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# Three-dimensional phase-field simulation on the deformation of metallic glass nanowires

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ABSTRACT

It is very challenging to investigate the deformation mechanisms in micro- and nano-scale metallic glasses with diameters below several hundred nanometers using the atomistic simulation or the experimental approaches. In this work, we develop the fully three-dimensional phase-field model to bridge this gap and investigate the sample size effects on the deformation behaviors of metallic glass nanowires. The initial deformation defects on the surface are found to significantly affect the mechanical strength and deformation mode of nanowires. The improved ductility of metallic glass nanowires could be related with the multiple shear bands initiated from the nanowire surfaces.



## 1. Introduction

In the past several years, there were a lot of investigations on the mechanisms of sample size effects on the deformation modes of metallic glasses (MGs). Several possible factors are accounted for the improved ductility and mechanical strength of MGs with sizes that are reduced from microns to several hundred nanometers, such as the energy balance between surface energy and strain energy or the size effects on plastic zone [1,2], stress states [3], surface constraint effects or surface unevenness effects [1,4–7], and the effects of surface atoms on shear transformation zones [8]. However, it is noted that there were some inconsistent and controversial results in those theoretical and experimental investigations. For the samples with sub-micron sizes, some researchers reported that the yield strength was size-independent [9–11]. Nevertheless, Jang and Greer indicated that the yield strength was size-dependent above 500 nm and size-independent below 500 nm [2]. Lai et al. stated that the yield strength should increase with decreasing size [12]. It was also found that the critical size at which the localized deformation transformed to the homogeneous deformation was significantly divergent. The critical size was reported to vary from 50 nm to 400 nm [1,3,11,13]. On the contrary, it was found that the localized shear deformation was less important and global plasticity could be significant when the size was decreased to 250 nm [14] or 150 nm [9]. These divergences are not surprising since it is very challenging to investigate the deformation mechanisms in MGs with sizes in the critical size region using the atomistic simulation or the experimental methods. In particular, although computer simulations such as molecular dynamics (MD) and finite element method (FEM) have played important roles in the investigations of the mechanical behaviors of metallic glasses, metallic glasses with their dimensions falling into the critical size region (40–400 nm) are either too large for the MD simulation to simulate their deformation processes, or too small for the FEM to capture their deformation details in the atomistic scales.

In this study, we investigate the three-dimensional (3D) nanowire samples with diameters ranging from 40 nm to 400 nm in tensile conditions based on the phase-field model, which was first developed by Zheng and Li [15] to model the shear banding in bulk metallic glasses (BMGs) under plane stress/strain loading conditions. The article is arranged as follows. In Section 2, the phase-field model is extended to investigate the deformation of fully 3D MG systems. In Section 3, the effectiveness of phase-field model in studying the fracture of 3D MG nanowires is demonstrated. Deformation mechanisms of MG nanowires with diameters of 40 nm and 400 nm are investigated in detail and are compared to elucidate the sample size effects on the mechanical properties of MGs.

## 2. Details of simulation methods

According to the characteristics of shear bands, the strain energy in the regions around the shear bands is a function of local deformation defect density $\rho$ ($\mathbf{r}$) and strains $\varepsilon_{ij}$, where $\varepsilon_{ij}$ are components of the strain tensor defined by the displacement field $\boldsymbol{u}$, as follows

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$$\varepsilon_{ij} = (\partial u_j/\partial x_i + \partial u_i/\partial x_j)/2, \quad i,j = 1,2,3. \tag{1}$$

According to the dynamic model built by Zheng and Li [15], the shear-band propagation and evolution could be simulated by solving the governing equations of deformation defect density $\rho$ ($\boldsymbol{r}$) and displacement field $\boldsymbol{u}$, as follows,

$$\rho_0 \frac{\partial^2 \mathbf{u}}{\partial t^2} = -\nabla \cdot \left[\frac{\delta F}{\delta \varepsilon_{ij}}\right] = \mu \nabla \cdot \left[\left(1 + \frac{a_1}{2}\rho^2 + \frac{b_1}{3}\rho^3\right)\nabla \mathbf{u}\right], \tag{2}$$

and

$$\tau_\rho \frac{\partial \rho}{\partial t} = -\frac{\delta F}{\delta \rho} = \kappa \nabla^2 \rho - (a_0\rho + b_0\rho^2 + c_0\rho^3) - \rho(a_1 + b_1\rho)(e[\varepsilon_{ij}] - e_0), \tag{3}$$

where $\tau_\rho$ is the characteristic time for deformation defects activation. Eq. (3) describes the local structural evolution of the MG, especially the accumulation of the deformation defects under the local plastic strain. $\rho_0$ is the mass density of the sample, $k$ is the interfacial energy between the regions with or without the deformation defects. The coefficients $a_0$, $b_0$ and $c_0$ in Eq. (3) depend on external state variables except the strain. $\Delta e = e[\varepsilon_{ij}] - e_0$; $e_0$ is the strain energy at the elastic limit when the applied stress $\sigma$ is close to the fracture strength $\sigma_f$. $e[\varepsilon_{ij}] = \frac{1}{2} C_{ijkl}\varepsilon_{kl}\varepsilon_{ij}$, where $C_{ijkl}$ is the component of the stiffness matrix defined as $C_{ijkl} = \mu(\delta_{ij}\delta_{kl} + \delta_{il}\delta_{jk}) + \lambda\delta_{ik}\delta_{jl}$. $\mu$ is the shear modulus and $\lambda$ is Lamé constant.

In this work we shall solve Eqs. (2) and (3) in fully 3D samples. The samples are chosen as the cylinder with a fixed height of 800 nm as shown in Fig. 1(a). The different sample sizes are characterized by the diameter of the cylinder, which ranges from 40 nm to 400 nm. Hence the 3D MG samples could be considered as nanowires with fixed length. The effects of aspect ratio on the deformation are not observed in the present simulation. Vitreloy 1 ($Zr_{41}Ti_{14}Ni_{10}Cu_{12.5}Be_{22.5}$) is chosen as the material in the present simulations. The material properties are listed as follows [16–17]: Glass Transition Temperature $T_g = 625$ $K$; Young's modulus $E = 95$ GPa; Poisson's ratio $v = 0.35$; Mass density $\rho_0 = 6050$ kg/m$^3$. The elastic strain limit under uniaxial tension is $\varepsilon_f \sim 2\%$. The characteristic time for deformation defect activation is $\tau_\rho = 0.25$ ns [18]. The coefficients in Eq. (3) are given by $a_0 = -4\Delta G\ (T_g - T)/T_g$, $b_0 = -24\Delta G$, $c_0 = 16\Delta G$, where the deformation defect activation energy $\Delta G$ is estimated as 4.6 eV at room temperature [19]. The coefficients $a_1 = -6$ and $b_1 = 6$ are chosen to quantitatively characterize the structural transformation of deformation defects in glassy alloy under plastic deformation such that $\rho(\boldsymbol{r})$=0 and 1 represent the ideal glassy state and the cracking state of the MG, respectively. The shear modulus tends to zero when $\rho(\boldsymbol{r}) \to 1.0$, which can be the indication of fracture in the glassy alloy. The critical density of deformation defect is defined as $\rho(\boldsymbol{r})$=0.8 to distinguish the shear softening regions from the remaining elastic region of ideal randomly close-packed solid structures.

Eqs. (2) and (3) can be solved numerically. Tetrahedra are used to discretize the space in nanowire interiors and the backward differentiation formula (BDF) scheme is employed to discretize and integrate time in the numerical analysis. The uniaxial tension is applied on the top surface of nanowire. The displacement constraint in $Z$-direction is imposed on the bottom surface, and the other surfaces are kept free as shown in Fig. 1(a). Before the simulation, the initial deformation defects (defined as the points with $\rho(\boldsymbol{r}) = 1.0$ at time $t = 0$) are randomly distributed in nanowire interior and on sample surfaces except the top and bottom surfaces. The remaining regions of nanowire are defined as the ideal glassy structures with $\rho(\boldsymbol{r}) = 0$.

## 3. Results and discussions

### 3.1. Phase-field simulation on the deformation of fully 3D MGs

As mentioned above, fully 3D simulation on the deformation of MGs based on the phase-field theory has not been reported in literature. Therefore, we shall first present a simple 3D case study for the analysis of fracture and shear-band propagation in the metallic glasses to verify the effectiveness of the phase-field model in the simulation of mechanical deformation. The sample is in cylinder shape with a diameter of 400 nm and a height of 800 nm as shown

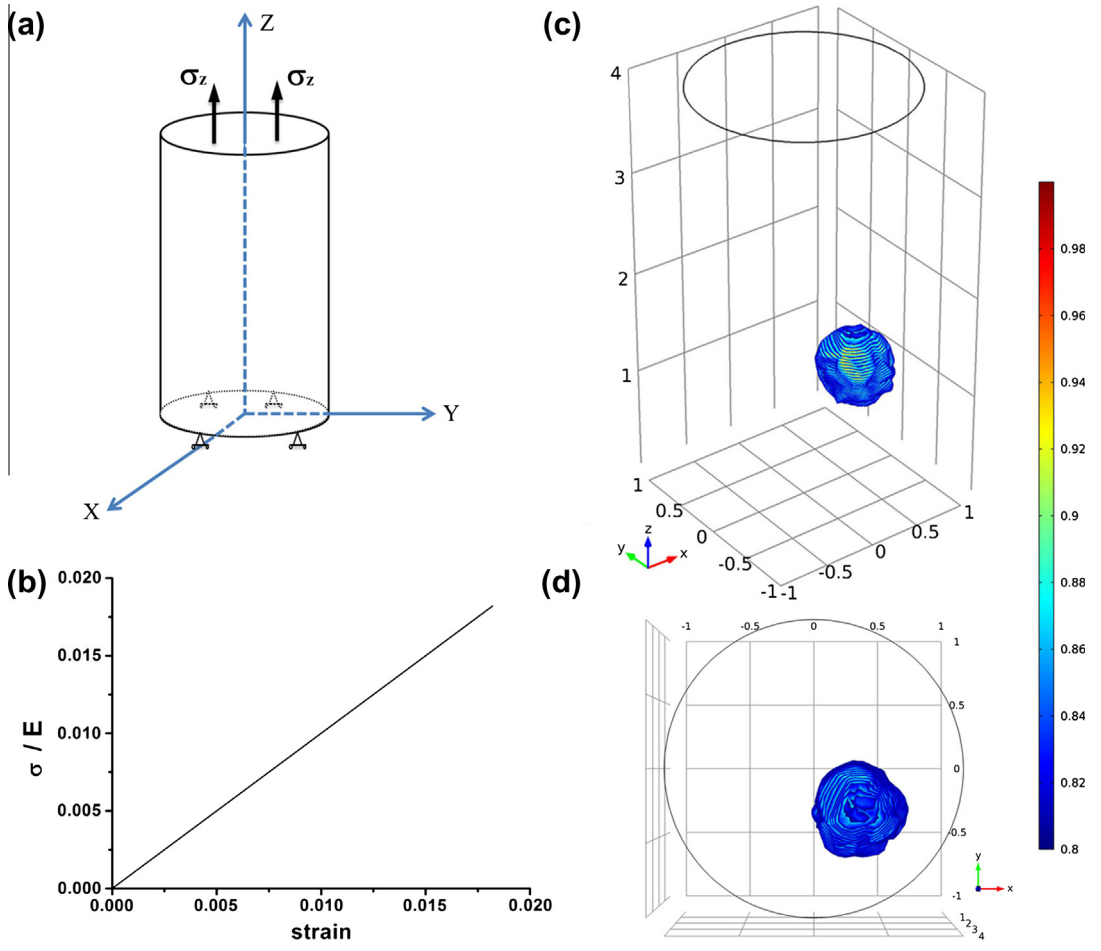


**Fig. 1.** (a) The model system of MG ($D$ = 400 nm, $h$ = 800 nm). Tensile stress is applied along the $Z$ direction. (b) Stress–strain relation of the model system. (c) Side, and (d) top views on the surface plots of deformation defects with density $\rho(\boldsymbol{r}) > 0.8$. The color bar represents the values of $\rho(\boldsymbol{r})$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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