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Effects of cooling rate on the atomic structure of $Cu_{64}Zr_{36}$ binary metallic glass

Feng Li [a,b], Huajian Zhang [a], Xiongjun Liu [b,*], Chunyan Yu [c], Zhaoping Lu [b]

[a] College of Materials Science and Engineering, Nanjing Tech University, Nanjing 210009, China
[b] State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing 100083, China
[c] College of Physics and Energy, Shenzhen University, Shenzhen 518060, China

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ABSTRACT

In this study, molecular dynamics simulations based on the embedded atom model (EAM) potentials were carried out to investigate influences of cooling rate on the ordered atomic structure, especially icosahedral short- and medium-range orders (ISRO and IMRO) in the $Cu_{64}Zr_{36}$ metallic glass (MG). It is found that potential energy of the system is strongly dependent on the cooling rate during the rapid solidification, and so does the glass transition temperature (T_g) which rises with increasing cooling rate. Both Honeycutt-Anderson bond pair and Voronoi polyhedra analyses indicate that icosahedral clusters are prominent in the $Cu_{64}Zr_{36}$ MG and the population of icosahedral polyhedra increases with decreasing cooling rate. The size of IMROs constructed by ISROs via the linkage of vertex-, edge-, face-, and intercrossed-shared atoms becomes larger as the cooling rate and temperature descend. The structural evolution with temperature manifests that the development of icosahedral ordering is the structural origin of the glass transition of the modeled alloy. Moreover, we found that the major structural units in the $Cu_{64}Zr_{36}$ MG are Cu_8Zr_5 and Zr_6Cu_{10} polyhedra for Cu- and Zr-centered clusters, respectively, which are different from the main competing crystalline phase upon cooling. The good glass-forming ability of the modeled alloy is originated from the chemical and structural discrepancy between these main clusters and the competing phase, which effectively retards the crystal nucleation in the $Cu_{64}Zr_{36}$ alloy during rapid solidification.

1. Introduction

Bulk metallic glasses (BMGs) have attracted much attention due to their unique structural, physical and chemical properties [1–3]. MGs can be considered as solids with frozen-in liquid structures, with no long-range ordering [4]. Thermodynamically, MGs are metastable and thus their microstructure and mechanical properties depend on preparation conditions, such as cooling rate and overheating degree [5,6], among which the cooling rate plays a crucial role in glass formation [7,8]. MGs can be formed only if the metallic liquid is cooled fast enough to avoid crystallization, i.e., at a cooling rate faster than the critical one. Recently, experimental studies indicate that physical and mechanical properties of MGs are also sensitive to the cooling rate [9,10]. It is known that cooling rate can affect the atomic structure and thus may affect the mechanical properties of MGs. For instance, higher cooling rates generally lead to looser atomic packing structure and more free-volume [11,12], which therefore gives rise to the larger plasticity [13,14]. Obviously, it is of importance to unveil the effect of cooling rate on local atomic structure.

Although considerable experimental efforts have been devoted to revealing the influences of cooling rates on glass formation and mechanical properties of BMGs [11,15–18], cooling rate-dependence of the detailed atomic-level structure, especially the icosahedral clusters, during glass formation is still unclear due to the intrinsic limitation of currently available experimental techniques. On the other hand, molecular dynamics (MD) simulation is a powerful tool to investigate the atomic-scale structural evolution from liquids to glasses as it can monitor the atomic trajectory as a function of time and temperature conveniently. Actually, MD simulations have been extensively applied in studying the atomic structure of amorphous alloys [19–22]. Nevertheless, most of them are focused on the structural evolution and local atomic packing of amorphous solids, while the relation between cooling rate and atomic structure is less concerned. Therefore, it is necessary to fully understand the influence of cooling rate on ordered clusters of MGs via MD simulations.

* Corresponding author.
E-mail address: xjliu@ustb.edu.cn (X. Liu).

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A typical binary $Cu_{64}Zr_{36}$ alloy with good glass-forming ability (GFA), which is able to form a BMG with a critical casting thickness of 2 mm [23], was selected for this study. The aim of this work is to investigate the cooling rate effects on the ordered atomic structure especially icosahedral short- and medium-range orders (ISROs and IMROs) of the amorphous $Cu_{64}Zr_{36}$ model alloy by MD simulations. Moreover, structural origin of good GFA for the $Cu_{64}Zr_{36}$ alloy was also explored.

2. Simulation methods

With the help of Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [24], MD simulations of the rapid solidification process of liquid $Cu_{64}Zr_{36}$ alloy were carried out. A classical embedded atom model (EAM) potential [25] was exploited to describe the interatomic interactions in the Cu-Zr system. This potential has been proved to be consistent with experimental measured structure factors [25,26] and has been extensively used to investigate the glass formation Cu-Zr MGs [27,28]. The simulations were performed with the system consisting of 8000 atoms (5120 Cu and 2880 Zr atoms) in a cubic box with periodic boundary conditions along all the three directions and their motion equations were solved by velocity-Verlet algorithm in the velocity form. The time-step was chosen to be 2 fs. The isothermal-isobaric ensemble (i.e., NPT) with a constant particle number (N), pressure (P) and temperature (T) and the Nose-Hoover thermostat [29] were used throughout the glass formation process.

During the MD simulation, the model alloy system was firstly run for 1000,000 MD steps (2 ns) at 1800 K (much higher than the melting point of the $Cu_{64}Zr_{36}$ alloy, T_m = 1224 K [30]) to obtain an equilibrium liquid phase for the initial configuration. Subsequently, the liquid was cooled down to 300 K at five different cooling rates (i.e., Q_1 = 0.1 K/ps, Q_2 = 0.5 K/ps, Q_3 = 1 K/ps, Q_4 = 5 K/ps, Q_5 = 10 K/ps) with the temperature interval of 50 K. During the relaxation process at any given temperature, 50 configurations were collected to get statistically structural and thermodynamic quantities during the process of solidification. In this work, the detailed structural information was characterized by means of pair distribution function (PDF) [31,32], Honeycutt-Andersen (HA) bond pair [33], coordination number (CN) and Voronoi polyhedra (VP) [34,35].

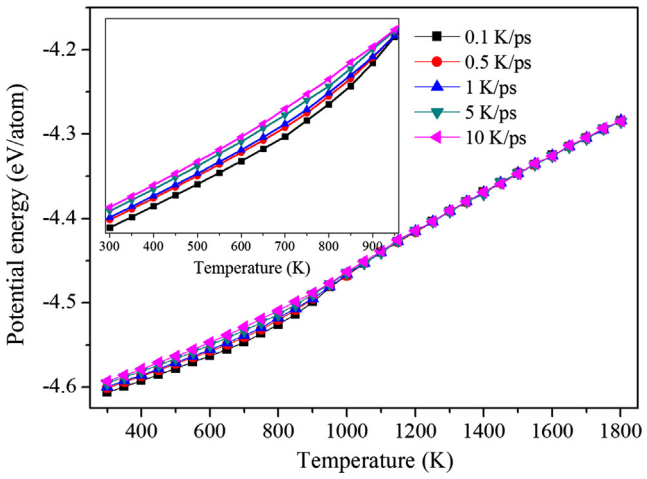

Fig. 1. Temperature dependence of potential energy at various cooling rate for the $Cu_{64}Zr_{36}$ alloy. The inset is the potential energy as a function of the temperature from 300 to 900 K.

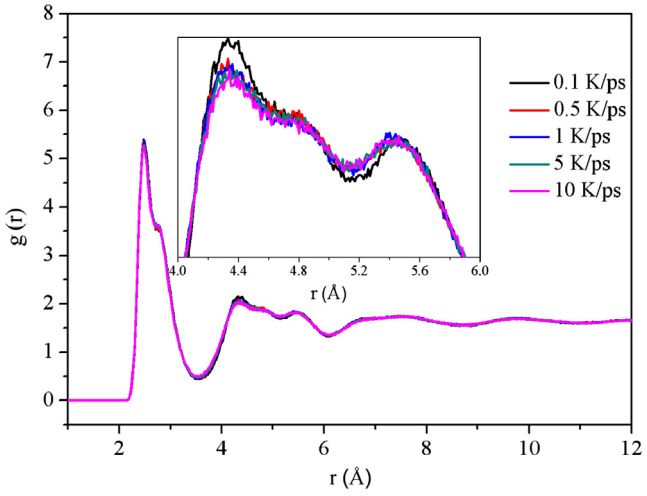

Fig. 3. The total pair distribution function (PDF) curves under various cooling rate for the $Cu_{64}Zr_{36}$ metallic glass at 300 K. The inset is the splitted second peak of total PDF curves.

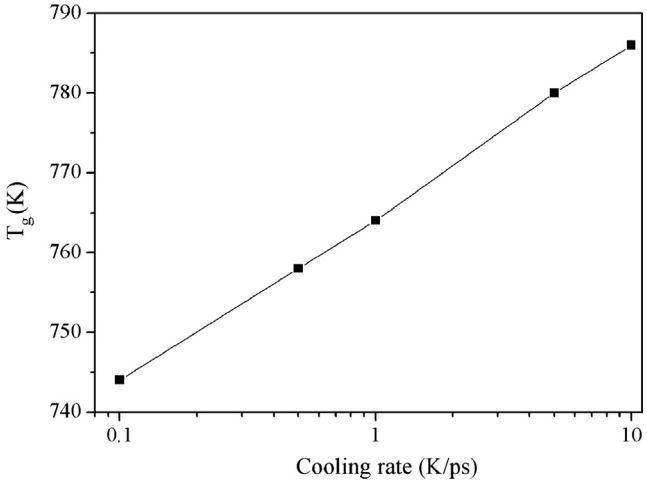

Fig. 2. The glass transition temperature as a function of cooling rate for the $Cu_{64}Zr_{36}$ metallic glass.

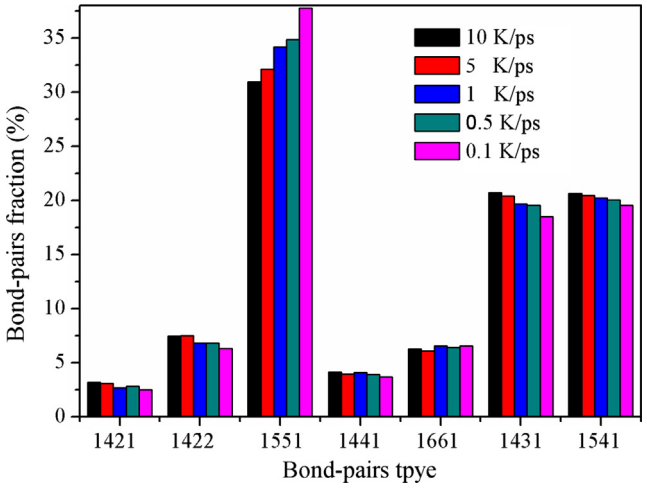

Fig. 4. The variation of relative concentration of dominant bond-pairs type under various cooling rates in the $Cu_{64}Zr_{36}$ metallic glass at 300 K.