

Networked interpenetrating connections of icosahedra: Effects on shear transformations in metallic glass

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Abstract

The local structures of metallic glasses have been analyzed previously in term of various types of short-range order (SRO). However, the SRO alone, neglecting the interconnection of neighboring icosahedra to medium range and beyond, is insufficient to account for the structure–property relationship in metallic glasses. In this study, we use molecular dynamics (MD) simulations of Cu–Zr binary metallic glasses to examine the effects of the next level of structural hierarchy: the interpenetrating connection of icosahedra (ICOI) and the linkage of the medium-range ICOI patches to form networks of icosahedra over extended range. The mechanical properties of these metallic glasses, especially the shear transformations that mediate plasticity, are found to be dependent on the degree of ICOI and development of the ICOI network. The evolution of the ICOI network during shear deformation, as well as the composition dependence, has been monitored and discussed.

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1. Introduction

The mechanical properties, especially plasticity, of metallic glasses depend largely on their atomic-scale structures, to an extent similar to that of crystalline materials. However, the details of the atomic-scale structures of the metallic glasses, and especially those that are responsible for their properties, remain to be elucidated. In 1928, Ramsey [1] proved that every complex structure, while seemingly random, necessarily contains ordered substructures. Nevertheless, it was not until much later that researchers began to recognize the existence of short-range-ordered structures (SROs) in metallic glasses, and relate these fundamental structural motifs to macroscopic properties. In recent years, Miracle [2], Sheng et al. [3] and Yang et al. [4] described the

local structures of the amorphous solid based on quasi-equivalent clusters of various fractions, while Shi and Falk [5] related the SRO structure, and different degree of SROs obtained by changing the cooling rate, to the strain localization in the metallic glasses. Subsequently, Wakeda et al. [6], Lee et al. [7], Park et al. [8], and Cheng et al. [9] performed extensive studies to clarify the composition dependency of the SRO structures in Cu–Zr-based metallic glasses and to relate these SROs to the observed mechanical properties. Shi and Falk [5,10] also assessed the effects of another important structural parameter, i.e., the spatial distribution and percolation of SRO, on the mechanical response. However, for this latter issue, much remains to be uncovered and analyzed in detail, as discussed below.

Recent atomic simulations revealed that the local structure of metallic glasses can comprise more than 100 different types of polyhedra. These local motifs, representing different SROs, are the building blocks of the three-dimen-

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sional glassy structure. Intuitively, even with the same fractions of the various SROs, innumerable numbers of different structures can be made by simply rearranging these SROs, which in turn can produce different mechanical properties. As such, the structure–property relation cannot be established by considering the SROs alone. It is therefore necessary to consider the glassy structure in a hierarchical sense. From this perspective, naturally the next task is to examine the structural organization beyond SROs (the first level clusters), to probe into the next level of the structural hierarchy. In other words, it is of importance to uncover the various ways the SROs are connected with one another and how the type and degree of connections affect the mechanical response of the amorphous material. This will be attempted in this paper, and can be viewed as a stepping stone before probing into an even higher hierarchical level, i.e., the percolation of structural order throughout the entire sample, to quantitatively establish if the amorphous solid has a backbone and how that influences the properties [11].

SROs generated during cooling tend to fill the 3D space of the metallic glasses in an efficient way to attain the lowest possible energy state under the kinetic constraints. As will be discussed later, this can be achieved by forming a densely packed structure, in which SROs connect with neighboring SROs to construct the medium-range-ordered structures (MROs). These MROs are atomic-scale structures with length scales typically longer than the diameter of the third coordination shell but shorter than the scale at which ordering becomes long-range and Bragg peaks appear in the structure factor [12]. It has been difficult to observe the MROs experimentally using conventional electron microscopy and diffractometry. Recently, the existence of MROs within disordered materials was suggested in fluctuation electron microscopy experiments [13,14]. Some specific types of MROs in metallic glasses were proposed from the model studies on efficient packing [15,16]. Several configurations of MROs have also been identified via the combined use of experiments (such as X-ray scattering) and atomistic simulations [16–22]. However, many other types of medium-range structures are possible, beyond the examples of MROs reported in earlier studies. Further, it has not been established whether the reported MROs are the major structural organization that plays a key role in determining the mechanical properties.

In this study, using molecular dynamics (MD) simulations of Cu–Zr binary alloys, we illustrate a conceptual structural organization, i.e., interpenetrating connection of icosahedra (ICOI) over an extended range. The characteristics of the networked structure based on ICOIs are quantitatively assessed in terms of their connectivity and rigidity. We also explore how the ICOI networks are created during cooling and destroyed during shear deformation, in order to qualitatively relate their evolution behaviors to the mechanical properties of metallic glasses, in the context of the nucleation of local shear deformation and the strain localization.

2. Molecular dynamics (MD) simulations and structural analysis

Atomic simulations, due to their ability to depict the atomic-scale structures and the corresponding mechanical properties, have been a powerful technique to explore the structure–property relationship in metallic glasses [2,5,6,9–11]. Of the various simulation techniques presently available, the first-principles calculations provide the most reliable interatomic interactions. However, these calculations are based on the NVT (constant numbers of atoms, volume and temperature) ensemble, which is different from the real-world laboratory conditions. In addition, the typical size that can be handled by this method is too small (normally less than ~ 200 atoms), and thus produces significant statistical scatter and is inadequate to investigate the mechanical behaviors of materials. Another approach is to use classical MD simulations employing (semi-)empirical interatomic potentials that can manage millions of atoms and the NPT (constant numbers of atoms, pressure and temperature) ensemble. Although MD simulations suffer from severe spatial and temporal limitations and their accuracy relies critically on the potential, this technique has been widely used to explore the structure–property relation by describing the general features of the local structure and its evolution associated with shear deformation [7–9,11], which cannot feasibly be obtained experimentally.

To investigate the structural changes and associated deformation behaviors of metallic glasses, we selected two model alloys from the Cu–Zr binary system: Cu₅₀Zr₅₀ and Cu₆₅Zr₃₅. These alloys possess a pronounced difference in their initial packing densities (or atomic-scale packing structures) and thus exhibit clearly different structural evolutions and associated flow behaviors [7,8]. These alloy characteristics enabled the investigation to focus on the effects exerted by the atomic packing structures of these alloys on both the structural evolution and the corresponding mechanical responses.

The 3D binary alloys were constructed using MD simulations employing the embedded atom method (EAM) potential developed by Cheng et al. [9,23]. Approximately 32,000 atoms corresponding to the Cu₅₀Zr₅₀ and Cu₆₅Zr₃₅ compositions were first packed into the simulation cell with approximate dimensions of $7.9 \times 10.1 \times 6.4$ nm and then heated to 2000 K. After allowing a sufficient relaxation time of 1 ns (time step 1 fs), the alloys were cooled to 300 K at a rate of 5×10^{12} K s⁻¹ to produce the 3D amorphous solids. The NPT ensemble was used for quenching, with the temperature controlled by a Nose–Hoover thermostat [24] and the pressure controlled at zero using a Nose–Hoover barostat [25]. A periodic boundary condition (PBC) was applied to the 3D directions in order to eliminate surface effects.

The model alloys with PBC were deformed at 300 K by applying simple shear with a strain rate of 10^8 s⁻¹ to induce plastic deformation and structural disordering. The

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