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Free volume gradient effect on mechanical properties of metallic glasses

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ABSTRACT

Gradient of free volume distribution in metallic glasses is omnipresent either naturally or artificially in synthesis and application. But how the spatial inhomogeneity affects mechanical properties remains poorly understood. Here we probe this issue using finite element modeling. We find that the strength and toughness improves with increasing gradient; and the larger the gradient, the more effective. But the plasticity is marginally enhanced or even decreases. Too high the gradient value leads to brittle fracture caused by abrupt release of the large stress concentrated at the gradient region. The effects are represented in their relations with the gradient energy coefficient.

Inhomogeneity is undesirable in many materials for its contribution to local stress concentration that eventually leads to fracture and failure. But in metallic glasses (MGs), it is the quantity of choice in tailoring mechanical properties. In crystalline materials, chemical composition variation, second phase with different crystal structures, and defect density and microstructure are the common examples of inhomogeneity and can be varied to alter properties. In MGs there are fewer choices in introducing "heterogeneity". But there is an internal state variable, free volume (FV) that can be varied more readily [1–5]. This unique representation of inhomogeneity in MG is omnipresent either naturally or artificially in synthesis and applications, for example, during rapid cooling of glass forming liquid in copper mould, [6] in surface treatment either using pulse laser, ion irradiation, or mechanical deformation such as shot peening or grinding, [7–12] and in the heavy mechanical deformation such as high pressure torsion [13,14], rolling, [15–17] and wire drawing [18–20]. These FVs are inhomogeneous in spatial distribution, resulting in gradient between different FV regions.

To reduce the undesired brittleness in monolithic MGs, inclusions with various structures, composition and properties are introduced [21]. They could be effective in reducing the brittleness by blocking shear bands [22]. FV gradients are introduced into MGs either in the interface regions between the inclusion and the matrix or inside the inclusion itself [23]. Although a large body of knowledge is available for the roles played by the average FV density in mechanical properties in MG composites, the FV gradient effect remains largely unknown quantitatively. In this work we attempt to address this problem using numerical modeling on the continuum scale.

FV gradient is defined as the variation of the FV density $v_f(\vec{r})$ in space, $\vec{\nabla} v_f$. It appears whenever v_f is not distributed homogeneously. The occurrence of the FV gradient indicates change in the local mechanical energy – more work is needed if one deforms a region with lower FV and vice versa. Usually the scalar quantity $|\vec{\nabla} v_f|^2$ out of the vector $\vec{\nabla} v_f$ is considered as the gradient contribution to the mechanical energy. The same argument has been applied in phase transitions: [24–28] To form a new phase, the interface containing the gradient interface (GI) between the new and old phase must be created, which demands additional energy. For mechanical deformation of MGs, the same concept should apply: In addition to the abovementioned example of deforming existing high and low FV regions with a GI, deformation also generates high FV density in certain regions such as surface and around inclusions, resulting in new GIs. To extend the high FV density region further requires more external applied stress. Thus one expects that the larger or stepper the FV gradient, the higher mechanical work is required, or the higher the strength and toughness of the sample could be. Here we examine whether or not this thinking is pertinent.

The interface region contains varying degrees of FV gradients depending on processing and application conditions. In MGs containing crystalline inclusions, the FV gradient at the crystal-glass interface is sharp, while a shallow gradient should exist at the surface region in contact with the copper mould in rapidly cooled samples; and shot peened or pulse laser treated surface has relatively diffusive FV gradient

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interfaces. The key question is how these varying degrees of FV gradients contribute to the overall mechanical properties. To address this question, we use the finite element modeling (FEM) in conjunction with the constitutive model that explicitly incorporates the FV variation in MGs [29–31].

The gradient is introduced through the initial FV distribution in the sample. Presently, we only deal with the gradient in one dimension across the two dimensional plane in the sample under plane strain condition. Operationally, we assign FV values in the mesh points according to certain *spatial distributions*; and the FV value itself is drawn from two types of *statistical distributions*. One is from uniform Gaussian distribution and another non-uniform bimodal distribution [32], which results in four cases: (a) spatially homogeneous (without gradient) and statistically uniform, (b) spatially homogeneous but statistically non-uniform, (c) spatially inhomogeneous and statistically uniform, and (d) spatially inhomogeneous and statistically non-uniform distributions. Case (a) and (b) have been studied previously and the results show that the statistically different but spatially homogeneous distributions of FVs alone can dramatically changes mechanical properties in samples without FV gradient [32]. To systematically examine the FV gradient contributions to mechanical properties, here we investigate the other two cases, (c) and (d). As shown below, (a) and (b) are the extreme cases of (c) and (d).

In the insets of Fig. 1(a)–(c), we show three typical cases of the initial FV gradient: (A) (Fig. 1(a)) and (B) (Fig. 1(b)) have higher FV at the sides and lower in the center with gradual variation in between, and (C) (Fig. 1(c)) has a sharp interface between the high and low FV regions. The FV values in case (A) are drawn from the uniform distribution, (B) a uniform random distribution, and (C) a non-uniform bimodal distribution. All statistical distributions are kept at the same mean FV value of 0.05. For each case, we also have a series cases for intermediate FV gradients (see the insets in Fig. 1(a)–(c)) with decreasing values. The extreme cases are these without gradient, that is, the uniform FV spatial distribution.

With the given initial FV distributions, by solving the equations of FV change and the strain and stress under a given external load, we can obtain the mechanical properties of the samples containing various gradients. In particular, the material tangent $D^{ep}_{ijkl} = \partial\Delta\sigma_{ij}/\partial\Delta\varepsilon_{kl}$ is implemented in ABAQUS finite element software through a UMAT subroutine. The material parameters of bulk MG $Zr_{41.25}Ti_{13.75}Ni_{10}Cu_{12.5}Be_{22.5}$ are used. The samples have 7500 regular mesh elements and the periodic boundary conditions. Since our focus is on the gradient, the sample is setup such that the high and low FV regions have the same volume fraction. Plane strain tension load are applied to the samples along the interface direction with the effective strain date of 0.1/s. Because tension measures ductility truthfully and the sample with the periodic boundary condition in FEM does not break if a local shear band passes through, which is not the case in experiment, we chose to use tension in our modeling. For more technical details, the reader is referred to Ref. 29–32.

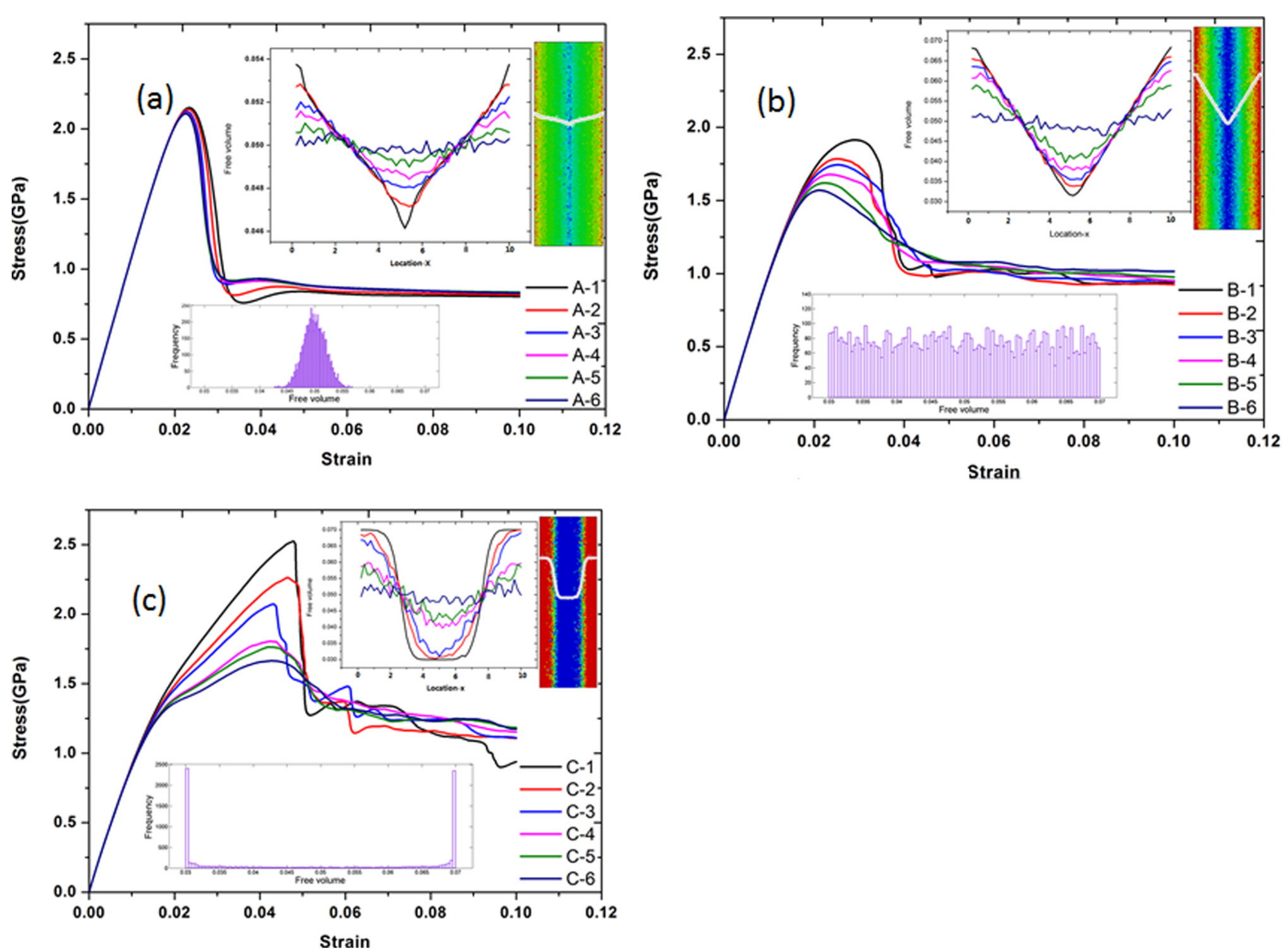

Fig. 1. The stress-strain relations for samples with different FV distributions from (a) a homogeneous Gaussian-like statistical distribution described by a beta distribution with the transformation relation through a beta function, beta(50,50)*0.04 + 0,03, (b) a uniform random statistical distribution described by beta(1,1)*0.04 + 0.03, and (c) an inhomogeneous bimodal statistical distribution described by beta(0.1,0.1)*0.04 + 0,03. The statistical distributions are shown in the lower inset. The upper left inset shows the different intermediate initial spatial FV distributions across the sample with different FV gradients. The upper right inset shows the intial FV distribution and the FV density profile. The warmer the color, the high FV density; and the line is the mean FV profile. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)