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Bridging shear transformation zone to the atomic structure of amorphous solids

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ABSTRACT

To correlate the atomic structure and mechanical behavior of amorphous solids, bridging shear transformation zone (STZ) to the atomic structure is crucial. Referring to dislocation of crystals and according to the concept of shear transformation in amorphous solids, from a mean perspective, an atomic structure-based shear transformation zone (SSTZ) based on radial distribution function (RDF) where an average atom is surrounded by atoms of different shells, is proposed. The elementary deformation event of the disordered structure is considered as a mean atomic rearrangement, i.e., a concordant rearrangement process between the atom shells in the SSTZ. The SSTZ will introduce no necessary modification into the transition state theory-based flow equation of amorphous alloys and provide both the universal yielding criterion and the anelastic deformation of amorphous alloys with a structure basis in terms of the shift of the peak on RDF under loading. Besides, regarding with issues like shear dilation and Poisson ratio etc., profound understandings can be achieved for the clear structural characteristic of the SSTZ.

1. Introduction

The elementary deformation unit, or more exactly deformation event, of disordered structure is of great importance to elucidate the mechanical behaviors of amorphous solids on the atomic structure level [1–3]. The effort to clarify such a unit can find its trail dating back to the 1930s [4–6], i.e., the concept of dislocation [7,8], a line defect defined on the crystal lattice, of which the glide on the lattice is the primary deformation mechanism of crystals [9]. Coming to amorphous solids, a concept of shear transformation in local atomic configuration, lately named shear transformation zone (STZ), is proposed by analogy to dislocations [10,11]. Although dislocation is undoubtedly observed with modern microscopy technology and the related theory on the various deformation behaviors of crystals is developed, the STZ in amorphous solids is still obscure and confusing for the isotropic and homogeneous contrast of the image of amorphous solids under high resolution electron microscopy [3,12–14]. However, many issues in the deformation of amorphous solids, like yielding and shear dilation, reckon on the structural characteristic of STZ [10]. What makes the situation more confusing, widespread consensus has been reached that STZ seems "event-oriented" rather than an entity of a specific structure like the clearly observed dislocation of crystals [2]. Computer simulations have also indicated that the size of STZ "events" follows a power law distribution and exhibits no characteristic size [15]. This dilemma of STZ stands as an unavoidable obstacle in correlating the mechanical behavior of amorphous solids to their atomic structure, especially for the clear structure variation in deformation observed in recent studies [16,17].

Besides electron microscopy, examination on amorphous structure is carried out mainly with synchrotron X-ray scattering tests [18–20], by which the atom packing characteristic can be obtained from the scattering pattern in the form of structure factor in the reciprocal space or radial (or pair) distribution function (RDF or PDF) in the real space. With enhanced X-ray intensity, scattering tests with in-situ loading circumstance in which the shift of the RDF or structure factor can be measured showing the length scale dependent atomic strain have been performed and provide important structure messages of amorphous alloys in deformation [21–23] whereas, the length scale dependent atomic strain obtained in scattering tests is averaged over the part of sample that participates in scattering the incident X-ray beam and individual STZs cannot be resolved. Therefore, in spite that the concept of STZ observed in the rearrangements of amorphous systems, like foam-craft model [24] and colloids [25], presents an important picture of the deformation of amorphous solids, the structural characteristic of STZ remains vague with nowadays structure characterization technique in understanding the mechanical behaviors of amorphous solids.

In this work, to make the best of the structure messages from in-situ loading scattering tests in understanding the mechanical behavior of amorphous solids, referring to dislocation of crystals and according to the concept of shear transformation, from a mean perspective, an atomic structure-based STZ (SSTZ) is proposed based on RDF to make up the

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missing structural characteristic of STZ in Part 2. The concept of SSTZ is justified in Part 3, and the applicability and application of the SSTZ are discussed in Part 4. The main conclusions are summarized in Part 5.

2. Method

Looking into the works on dislocation, it is important to note that the elementary deformation ψ of crystals induced by the glide [7] of mobile dislocations is calculated as [26]: $\psi = b\rho_m/\sqrt{\rho_f}$, where ρ_m is the mobile dislocation density (the length of the mobile dislocation line in unit volume); ρ_f is the forest dislocation density; b is the modulus of the Burgers vector of dislocation [9]. However, the glide of a dislocation, similar to the operation of a STZ surrounded by its matrix in amorphous solids, will not change the shape of the grain until it reaches the grain boundary. Hence, understanding the strain of dislocation glide from the perspective of individual dislocation glide [4] seems inappropriate and so does understanding the strain induced by the operation of an individual STZ in amorphous solids. Noting the coefficient $\rho_m/\sqrt{\rho_f}$, where $1/\sqrt{\rho_f}$ is the *mean* space between the forest dislocations in a glide plane which act as obstacles to resist the glide of the mobile dislocations, it means that the macroscopic plastic deformation of crystals is actually calculated as a mean dislocation gliding along its Burgers vector in the glide plane, i.e., a mean dislocation of ρ_m in length and of a Burgers vector of modulus b sweeps through an equivalent crystal grain of a size of $\sqrt{\rho_f}/\rho_m$ in the dislocation glide direction and induces a macroscopic strain of ψ. From this aspect of view, in amorphous solids, it would also be more appropriate to understand the deformation mechanism from a similar mean perspective to resolve the effect of the surrounding matrix in the operation of individual STZs. For the long range disorder, the mean atomic structure of amorphous solids is characterized with radial distribution function (RDF) $g(r)$ schematically illustrated in Fig. 1, where different shells of atoms around the average atom are shown, noting that the splitting of the second strong peak is not drawn for clarity. In the following part, we will justify the STZ based on RDF from the mean perspective with a structure basis, i.e., an atomic structure-based STZ (SSTZ), within the state of the art of researches on amorphous alloys.

3. Results

Firstly, we have calculated the average atom size of a series of amorphous alloys [27] that have been fabricated, which turns out to be of a radii of 0.14–0.2 nm as shown in Table 1. Meantime, it is important to note that the scale range of the RDF is 0 to 1.5–2 nm [18,28], a domain of about 10-atom size comparing to the average atom radii. Based on these results, the number of atoms in the range of 0–2 nm on the RDF is roughly 1000 atoms, encompassing the size (1–3 nm in diameter) and the number of atoms (100–500) of a nowadays recognized STZ quite well [29,30]. Secondly, it has been reported that the length scale

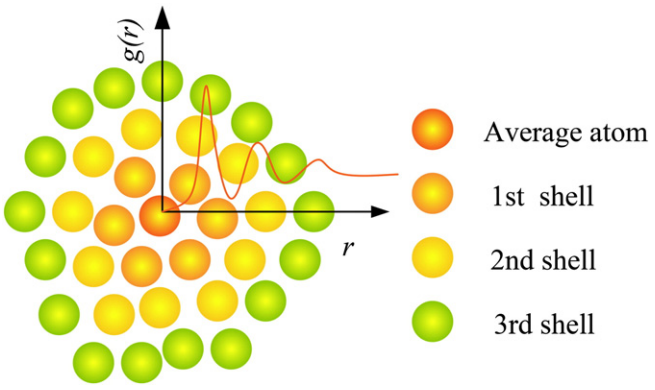

Fig. 1. (Color online) A schematic illustration of radial distribution function (RDF) $g(r)$.

Table 1
Average atomic radii of amorphous alloys.

Composition (at.%)	Average atomic radii (Å)
$Zr_{62}Cu_{15.4}Ni_{12.6}Al_{10}$	1.67
$Zr_{59}Ta_5Cu_{18}Ni_8Al_{10}$	1.67
$Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$	1.58
$Cu_{47.5}Zr_{47.5}Al_5$	1.61
$Cu_{60}Zr_{20}Hf_{10}Ti_{10}$	1.56
$(Ti_{0.5}Cu_{0.5})_{84}Ni_7Hf_5Zr_3Si_1$	1.54
$Ni_{62.5}Zr_{20}Nb_{15}Pd_{2.5}$	1.52
$Ni_{60}Zr_{20}Nb_{15}Pd_5$	1.52
$Ni_{57.5}Zr_{20}Nb_{15}Pd_{7.5}$	1.52
$Ni_{55}Zr_{20}Nb_{15}Pd_{10}$	1.53
$Ni_{52.5}Zr_{20}Nb_{15}Pd_{12.5}$	1.53
$[(Fe_{0.8}Co_{0.1}Ni_{0.1})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	1.40
$[(Fe_{0.6}Ni_{0.4})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	1.40
$Fe_{76}Si_{9.6}B_{8.4}P_6$	1.47
$(Fe_{0.76}Si_{0.096}B_{0.084}P_{0.06})_{99.9}Cu_{0.1}$	1.47
$Zr_{65}Cu_{10}Ni_{10}Al_{10}$	1.67
$Zr_{64.13}Cu_{15.75}Ni_{10.12}Al_{10}$	1.67
$Zr_{61.88}Cu_{18}Ni_{10.12}Al_{10}$	1.66
$Zr_{55}Cu_7Co_{19}Al_{19}$	1.66
$Zr_{57}Cu_{15.4}Nb_5Al_{10}Ni_{12.6}$	1.66
$Zr_{57}Cu_{20}Ti_5Al_{10}Ni_8$	1.66
$Au_{49}Ag_{5.5}Pd_{2.3}Cu_{26.9}Si_{16.3}$	1.63
$(Zr_{0.59}Cu_{0.22}Ti_{0.06}Ni_{0.13})_{85.7}Al_{14.3}$	1.62
$Zr_{45}Cu_{45}Gd_3Al_7$	1.62
$Au_{55}Cu_{25}Si_{20}$	1.62
$Zr_{54}Cu_{46}$	1.60
$Zr_{46.75}Ti_{8.25}Cu_{10.15}Ni_{10}Be_{27.25}$	1.59
$Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$	1.57
$Zr_{48}Fe_8Cu_{12}Nb_8Be_{24}$	1.59
$Ni_{45}Zr_{25}Ti_{20}Al_{10}$	1.56
$Pd_{77.5}Cu_6Si_{16.5}$	1.56
$Pd_{60}Cu_{20}P_{20}$	1.51
$Pd_{40}Cu_{40}P_{20}$	1.50
$Pd_{39}Ni_{10}Cu_{30}P_{21}$	1.47
$Fe_{53}Cr_{15}Mo_{14}Er_1C_{15}B_6$	1.47
$Fe_{74.5}Mo_{5.5}P_{12.5}C_5B_{2.5}$	1.47
$Fe_{70}Mo_5Ni_5P_{12.5}C_5B_{2.5}$	1.40
$Fe_{61}Mn_{10}Cr_4Mo_6Er_1C_{15}B_6$	1.40
$Pd_{64}Ni_{16}P_{20}$	1.44
$Pt_{57.5}Ni_5Cu_{14.7}P_{22.8}$	1.49
$Pt_{60}Ni_{15}P_{25}$	1.50
$Ni_{60}Nb_{35}Sn_5$	1.50
$Ni_{60}(Nb_{0.8}Ta_{0.2})_{34}Sn_6$	1.50
$Zr_{50}Cu_{50}$	1.51
$Zr_{48}Cu_{48}Al_4$	1.60
$Ca_{65}Mg_{8.54}Li_{9.96}Sn_{16.5}$	1.61
$Ca_{65}Mg_{8.31}Li_{9.69}Sn_{17}$	2.00
$Yb_{62.5}\ Mg_{17.5}Cu_5Zn_{15}$	2.00
$Ce_{70}Al_{10}Ni_{10}Cu_{10}$	1.97
$(Ce_{20}La_{80})_{68}Al_{10}Cu_{20}Co_2$	1.89
$Ce_{68}Al_{10}Nb_2Cu_{20}$	1.88
$(Ce_{80}La_{20})_{68}Al_{10}Cu_{20}Co_2$	1.88
$Ce_{68}Al_{10}Co_2Cu_{20}$	1.88
$Ce_{68}Al_{10}Ni_2Cu_{20}$	1.87
$La_{60}Al_{20}Co_{20}$	1.87
$Dy_{55}Al_{25}Co_{20}$	1.85
$Pr_{55}Al_{25}Co_{20}$	1.78
$Tb_{55}Al_{25}Co_{20}$	1.82
$Ho_{55}Al_{25}Co_{20}$	1.78
$Er_{55}Al_{25}Co_{20}$	1.76
$Tm_{55}Al_{25}Co_{20}$	1.75
$Tm_{39}Y_{16}Al_{25}Co_{20}$	1.75
$Lu_{39}Y_{16}Al_{25}Co_{20}$	1.75
$Lu_{45}Y_{10}Al_{25}Co_{20}$	1.74
$Lu_{55}Al_{25}Co_{20}$	1.74
$Mg_{65}Cu_{25}Gd_{10}$	1.74
$Mg_{65}Cu_{25}Y_9Gd_1$	1.71
$Mg_{65}Cu_{25}Y_{10}$	1.70
$Mg_{65}Cu_{25}Y_8Gd_2$	1.70
$Mg_{65}Cu_{25}Y_5Gd_5$	1.69
$Mg_{65}Cu_{25}Tb_{10}$	1.68