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Structural and Mechanical Characteristics of Metallic Glasses

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Metallic Glasses (MGs) are potential candidate for a myriad of structural and engineering applications [1-3] because of their unique properties due in part of the absence of crystalline lattice which is found in conventional metals. However, the amorphous structure in MGs are still not very well understood and recent studies have highlighted the importance of understanding the atomic-level structure of MGs and its correlation with the mechanical behaviors [4].

To understand the structure of MGs, binary systems such as Ni-P and Cu-Zr have been extensively studied [5-7]. Microscopically, the Short-Range Order (SRO) of MGs is characterized by the presence of similar solute-centered clusters [5,8]. The effective solute-to-solvent radius ratio plays an important role in determining the SRO in different systems [9-11]. The dominant SRO, or the structural order, could exhibit in the form of Kasper polyhedra with a large fraction of fivefold bonds [5]. However, any distortion to the fivefold bond will promote the formation of defective sites, which are energetically unstable [4,5]. Furthermore, the absence of direct solute-solute contact was confirmed by studying the partial Radial Distribution Functions (RDFs) [5]. At a larger scale, these similar clusters are efficiently packed and connected, forming the Medium-Range Order (MRO) in 3D space [5,8,12].

Unlike in crystalline alloys where the lattice and crystal defects could be easily identified, in MGs, there are a variety of cluster types [5] resulting in heterogeneity in the structure. For example, some clusters such as Kasper polyhedra could be the dominant structure, while other clusters are relatively unstable and irregular. Egami et al. [13,14] proposed the concept of atomic level stresses to explain the origins of these structural fluctuations. The size of each atom varies with its atomic level stress and leads to changes in the effective size ratio between the solute and the solvent atoms [13]. Since the effective size ratio determines the corresponding coordination number, therefore atoms with different stresses will possess different packing schemes. Furthermore, strain energy will be induced by the atomic level stresses [15], hence it is reasonable to conclude that atoms with lowest energy are stable and tend to form ordered clusters, whereas atoms with highest energy are likely to form structural defects.

The micro structural features of MGs are of fundamental importance for explaining their macroscopic properties, such as their strength, elasticity and deformation behavior. Although the mechanical performances of crystalline materials could be explained from the coexistence of lattice periodicity and crystal defects such as dislocations, the local topology varies from site to site in MGs, resulting in distinct mechanical behaviors at each site [4].

One interesting attribute of MGs is their ultrahigh strength–exceeding 1 GPa in most cases [16,17]. The typical yield strain of MGs is about 2%, which is far beyond that of crystalline alloys. While the strength of crystalline materials is determined by the sliding of dislocations, the strength of MG sis related to the strength of metallic bonds due to the absence of dislocations [4,16]. A well relaxed MG has a large fraction of unlike (solute-to-solvent) bonds which exhibit higher stability and bonding strength [4,5]. In other words, the solute atoms are likely to be surrounded by solvent atoms, leading to an improvement in strength [4].

At microscopic level, there are regions with low and high local stiffness in MGs [18]. This mechanical heterogeneity originates from the structural fluctuations in MGs, and has been confirmed by computer simulations [19-22]. Typically, Kasper polyhedra tend to percolate with each other, forming the structural backbone to sustain the entire matrix [5,22]. Consequently, regions with more Kasper polyhedra tend to form interpenetrating networks and exhibit higher resistance to external loads. Regions with less Kasper polyhedra are relatively unstable and are likely to undergo inelastic deformation. It is found that the shear resistance of MGs is enhanced with more rigid structural units. For instance, computer simulations on Cu-Zr MG confirmed that full icosahedra exhibits lower atomic strain energy and yields higher stiffness, which means that they are energetically more stable [15,23]. Furthermore, the icosahedra clusters tend to connect with one another, constituting the MRO in the system [12].

The yielding of MGs has been attributed to the percolation of Shear Transformation Zones (STZs) that undergo inelastic deformation and are characterized by the structural defects in MGs [24-26]. Typically, the STZs are dispersed in the matrix, which is supported by the structural backbone (networks of Kasper polyhedra). By applying a shear force onto the system, these STZs will experience inelastic deformations and gradually percolate with one another [27]. As long as the interconnection of these STZs does not exceed a critical length scale, they are reversible upon unloading. However, if the shear stress is sufficiently large, a variety of STZs will then connect with one another, giving rise to the destruction of the elastic backbone and irreversible plastic strain. At room temperature, shear deformation is concentrated in several localized shear bands, which is a catastrophic failure mode of MGs. Molecular Dynamics (MD) simulations have been applied to study the yielding and shear banding process of MGs [28,29]. For example, in Cu-Zr MG, regions with more unstable polyhedra are likely to undergo inelastic deformations, while those with the more stable full icosahedra will only be elastically deformed. Furthermore, it is also reported that the full icosahedra in STZ should be transformed into other unstable clusters during the yielding process.

In summary, the atomic structure of MGs has a broad distribution of networks that gives rise to their unique mechanical properties. Although the mechanical behaviors of MGs have been intensively analyzed through experiments, understanding of the underlying mechanisms of their mechanical performances is still inadequate.

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Henceforth, the atomic structure and structure-property relationship of MGs need further investigations to unravel and improve our understanding of the glassy state.

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