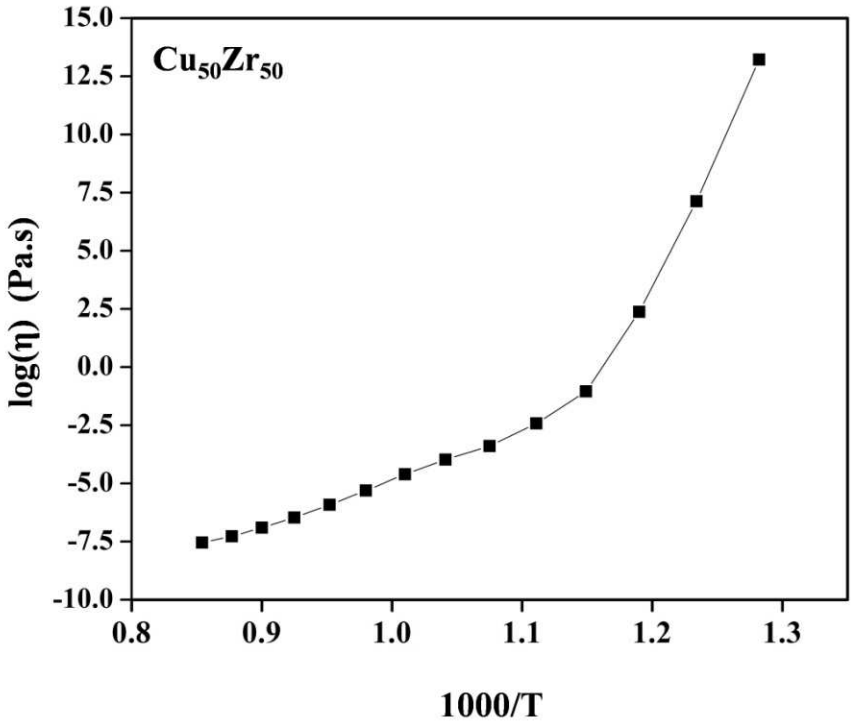


Figure 5 Simulated logarithm of the Viscosity vs. Inverse temperature curve for $Cu_{50}Zr_{50}$

CONCLUSION

In summary, we have presented an MD simulation for binary Cu50Zr50 BMG using embedded atom method (EAM) potential. The structural study has been carried out by means of volume temperature curve, radial distribution function (RDF) and Voronoi tessellation. The dynamic study was done by studying the glass transition temperature using WA parameter as well as looking at the evolution of the viscosity as a function of temperature using VFT law. Distinct splitting in the second Cu-Zr peak of Cu50Zr50 was found in different atom pairs. Voronoi tessellation analysis shows that icosahedral order is presented in the glassy alloy. The slope of logη Vs 1000/T shows that Cu50Zr50 is good glass former as it shows low fragility. Our finding matches well with the reported results in literatures. More over Molecular dynamics (MD) simulation provide an effective way to tackle the problem and help in screening the promising alloy compositions worthy of further experimental trials.

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