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Computer simulation of the strong surface effects on deformation behaviors of metallic glass nanowires

G.P. Zheng,[a,b,*] H.Y. Zhang[a] and J.H. Yang[b]

[a] *Department of Mechanical Engineering and Shenzhen Research Institute, Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong*

[b] *School of Materials Science & Engineering, University of Shanghai for Science and Technology, Shanghai, China*

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Size effects on deformation behaviors of metallic glass (MG) nanowires are found to be associated with their surface imperfections from phase-field modeling. Necking instead of shear banding is the dominant deformation mode in MG nanowire with diameter $d < 100$ nm, suggesting that nucleation and growth of the flow defects at the nanowire surface could be the deformation mechanism. The surface effect manifests itself by the finite-size scaling for the fracture strength and the critical intrinsic surface defect density.

Keywords: Metallic glass; Hall–Petch effect; Shear bands; Phase-field model; Fracture

In the past few years tremendous efforts have been devoted to understanding the sample size effects on the mechanical properties of metallic glasses (MGs). Mechanisms of sample size effects on the mechanical properties of MGs are believed to be related to the length scales of shear banding, the surface energy [1,2], the stress states [3] and surface roughness [1,4–7] of the samples, or the shear transformation zones affected by the surface atoms [8]. However, the results obtained from simulations and experimental investigations were inconsistent and controversial. Whether the yield strength depends on the sample sizes ranging from 100 nm to 500 nm is still a matter of debate [2,9–12]. In particular, the critical sample size at which the localized plastic deformation transformed to the homogeneous deformation was reported to vary from 150 nm to 500 nm [1,3,9,11,13,14]. In experiments these divergences could be ascribed to different sample conditions such as the imperfect sample geometry. Nevertheless, the differences in the intrinsic structural states on the sample surface are unavoidable, especially in nanosized samples prepared by top-down methods [15]. Thus understanding the effects of intrinsic or initial deformation defects on the deformation mechanisms of the sample not only benefits the nanotechnology applications of MGs but also sheds some light on the underlying physics of shear banding in the deformation of MG. Evidence from experiments has shown the mechanical strength of the as-cast and the annealed metallic glasses are very different, owing to the differences in the free-volume defect density in the sample interiors. On the other hand, surface imperfections on the sample surfaces significantly affect the mechanical properties of metallic glass nanowires usually fabricated by the focused ion beam (FIB) method or templates with nanosized channels [16].

In this work we use the phase-field model [17] to investigate the deformation behaviors of the MG nanowires. The density of deformation defects $\rho(\boldsymbol{r})$ is chosen as the order parameter. Such scalar quantity could indicate the occurrence of the shear band based on the assumption that it also reflects the changes of other quantities such as local atomic packing, chemical composition and short- and medium-range topological order, which have been verified by atomic simulations [5,8]. Compared with the ideal glass with random close packing structure, the loosely packed atomic clusters in the MG are defined as deformation defects [18].

* Corresponding author at: Department of Mechanical Engineering and Shenzhen Research Institute, Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong; e-mail: mmzheng@polyu.edu.hk

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Based on the Ginzburg–Landau formulism, the shear band propagation and evolution are simulated by solving the governing equations of $\rho(\mathbf{r})$ and displacement field $\mathbf{u}$, as follows [17]:

$$\rho_0 \frac{\partial^2 \vec{u}}{\partial t^2} = \mu \nabla \cdot \left[\left(1 + \frac{a_1}{2}\rho^2 + \frac{b_1}{3}\rho^3 \right) \nabla \vec{u} \right] \quad (1)$$

and

$$\tau_\rho \frac{\partial \rho}{\partial t} = \kappa \nabla^2 \rho - (a_0\rho + b_0\rho^2 + c_0\rho^3) - \rho(a_1 + b_1\rho) \times (e - e_0) \quad (2)$$

where ρ_0 is the mass density of the sample, κ is the interfacial energy between the regions with or without the deformation defects, τ_ρ is the characteristic time for deformation defects activation, e is the local strain energy, e_0 is the strain energy at the elastic limit when the applied stress σ is close to the fracture strength σ_F and μ is the shear modulus of a bulk sample. The definitions of coefficients a_0, b_0 and c_0, a_1 and b_1 can be found in Ref. [17].

We solve Eqs. (1) and (2) numerically in the MG nanowire system with a fixed height $L = 800$ nm and diameter $d = 30$–400 nm under uniaxial tension, as shown in Figure 1a. The simulation results are found to be independent of the aspect ratio of the samples. Vitrelloy-1 ($Zr_{41}Ti_{14}Ni_{10}Cu_{12.5}Be_{22.5}$) is chosen as the material [17,19–20]. The critical density of deformation defects defined as 0.8 is chosen to distinguish the shear softening regions from the elastic regions. Before the tensile deformation, the initial deformation defects (defined as the points with $\rho(\boldsymbol{r}) = 1.0$ at time $t = 0$) are randomly distributed in nanowire interiors and on sample surfaces except the top and bottom surfaces.

We first investigate the relation between the intrinsic volume fraction of deformation defects (N_0) in the interior of an undeformed MG sample and its mechanical strength. For comparisons, deformation behaviors of MG nanowires with $d = 400$ nm and 40 nm are simulated, and both nanowire samples have the same intrinsic deformation defect density on their surfaces ($n_0 = 15\%$). The normalized fracture strength (σ_F/μ, $\mu = 35$ GPa) decreases with increasing N_0, as shown in Figure 1b and c. The decrease of mechanical strength of MG with increasing N_0 has been well observed through atomic force microscopy and nano-hardness measurements [21].

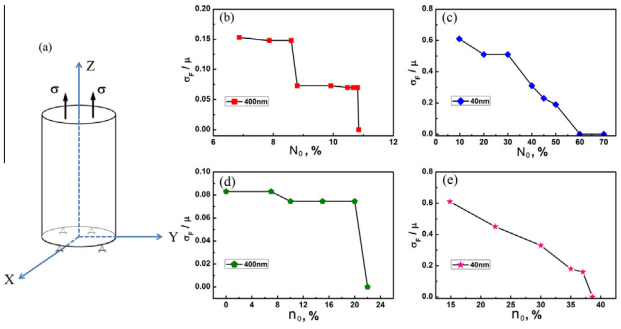

Figure 1. (a) The model system of MG nanowires under tension. Dependences of normalized fracture strength (σ_F/μ) on N_0 (a, b), and n_0 (d, e).

The influence of n_0 on σ_F/μ is shown in Figure 1d and e for MG nanowires with $d = 400$ nm and $d = 40$ nm, respectively, where N_0 of both samples is kept as 9.8%. As shown in Figure 1d, there is a slight change of σ_F when n_0 changes from 0 to 20% in nanowire with $d = 400$ nm. σ_F decreases rapidly when n_0 is close to 22%. For the MG nanowire with $d = 40$ nm, σ_F decreases gradually with the increasing n_0, as shown in Figure 1e. When n_0 increases to a critical value $n_c(d)$ ($\sim$38.6%), σ_F decreases to almost zero (0.01 GPa). Remarkably, σ_F decreases more than 75% when n_0 changes from 15.0% to 37%. This is because the larger n_0 leads to higher possibility of activated deformation defects which could induce the local cracking or fracture on the nanowire surface. From the simulation it is noted that the surface effect is very significant in nanowires with $d = 40$ nm. Keeping $n_0 = 20\%$ and $N_0 = 9.8\%$ for both samples, we can observe that σ_F of nanowires with $d = 40$ nm is much higher than that of nanowires with $d = 400$ nm, indicating significant size effects on the mechanical strength of MG. The simulation results are consistent with experiments [3].

Under the circumstance that the densities of intrinsic deformation defects in the interiors ($N_0 = 9.8\%$) and on the surfaces ($n_0 = 20\%$) of the MG nanowires are independent of their diameters, the sample size effect on the fracture strength is shown as the $\sigma_F/\mu \sim d$ curve (square symbols) in Figure 2a. σ_F increases significantly when d decreases from 400 nm to 100 nm. It seems that σ_F approaches the theoretical strength limit (0.45–0.5μ) if $d < 100$ nm. Quantitative analysis on the $\sigma_F \sim 1/d$ relation is illustrated in the inset of Figure 2a. The Hall–Petch like relationship $\sigma_F = \sigma_0 + Kd^{-1}$ is used for

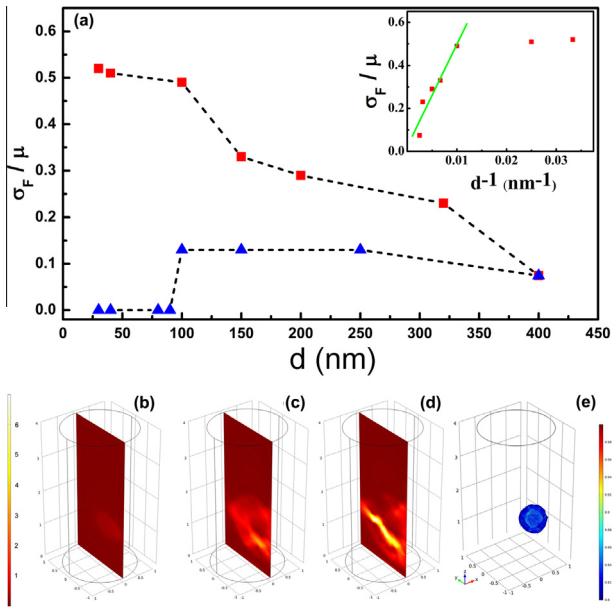

Figure 2. (a) The sample size effects on σ_F/μ. The inset shows the fits of σ_F/μ with respect to d^{-1}. (b–d) The equivalent plastic strain at the XZ cross-sectional plane ($d = 400$ nm) at time $t = 10$, 12.5, 13 ns, respectively. (e) The formation of shear band embryo at $t = 10$ ns. The color bar on the left represents the value of the plastic strains. The color bar on the right represents the value of $\rho(r)$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)