



Intrinsic structural defects on medium range in metallic glasses



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ABSTRACT

To get insight into the structural defects on medium range in metallic glasses, molecular dynamic simulations on cavitation instability are carried out. It is found that micro voids are prone to nucleate at the sites where atomic clusters are loose packing on medium range. Close-up observation on atomic clusters around the nucleation site shows that there are two kinds of defects on medium range: cavities among the atomic clusters and boundaries between medium range orders. Further investigation shows that the defects are significantly important in both cavitation and shear transformation, which are two intrinsic deformation modes of metallic glasses.

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1. Introduction

Intrinsic structural defects such as vacancies, dislocations and grain boundaries, usually play important roles in the mechanical behaviors of conventional crystalline materials. For example, plastic deformation is attributed to the motion of dislocations, and damage evolution process which leads to catastrophic failure is usually due to vacancy clustering, dislocation pileup, grain boundary sliding, etc. [1] In contrast, in metallic glasses (MGs) [2,3] which are relatively new kind of materials and exhibit excellent physical and mechanical properties, what the intrinsic structural defects are and how they influence the material properties still fascinates and challenges scientists.

MGs are amorphous metastable solids which are usually made by fast quenching process. For the unique disordered structures, MGs are lack of long-range translational order and have long-range homogeneity. Thus, unlike their crystalline counterparts, heterogeneities on mesoscopic scale do not exist in MGs and their properties are significantly influenced by atomic structures on microscopic scale [4–11]. To characterize the atomic-level structure of MGs, much work has been done over the past few decades [12–23]. The atomic structure of MGs are initially described as dense random packing of hard spheres [12]. Now it is widely accepted that they have short-range orders (SROs), which is constituted by the atomic configuration of the nearest-neighbor

shell, contributing to the first peak in the pair distribution function (PDF) [4,13]. They are the basic building blocks [14] characterized by different types of polyhedra, and icosahedral (or icosahedral-like) order is the most favourable local order [16–18]. Recently, medium-range orders (MROs) have been found to exist in MGs too. The dense packing of atomic clusters by sharing shell atoms (face sharing, edge sharing, or vertex sharing) forms MRO [20,24–27], thus the structural features are beyond the first peak in PDF to a distance up to 1–2 nm. Further investigation shows that the packing of clusters may be characterized as fractals [28,29]. Furthermore, on a length scale beyond MROs, the material is believed to consist of hard matrix and soft zones (or liquid-like regions) [10,11,23]. The hard matrix, which is rich in interpenetrating icosahedral-like orders, are the backbone of MGs. Soft zones, which contain disordered clusters with low packing efficiency, are regarded as heterogeneities.

The above works established a relatively clear picture of structural organization in MGs, but the defects in such kind of material are far from being understood. It is well known that there are no vacancies, dislocations or grain boundaries in MGs. Free volume [30] and disclinations [31] are believed to be the structural defects. Free volume is the “flow defect”, which can be described as local fluctuations of density. Disclinations are rotational defects, usually seen as sixfold and fourfold bipyramids. Now these concepts are widely used to understand the mechanical and physical behavior of MGs [32–39]. However, all of them can be regarded as defects on short range. As there are MROs which determine cluster packing over a longer length scale, they may be as important as SROs in

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affecting the material properties [4]. Then, are there any structural defects on medium range? How do they act during the deformation and failure processes of MGs [40–42]?

In this work, cavitation instability [43] in a binary metallic glass (MG) $\text{Cu}_{50}\text{Zr}_{50}$ is studied via dynamic molecular (MD) simulations. To characterize the intrinsic structural defects, micro-structure evolution under tensile pressure is analyzed, with special attention on evolution of the atomic clusters around void nucleation sites. The physical picture of intrinsic structural defects on medium range is presented, and the role that the defects play in cavitation process is discussed. Besides, via additional simulations on compression of the material, we also show how the shear transformation event is mediated by the defects. Thus, the recognized MRO defects are significantly important in both cavitation and shear transformation, which are two intrinsic deformation modes of MGs.

2. Simulation and methods

The MD simulations are carried out with the open source code LAMMPS [44]. A simple binary MG $\text{Zr}_{50}\text{Cu}_{50}$ is selected as the model material. We employ the Finnis-Sinclair type interatomic potential with parameters given by Mendeleev et al. [45] to describe the interactions in the Zr–Cu system. Glass samples are prepared via a melting-and-quenching process [46]. Simulations are performed in the constant number of particles, pressure, and temperature (*NPT*) ensembles, the time step for integration is chosen to be 1 fs, and three-dimensional periodic boundary conditions with ambient pressure are applied. The initial system with ~55,000 atoms is a fcc lattice in a cubic shape, with the sites randomly occupied by Zr and Cu atoms in accordance with the nominal composition. With different random seeds, several samples with different initial configurations are obtained. For each sample, temperature is raised gradually from 1 K to 2500 K, equilibrates for 100 ps and cools down to 300 K, with the same heating and cooling rate of 5 K/ps. After a further relaxation for 100 ps, glass samples with dimensions of $\sim 10 \times 10 \times 10 \text{ nm}^3$ are prepared. For simulations of cavitation instability, all the samples are subjected to uniform hydrostatic tension with the volumetric strain rate of $\sim 6 \times 10^{-4} \text{ ps}^{-1}$. The loading is carried out without temperature control, to capture temperature effects related to plasticity [47].

To analyze the atomic structures of MGs, the Voronoi tessellation method is employed [48]. With this method, each atom is indexed with the Voronoi indices $\langle n_3, n_4, n_5, n_6, \dots \rangle$, where n_3, n_4, n_5 and n_6 represent the number of triangles, tetragons, pentagons and hexagons on the Voronoi polyhedron, respectively. And the structure feature of the central atom and its nearest neighbors can be characterized.

3. Results and discussions

3.1. Micro-structure evolution during cavitation instability

Fig. 1 shows the evolution of atomic configuration of one sample (denoted as S1) before a void is nucleated with colors indicating the normalized local atomic number density ρ/ρ_{mean} . The red color represents lower values of ρ/ρ_{mean} , while the blue color represents higher values. Atomic density fluctuation is clearly observed in this CuZr MG. As the applied tensile volumetric strain increases, a void is nucleated in the sample. It should be noted that the void is not nucleated in a region with the lowest density (or the highest free volume content), but in a region with relatively lower density as shown in Fig. 1(a). Just before void nucleation, the density begins to decrease a lot at the nucleation site. As free volume is believed to play an important role during the void nucleation process [46,49],

this phenomenon is beyond our expectation. It implies that not only the free volume content but also the atomic packing has significant influence.

Fig. 2 show the change in population of polyhedra with increasing volumetric strain before void nucleation. Different types of polyhedra are sorted according to their population from large to small. Then the former 50 types are divided into 5 groups, each containing 10 types, and other types are counted in the rest group. As shown in Fig. 2, in the initial configuration, the total fraction of the first group which contains the top 10 major polyhedra approaches 40%, while the rest 60% is the fraction of all the other groups. With increasing the volumetric strain, the fraction of major polyhedra decreases, corresponding to the increase in the fraction of minor polyhedra with the same amplitude. The larger populations the polyhedra have, the more their fraction decrease. In the first group, most polyhedra are stable or solid-like clusters with high density of fivefold bonds. Such as $\langle 0, 0, 12, 0 \rangle$, $\langle 0, 2, 8, 2 \rangle$, $\langle 0, 3, 6, 4 \rangle$, $\langle 0, 1, 10, 2 \rangle$, $\langle 0, 2, 8, 1 \rangle$ and $\langle 0, 3, 6, 3 \rangle$ polyhedra, they are usually Cu-centered icosahedral-like clusters which lead to dense atomic packing and slow dynamics [50–52]. And $\langle 0, 2, 8, 5 \rangle$, $\langle 0, 1, 10, 4 \rangle$, $\langle 0, 2, 8, 6 \rangle$ polyhedra, which are usually Zr-centered clusters, are also stable clusters [51,52]. In contrast, most of the minor polyhedra are usually liquid-like clusters fragmented with high disclination density [4]. Thus, the variety in population of polyhedra implies that the atomic structure of the sample becomes more liquid-like under tensile pressure. As liquid-like clusters are more unstable, atom rearrangement easily occurs. This feature is expected to benefit void nucleation.

Are voids prone to nucleate in the liquid-like regions in MGs? To answer this question, we propose a simple parameter to distinguish the liquid-like regions and the solid-like regions in the amorphous structure, as follows:

$$F_n = \frac{N_n}{N_{\text{cut-off}}}, \quad (1)$$

where F_n is the fraction of the top n major polyhedra in the local structural environment, $N_{\text{cut-off}}$ is the total number of atoms within the cutoff distance, and N_n is the number of the top n major polyhedra within the cutoff distance. It is known that MG would tend to maximize its favourable SROs, which elevates the stiffness and slows down the relaxation dynamics, and leads to more ordered configurations [53]. For a well relaxed MG, the major polyhedra are just the most favourable polyhedra in MGs. Thus, the main difference of atomic structure between the solid-like regions and the liquid-like regions can be attributed to the different fraction of major polyhedra. For a larger F_n , it means that the local structural environment is dominated by the most favourable polyhedra and is dense packing in SRO.

For the CuZr MG in this letter, a value of $n = 10$ and a cutoff distance of 7.6 Å are used to obtain F_n . Fig. 3 illustrates the distribution of solid-like and liquid-like regions in S1. The red color represents lower values of F_n , while the blue color represents higher values. Liquid-like regions and solid-like regions of nanometer scale are clearly distinguished. As volumetric strain increases, all regions become to be more liquid-like gradually. Beyond our expectation, void nucleation occurs at a solid-like region in the initial configuration. Just before the void is nucleated, the region turns to be liquid-like.

Now the features of nucleation site in sample S1 can be concluded: it is located at a region with relatively lower density, but with relatively higher value of F_n . To find the common features, cavitation instability in several other samples are explored. Fig. 4 shows the initial configuration of each sample with green circles denoting the nucleation sites. It is found that there is a little

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