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Relationship between local geometrical factors and mechanical properties for Cu–Zr amorphous alloys

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Abstract

Cu_xZr_{1-x} ($x = 0.30–0.85$) amorphous alloy models were constructed using molecular dynamics simulations. In order to estimate the local structures characterized by pentagonal short-range order and free volume, Voronoi polyhedra analyses were performed for the initial states and also for the deformed states of the models. Both these geometrical factors are intimately related to each other and exhibit a large influence on mechanical properties. The elastic properties tend to increase as the free volume decreases. Moreover, flow stress drastically decreases with increasing free volume content. It was found that the non-pentagonal regions, which are sources for the generation of high free volume structures, preferentially undergo irreversible atomic rearrangements in the early stage of the deformation process.

Keywords: B. Elastic properties; B. Glasses, metallic; B. Plastic deformation mechanisms; E. Mechanical properties, theory; E. Simulations, atomistic

1. Introduction

Amorphous metals have received much attention due to their excellent mechanical properties, including high yield strength, high fracture toughness and high elastic limit. These properties arise from their disordered atomic structures. Unlike crystalline materials, amorphous metals have random closed-packed structures. Therefore, plastic deformation of amorphous metals is not dependent on dislocation-based mechanisms. Argon [1] first proposed the simplified plastic units, the so-called STZ (Shear Transformation Zone). From a microscopic viewpoint, it is hypothesized that the applied stress generates local shear shuffling among the atoms within a STZ, and chain-reactions of STZs occur in sequence [2]. The macroscopic shear bands observed in some previous experimental studies [3,4] have been recognized to form due to self-assembly of STZs. This suggests that the local structure variation observed in amorphous alloys is crucial, and atomistic modeling, taking microscopic inhomogeneities into account, is necessary to understand the deformation mechanism. The question arises as to what kind of local structure preferentially undergoes irreversible atomic rearrangement in the early stages of the deformation process. Some studies have pointed out the role of the density and the free volume variation on the deformation process. Spaepen [5] indicated that shear viscosity can be appreciably reduced in the locally dilated region of a high free volume, and predicted the localized deformation by the increase in the free volume induced by the plastic deformation. Argon and Kuo [6] also showed that plastic deformation in the local shear zone was accompanied by an increment in free volume. However, since free volume can be defined as the global volume difference with respect to the reference state, its extension to the atomic-level specific structure is not clearly understood. In addition, the evolution process of local short-range structure, such as the non-periodic icosahedron in the deformation process, is still not clear, although such a geometry-specific factor is thought to play a critical role in the early stages of deformation.

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Our aims in the present study are, therefore, to identify the geometrical factors characterizing the free volume structure, and to clarify the role of these factors in the deformation process. We computationally modeled the atomic Cu_xZr_{1-x} amorphous alloys, with x ranging from 0.30 to 0.85, using molecular dynamics simulations. These models are enforced by uniaxial tension and simple shear loading to determine internal structural evolution. Voronoi analyses were applied to link these stress states to the mechanical properties of the amorphous alloys with the local geometrical factors.

2. Atomic amorphous alloy model

Our intention here is not to obtain precise physical properties but rather to investigate the general principles of the relationship between the locally inhomogeneous structure and the complex deformation mechanism. The simple pair potentials [7], which refer to short-range two-body effects, are thus thought to be sufficient to describe Cu–Cu, Cu–Zr and Zr–Zr interactions. These potentials are based on the Lennard–Jones 4–8 potential, and the potential parameters are determined so as to satisfy the equilibrium values of the nearest neighbor distances of the FCC lattices of Cu and Zr, the elastic constants of crystalline Cu and Zr, and other conditions.

Cu_xZr_{1-x} amorphous alloy models with values of x of 0.30, 0.40, 0.50, 0.57, 0.64, 0.75, 0.80, and 0.85 were prepared as follows. The source model was randomly packed with Cu and Zr atoms with the specific composition into the simulation cell. It was numerically heated to 2000 K, which is much higher than the melting point. After a sufficient relaxation of 20 ps, it was cooled to 0 K at a rate of 10^{12} K/s. The external pressure during this heat treatment was kept at zero by the Parrinello–Rahman ensemble [8], and the temperature of the whole cell was controlled by scaling the velocity of each atom. Periodic boundary conditions were applied to the three dimensional directions in order to eliminate surface effects. The radial distribution functions and the density of the constructed $Cu_{57}Zr_{43}$ model were in good agreement with the experimentally obtained data [9,10], as shown in Table 1.

To understand the local structural evolution during deformation, we performed Voronoi analyses [11], indicating the 3D atomic configuration between the centered and the surrounding atoms. As an example, we represent the Voronoi polygon and its atomic configuration that existed in the $Cu_{57}Zr_{43}$ model in Fig. 1 and also the Voronoi index list in Fig. 2. The Voronoi index shows that most of the Voronoi polygons have a specific kind of center atom. In the (0,0,12,0) case, the Cu atom accounts for more than 99% of the center atom. Therefore, the contents of the Voronoi polygon are expected to largely depend on the global atomic composition.

Table 1
Density and the first peaks of the radial distribution function (RDF) of the $Cu_{57}Zr_{43}$ model along with the experimental values

Density (g/cm^3)		First peaks of RDF (Å)		
		Cu–Cu	Cu–Zr	Zr–Zr
Model	7.366	2.53	2.83	3.13
Exp.	7.382 [9]	2.65 [10]	2.80 [10]	3.15 [10]

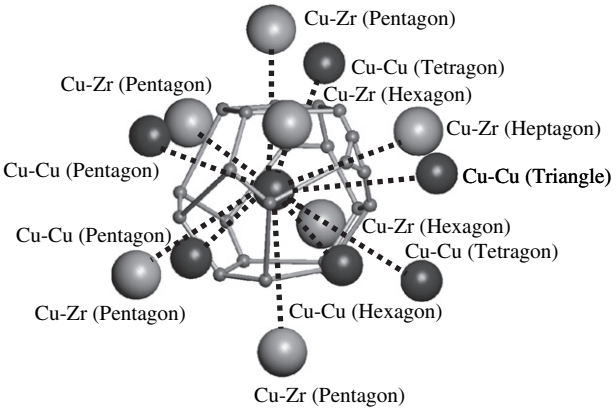

Fig. 1. Voronoi polyhedron, its center and surrounding atoms. This polyhedron consists of one triangle, two tetragons, six pentagons, three hexagons and one heptagon, representing as the Voronoi index of (1,2,6,3,1).

3. Results

3.1. Structural analyses of initial states

The fraction of Voronoi triangles, tetragons, pentagons, hexagons, and heptagons in the quenching process is shown in Fig. 3. Similar to some previous computational results [12,13], only the fraction of pentagons increased with

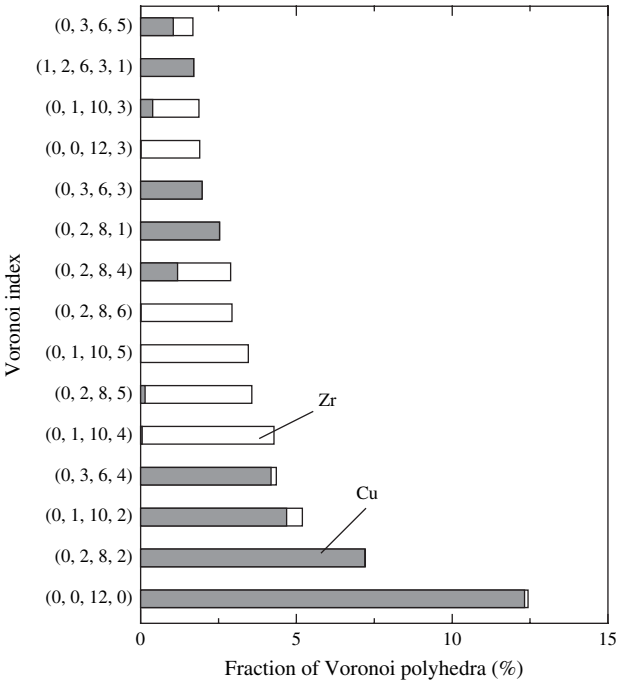

Fig. 2. Voronoi index list of the constructed $Cu_{57}Zr_{43}$model. These are the major components among the more than 100 kinds of Voronoi polygons contained in the model. Dark and light parts represent the ratio of Cu and Zr centers, respectively.