

## Correlation Between Local Atomic Symmetry and Mechanical Properties in Metallic Glasses



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The local atomic symmetry was investigated and discussed for understanding mechanical, vibrational and dynamical properties in metallic glasses. Local five-fold symmetry was defined based on the ratio of pentagons to the total number of faces in a Voronoi cluster analyzed by Voronoi tessellation method. It is found that the plastic deformation prefer to be initiated in the regions with less degree of local five-fold symmetry (LFFS) and propagate gradually toward the region with more degree of LFFS. On the other hand, the local structures having less degree of LFFS contribute more to the soft low-frequency modes, and thus the so-called boson peak, while those with more degree of LFFS participate more in moderate- and high-frequency modes in metallic glasses. The relationship between local atomic symmetry and structural heterogeneity, mechanical heterogeneity, and glass transition was also discussed. It is shown that local atomic symmetry could be a general structural indicator in metallic liquids and glasses for better understanding the structure-property relationship in amorphous alloys.

**KEY WORDS:** Metallic glasses; Atomic symmetry; Deformation; Molecular dynamics

### 1. Introduction

It has been well known that the discovery of dislocation and the development of dislocation theory established the relationship between structure and mechanical properties of crystalline materials, such as the structure origin of strength and plasticity. However, for amorphous solids, such as metallic glasses, due to the disordered nature and lack of a structural indicator such as dislocation in crystalline counterparts, it is difficult to define a local geometrical parameter as energy dissipative units for understanding the microscopic mechanism of mechanical behavior<sup>[1–4]</sup>.

The model of shear transformation zone (STZ) proposed by Argon provides a dynamical picture for the understanding of deformation mechanism in metallic glasses<sup>[5–7]</sup>. Falk and Langer introduced mean-field equations of motion for the number density of STZs and their two-state transition<sup>[6]</sup>. All these efforts have been successful in explaining many phenomena, such as shear localization and emergence of yield in amorphous solids<sup>[2,3]</sup>. However, STZ theory did not provide any information

on the specific structural feature accounting for plastic domains in amorphous solids. Based on the potential energy landscape theory and Frenkel's analysis for the shear strength of crystal solids, Johnson and Samwer introduced a cooperative shearing model of STZs for predicting the temperature dependence of yield strength of metallic glasses<sup>[8]</sup>, correlating STZs with potential energy barrier and thus providing a simple explanation of plasticity of metallic glasses at low temperatures.

So far, a couple of structure indicators have been proposed for understanding the mechanical behavior in metallic glasses, such as free volume and icosahedral short-range order<sup>[9–11]</sup>. Based on the concept of free volume envisioned by Turnbull and Cohen<sup>[12]</sup>, the free volume is defined as excess atomic volume surrounding each atom in amorphous states. Based on a competition between creation and annihilation of free volumes in metallic glasses driven by shear stress, Spaepen developed a steady-state inhomogeneous flow model to investigate the mechanical behavior of metallic glasses<sup>[8]</sup>. Because of simple and clear physical picture, free volume model has been widely adopted to understand various mechanical properties in metallic glasses<sup>[2,4,13]</sup>. However, as a structural indicator, free volume is a statistical or average variable, unable to provide specific structure information of the atomic symmetry or chemical ordering of local environments<sup>[11]</sup>. On the other hand, free volume model did not provide a clear picture for the atomic rearrangements during mechanical deformation<sup>[4,11]</sup>.

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Although amorphous alloys lack of long-range order, it has been demonstrated that metallic glasses contain significant short-range order<sup>[10,14,15]</sup>. Icosahedral short-range order (ISRO) with five-fold symmetry has been suggested as the most favorable local structural unit in metallic liquids and glasses, because of its specific close-packed atomic arrangement<sup>[16]</sup>. So far, ISRO and its spatial distribution have been found to closely correlate with structural heterogeneity, glass-forming ability, dynamical and mechanical properties in metallic liquids and glasses<sup>[11,14,17–22]</sup>. Therefore, ISRO is also adopted as a structural indicator for the fundamental process underlying structural relaxation and atomic rearrangements<sup>[11,23]</sup>. The effect of ISRO characterized by icosahedral clusters on the mechanical behavior of Cu–Zr-base metallic glasses has been widely investigated with computer simulations and found that ISRO is responsible for the local stiffness, yield strength and mechanical stability<sup>[13,24,25]</sup>. However, the so-called ISRO is mainly represented by the icosahedral clusters characterized in terms of Voronoi tessellation method<sup>[14]</sup>. Most icosahedra in metallic glasses are not perfect, but distorted<sup>[21]</sup>. Perfect icosahedron is five-fold symmetric. However, the distorted icosahedra even contain partial face-centered cubic symmetry<sup>[21]</sup>. The local atomic packing of perfect and distorted icosahedra may not be the same, either. Thus, they may exhibit significantly different mechanical behavior. On the other hand, ISRO may not be the representative of main local structures or may be even absent in some metallic glasses<sup>[14,26,27]</sup>.

## 2. Local Atomic Symmetry in Metallic Glasses

In fact, local atomic symmetry may be a more general concept in metallic liquids and glasses. Recently, direct experimental evidence for the existence of five-fold symmetry has been obtained in liquid Pb<sup>[28]</sup>. Nuclear magnetic resonance (NMR) experiments have also shown that local cluster symmetry plays an important role in glass-forming ability (GFA) and anelastic deformation in metallic glasses<sup>[29,30]</sup>. Recent statistical analysis of pair distribution functions of many metallic glasses shows the local translational symmetry feature in atomic packing in metallic glasses<sup>[31]</sup>. Even for the icosahedral clusters in metallic glasses, they may contain both local five-fold symmetry and face-centered cubic symmetry<sup>[21]</sup>. In addition, the degree of local five-fold symmetry in local structures has been demonstrated to correlate with the initiation and propagation of plastic deformation in metallic glasses<sup>[32]</sup>. Therefore, local atomic structures in metallic glasses may contain both local five-fold and translational symmetries.

For an atomic cluster, the structural configuration can be characterized by the Voronoi tessellation which divides the space between central atom and its nearest neighbors by construction of bisecting planes along the lines joining the central atoms and all its neighbors. The constructed polyhedron can be identified by the Voronoi index  $\langle n_3, n_4, n_5, n_6, \dots \rangle$ , where  $n_i$  ( $i = 3, 4, 5, 6, \dots$ ) denotes the number of  $i$ -edged faces of the polyhedron. Apparently, an  $i$ -edged face in a Voronoi polyhedron reflects the atomic packing nature and local atomic symmetry of the central atom with some nearest neighbor atoms in the direction normal to the face. Therefore, the triangle, tetragon, and hexagon faces should reflect the local translational symmetry feature, while pentagon faces reflect the local five-fold symmetry. Computer simulations for some realistic metallic glasses have demonstrated that the evolution of the fraction of pentagons with temperature or shear stress is totally different from that of other type faces<sup>[24,33]</sup>, implying the competition and transformation between local five-

fold symmetry and local translational symmetry in local structures during glass formation or deformation process. Therefore, local atomic symmetry could be a more general structural indicator in metallic liquids and glasses for better understanding the structure-property relationship in amorphous alloys.

Currently it is difficult to measure the local atomic symmetry in metallic glasses in experiments. It is not easy for numerical analysis, either. Several structural parameters have been proposed to characterize the atomic symmetry feature for local atomic clusters, such as bond-orientational order<sup>[34]</sup>, common-neighbor analysis<sup>[35]</sup>, and Honeycutt–Andersen (HA) index<sup>[36]</sup>. Common-neighbor analysis and HA index are quite similar. Steinhardt et al. proposed bond-orientational order based on spherical harmonics to quantify the bond-orientational symmetry around the central atom<sup>[34]</sup>. The normalized parameter  $\hat{W}_l$  ( $l = 2, 4, 6, 10$ ) was derived, which is able to differentiate various local atomic clusters. Different atomic clusters may correspond to different values of  $\hat{W}_l$ . For example,  $\hat{W}_6$  values of fcc, bcc, hcp, and icosahedron clusters are  $-0.01316$ ,  $0.01316$ ,  $-0.01244$ , and  $-0.16975$ , respectively. For local structures in metallic glasses, however,  $\hat{W}_6$  exhibits a broad distribution between  $-0.2$  and  $0.1$ <sup>[20]</sup>. Thus, it is not so clear how to quantify the local atomic symmetry for an atomic cluster with irregular configuration in the frame of bond-orientational order.

HA index was proposed by Honeycutt and Andersen by using four integers  $ijkl$  to characterize local atomic arrangements<sup>[36]</sup>. The first index denotes the root pair of two atoms.  $i = 1$  if two atoms are the nearest neighbors, otherwise  $i = 2$ . The second one represents the number of near neighbors shared by the root pair. The third index denotes the number of the nearest neighbor bonds formed among the shared neighbors. The fourth index is used to distinguish configurations with the same first three indices but with different topologies. Typically the first minimum of the pair correlation function is taken as the distance cutoff to determine whether a bond is formed between root pairs or two common nearest neighbor atoms. This method is able to distinguish between various local structures like fcc, hcp, bcc, and icosahedral environments. In most analyses, only the case of  $i = 1$  is often considered. Thus, the 1551 index represents a five-fold ring of common neighbors with all nearest neighbors bonded. 1541 or 1531 corresponds to the five-fold ring with one or two bonds broken because the distance between them is beyond the cutoff. The types of 1661, 1651, 1441, 1421, and 1422 are present in the bulk bcc, fcc, and hcp crystals, respectively. For an atomic cluster, HA index characterizes the local atomic packing and symmetry feature between the central atom and a part of nearest neighbor atoms, does not provide full atomic symmetry information for an atomic cluster.

To quantify the local atomic symmetry of an atomic cluster, we simply define the degree of local five-fold symmetry (LFFS) in a cluster as the ratio of the number of pentagons to the number of the nearest neighbor atoms<sup>[29]</sup>,

$$d_5 = \frac{n_5}{\sum_{i=3}^6 n_i} \quad (1)$$

As mentioned above,  $n_i$  ( $i = 3, 4, 5, 6$ ) denotes the number of  $i$ -edged face of a polyhedron. In this work, we used the degree of LFFS,  $d_5$ , as structural indicator to investigate structural signature of plastic deformation in metallic glasses and the relationship between normal modes and local atomic symmetry.

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