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Low-cycle fatigue of metallic glass nanowires

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Abstract—Low-cycle fatigue fracture of metallic glass nanowires was investigated using molecular dynamics simulations. The nanowires exhibit work hardening or softening, depending on the applied load. The structural origin of the hardening/softening response was identified as the decrease/increase of the tetrahedral clusters, as a result of the non-hardsphere nature of the glass model. The fatigue fracture is caused by shear banding initiated from the surface. The plastic-strain-controlled fatigue tests show that the fatigue life follows the Coffin–Manson relation. Such power-law form originates from plastic-strain-dependent microscopic damage accumulation. Lastly, the effect of a notch on low-cycle fatigue of nanowires in terms of failure mode and fatigue life was also discussed.

Keywords: Metallic glasses; Nanowires; Low-cycle fatigue; Fracture; Work hardening

1. Introduction

Nanometer-scaled metallic glasses have emerged as a scientifically interesting and technologically useful structural material [1,2]. They possess an unusual suite of properties, such as excellent formability [3], high elastic limit [4–6], high strength [4,7] and high ductility [4,7,8]. Therefore, metallic glasses have great advantages for applications in the fields of microelectromechanical [9], nanoelectromechanical systems [10], micromachines [1] and biomedical applications [11]. To utilize the extraordinary properties of nanometer-scaled metallic glasses, bulk metallic glass composites with nanometer-scaled microstructure [12,13], or bulk metallic glass foams [14] with ligaments of nanometer-sized cross-sections have been developed, significantly enhancing the application prospects of metallic glasses. In the context of the above real-world applications, the fatigue behavior of nanometer-scaled metallic glasses, however, has received much less attention. Such omission is significant, since fatigue failure accounts for more than 90% of all mechanical failures [15].

The fatigue limit of the submicron-sized metallic glasses was found to be as high as the yield stress [16]. Bulk metallic glass composites with micron-sized microstructures also exhibit enhanced fatigue endurance limit [17]. In the few experiments devoted to the cyclic deformation of nanometer-scaled metallic glasses, work-hardening was observed under cyclic tension [4,5] or in nanoindentation testing [18]. However, the exact fatigue fracture mechanism and the quantitative description of the fatigue life of nanometer-scaled metallic glasses are largely unknown.

Molecular dynamics (MD) simulations can provide important atomistic insights on fatigue failure. In existing MD simulations on the fatigue behavior of metallic glasses, directional localization of free volume [19] and defects [20] were suggested to be important for the initiation of fatigue damage. Cyclic loading induced hardening [21] and crystallization [22] have also been observed in recent atomic simulations. However, it is challenging to directly simulate fatigue fracture in MD simulations. The foremost challenge arises from the deficiency of the available atomic force fields [23], which usually lead to model metallic glasses that are significantly more ductile than experimental metallic glass systems. For instance, the amorphous nanowire modeled by the widely used Lennard–Jones (LJ) force field [24] exhibits little damage, let alone fracture, even after extensive push–pull cyclic loading with a strain amplitude as high as 36% in our preliminary testings. Moreover, it has been shown that the sample preparation can significantly affect the deformation mode of nanoscale metallic glass samples [25]. Specifically, nanoscale metallic glass samples made from the traditional cutting method (vitrify a bulk liquid to bulk glass, then cut to a nanowire) have unrelaxed surfaces, which will in turn suppress the shear band formation and likely fatigue fracture. As a result, to the best of our knowledge, no direct fatigue fracture process of metallic glass nanowires has been observed in MD simulations.

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In this study, we conducted cyclic compression tension tests with a large strain range to directly examine the low-cycle fatigue fracture behavior of metallic glass nanowires at the atomic level. During the cyclic loading, the nanowire hardens under low strain amplitude and softens under higher strain amplitude. The final fracture of the nanowires is caused by rapid shear band formation, true for the entire range of strain amplitudes explored in this study. In the plastic-strain-controlled fatigue tests, the fatigue life of the nanowire follows the Coffin–Manson relation. This power-law form can be rationalized from the microscopic deformation damage accumulation, which depends on the macroscopic plastic strain amplitude.

2. Simulation methodology

MD simulations were carried out with the LAMMPS package (Large-scale Atomic/Molecular Massively Parallel Simulator, http://lammps.sandia.gov) [26] with a modified binary Lennard–Jones (mBLJ) potential upon the Wahnstrom system [23]. The alloy consists of two equimolar species, which will be referred to as *S* and *L* for small and large atoms, interacting via a modified LJ potential of the form:

$$\phi_{mBLJ}(r) = \begin{cases} 4\varepsilon_{\alpha\beta}\left(\frac{\sigma_{\alpha\beta}^{12}}{r^{12}} - \frac{\sigma_{\alpha\beta}^{6}}{r^{6}}\right) - \varepsilon_{cutoff}, & \mathrm{r} < r_{\alpha\beta}^{s} \\ 4\varepsilon_{\alpha\beta}\left(\frac{\sigma_{\alpha\beta}^{12}}{r^{12}} - \frac{\sigma_{\alpha\beta}^{6}}{r^{6}}\right) - \varepsilon_{cutoff} & \\ \qquad +\varepsilon_B\varepsilon_{LL}\cdot sin^2\left(\pi\frac{r_{\alpha\beta}^{c}-r}{r_{\alpha\beta}^{c}-r_{\alpha\beta}^{s}}\right), & \mathrm{r} \geqslant r_{\alpha\beta}^{s} \\ 0, & \mathrm{r} \geqslant r_{\alpha\beta}^{c} \end{cases} \tag{1}$$

The modification is a “bump” energy penalty extending from $r_{\alpha\beta}^{s}$ to the cutoff. $\varepsilon_{\alpha\beta}$ and $\sigma_{\alpha\beta}$ (α, β denotes species of *S* or *L*) provide the energy and length scales, respectively. $r_{\alpha\beta}^{s}$ is taken as $1.5\sigma_{\alpha\beta}$, which is outside the first neighbor shell. The cutoff values $r_{\alpha\beta}^{c}$ were chosen to be species dependent, such that all pair interactions are precisely 0.0163 ε_{LL} at the cutoffs of $r_{LL}^{c} = 2.5\sigma_{LL}$, $r_{LS}^{c} = 2.2917\sigma_{LL}$, $r_{SS}^{c} = 2.0833\sigma_{LL}$. The *SS* and *LL* bond energies are equal to that of the *SL* bond energy: $\varepsilon_{SS} = \varepsilon_{SL} = \varepsilon_{LL}$. The *SS* and *LL* length scales are related to the *SL* length scale by:

$$\sigma_{SS} = \frac{5}{6}\sigma_{LL}\ ,\sigma_{SL} = \frac{11}{12}\sigma_{LL}. \tag{2}$$

The two types of atoms have different masses: $m_L = 2m_0\ , m_s = m_0$, where m_0 is the mass unit. The reference time scale is $t_0 = \sigma_{LL}\sqrt{m_0/\varepsilon_{LL}}$. All physical quantities will therefore be expressed in SI units following the conversion in a previous report [27]: $\sigma_{LL} \approx 2.7$ Å; $m_0 \approx 46$ amu; $\varepsilon_{LL} \approx 0.151$ eV; $t_0 \approx 0.5$ *ps*.

This force field is inspired by the Dzugutov potential [28], which features an energy bump to mimic the Friedel oscillations [29,30,28,31] and to control the bonding covalency, and thus can reduce the excessive ductility commonly present in model metallic glasses. In this study, the bump height parameter ε_B used is 0.3. The corresponding model glassy nanowire fractures via shear banding (i.e. lose half of the tensile stress at ∼20% strain) in a uniaxial tensile test [23]. A standard velocity Verlet integrator with a time-step of 5 fs was used. The temperature control and stress control used in the MD simulations follow the standard Nosé–Hoover formulation [32,33]. Similar to a previous study [23], glassy nanowires 24.3 nm long and 11.3 nm in diameter (∼0.13 million atoms) were chosen. Due to the high loading cycles required in fatigue tests, a study with an even larger sample size is very demanding at present. The nanowires were melted and equilibrated at a high pressure (9.4 GPa) and high temperature (2000 K) in a cylindrical container and quenched into the form of nanowire with zero pressure and at 60 K, with a cooling rate of $8.7 \times 10^{11}\ K/s$. The quenching process mimics the experimental casting [25]. Thus, the as-quenched glassy nanowires have relaxed surfaces [25]. The periodic boundary condition applies only in the axial direction. During fatigue tests, the nanowire was uniaxially loaded by rescaling the simulation box with a strain rate of 0.4 ns^{-1}. The temperature was maintained at 60 K (20% of the glass transition temperature $\mathrm{T_g}$) during the fatigue tests.

3. Total-strain-controlled fatigue tests

First, we applied total-strain-controlled symmetric compression–tension fatigue tests on the nanowires, in which the strain amplitude in tension or compression spans from 4% to 6% with an interval of 0.5%. Five independent samples were tested for each strain amplitude to investigate the statistics of the fatigue behaviors. Fig. 1a shows that at total strains of 4% and 4.5% the stress exhibits a slightly cyclic-hardening behavior before fracture (upon which the stress drops significantly). However, at higher strain levels, there is generally a cyclic-softening behavior before the stress significantly drops. Such behavior is likely due to the competition between aging-induced hardening (possibly mechanically assisted) and deformation-induced softening. At low loads, aging dominates; while at high load, deformation dominates. The fatigue life of the sample was identified as the first cycle in which the peak tensile stress reduces to half of the initial stress amplitude. The tensile stress was chosen here since the fractured sample might still be able to sustain a certain amount of compressive stress. The plastic strain ε_p of every cycle is defined to be half of the strain difference between the two zero-stress points, as shown in Fig. 1b. As shown in Fig. 1c, the higher the applied total strain amplitude ε, the higher the plastic strain ε_p observed. Similar to the stress evolution, ε_p also exhibits either softening or hardening behavior, depending on the strain amplitude. For samples with total-strain amplitudes lower than 4.5%, ε_p decreases during the majority of the cyclic loading, before surging rapidly upon failure. Cyclic strain induced work-hardening behavior was also observed in nanoindentation tests [18,21] and in cyclic tensile tests on metallic glass nanowires [4,5]. With the total-strain amplitude of 5%, the plastic strain, ε_p, maintains a constant level until fracture. For samples with total-strain amplitudes >5%, the plastic strain increases during the whole fatigue tests, indicating strain-softening behavior.

The sudden increase in the plastic strain marks the onset of fracture in all of the total-strain-controlled fatigue tests. The atomic deformation morphology further reveals that the onset of fracture is caused by the rapid shear band formation and propagation process as shown in the side views of the nanowires of Fig. 2. The color coding follows the local atomic shear strain according to a previous study [34]. The top views of the nanowires during fatigue tests evidently show that the shear band initiates at the surface and floods into the nanowire at the later stage of the fatigue