Journal of Non-Crystalline Solids 428 (2015) 146–150

Contents lists available at ScienceDirect

Journal of Non-Crystalline Solids

journal homepage: www.elsevier.com/ locate/ jnoncrysol

Mesoscopic examination of cyclic hardening in metallic glass

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ARTICLE INFO

Article history:
Received 27 May 2015
Received in revised form 28 July 2015
Accepted 6 August 2015
Available online 29 August 2015

Keywords:
Metallic glass;
Cyclic hardening;
Shear transformation zone;
Free volume;
Modeling

ABSTRACT

The deformation behavior of metallic glass (MG) under cyclic nanoindentation tests has been investigated using a meso-scale model, shear transformation zone (STZ) dynamics, which incorporates excess free volume as a state variable. The yield load of MG is found to increase after cyclic indentation in the microplastic regime. The cyclic hardening behaviors are demonstrated to be directly related to the glass structural relaxation reflected by a decrease of excess free volume, which results from the dynamical competition between microplastic events during the cyclic indentation.

1. Introduction

Metallic glasses (MGs) featured with the high yield strength and the large elastic limit have a great potential to be used as actuators, springs, gears and micro- and nano-electromechanical systems (MEMS/NEMS) [1–3]. Among these applications, the mechanical behaviors of MGs under cyclic loading become a key issue due to fatigue failure, and yet the MGs were reported to exhibit a low fatigue limit (~10%–50% of the yielding stress) [4,5]. Both experiments and computational simulations have been employed to investigate the cyclic deformation behaviors of MGs [6–17]. Packard et al. [7,15] found that the MGs were hardened after cyclic nanoindentation in the nominal elastic range. Tian et al. [16] observed a work hardening behavior of CuZr MG nanopillars under cyclic tension. The molecular dynamics (MD) simulations by Deng et al. [9] also found a cyclic indentation hardening of the MG and further revealed a selection of secondary yield path that can be ascribed to the hardening. Most recently, Luo et al. [11] investigated the low cycle fatigue behavior of MG nanowires via MD simulations, in which both cyclic hardening and softening were observed. They associated the hardening/softening response with the change of population of tetrahedral clusters, which were viewed as liquid-like regions in the amorphous solid. Lo et al. [17] proposed an atomistic picture on the structural relaxation under cyclic loading based on the MD results. Atoms in the irreversible relaxation centers [18] prefer to occupying lower energy position by annihilating free volumes and forming tighter bonds. Till now, however, the dynamic nature of structural evolution with respect to cyclic deformation still remains a challenging question, given that the details of MG structure are rather complicated.

In this work, we employ a recently developed STZ dynamics model [19], which incorporates excess free volume as a state variable, to study the interplay of glass deformation and structural evolution under cyclic indentation tests at an experimentally relevant time scale. We simulate the structural evolution through the competition of shear transformation induced excess free volume creation vs. diffusion-relaxed excess free volume annihilation [19–22]. We observe a progressive hardening of MG after the cyclic indentation in the microplastic regime and associate the hardening effect with the decrease of excess free volume, which is a consequence of annihilation outpacing creation during the cyclic loading.

2. Methods

The developed STZ dynamics model [19] is an extension of the initial work by Homer and Schuh [23], and it considers the MG deformation as a Markov chain of STZ activations that leads to deformation on a larger scale. In particular, a simulated volume of material is partitioned into an ensemble of potential STZs which are mapped onto a finite element mesh. Associated with each mesh point there is an internal state variable, *excess free volume* f_v. The system evolves via two types of *local* competing events, i.e., STZ activation that creates f_v vs. diffusive rearrangement that annihilates it. The activation rate for a potential STZ to shear in one direction is given as

$$\dot{s}_{STZ} = \upsilon_{STZ}\exp\left(-\frac{\Delta F_{STZ}(f_v) - \tau\gamma_0\Omega_0/2}{kT}\right) \quad (1)$$

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http://dx.doi.org/10.1016/j.jnoncrysol.2015.08.007
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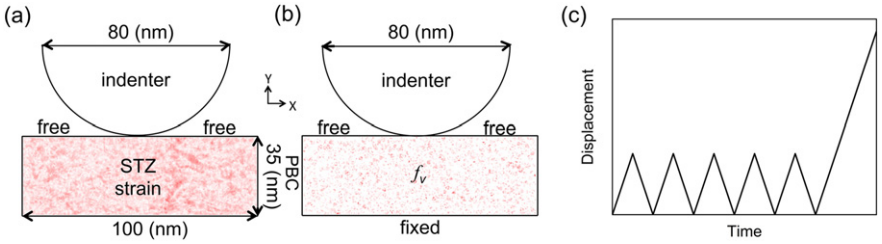

Fig. 1. (a) (b) A two-dimensional (2D) FEM model setup for nanoindentation. The simulated sample has preexisting strain in (a) and excess free volume f_v in (b). (c) Schematic displacement-time function curve of 5-cycle triangular loading.

and the resultant *local* excess free volume creation rate in an activated STZ region is

$$\dot{f}_v^{+} = \varepsilon_v(1-f_v)\upsilon_{STZ}\exp\left(-\frac{\Delta F_{STZ}(f_v)-\tau\gamma_0\Omega_0/2}{kT}\right) \quad (2)$$

where τ, T, f_v are the *local* shear stress, temperature and excess free volume, respectively; γ_0, ε_v and Ω_0 represent the characteristic shear strain, dilatation strain, and activation volume associated with an STZ activation; ν_{STZ} is the attempt frequency; k is the Boltzmann's constant. ΔF_{STZ} is the activation barrier for shearing an STZ and is reduced with f_v increasing [24]. In parallel, diffusive rearrangement takes place at a rate

$$\dot{s}_D = (1-f_v)\upsilon_D\exp\left(-\frac{\Delta G_D(f_v)}{kT}\right) \quad (3)$$

and the resultant *local* excess free volume annihilation rate in the activated region is

$$\dot{f}_v^{-} = \varepsilon_v f_v(1-f_v)\upsilon_D\exp\left(-\frac{\Delta G_D(f_v)}{kT}\right) \quad (4)$$

where ν_D is the frequency of diffusive rearrangement. The activation energy of the annihilation event ΔG_D can be reduced through a linear function of f_v [24].

The standard kinetic Monte Carlo (kMC) algorithm is employed to evolve the system by choosing a time step and controlling the activation sequence of STZ and diffusive rearrangement events. In each kMC step, only one *local* event is selected based on the activation rates determined by the local conditions. The activation of the event in turn leads to the change of local states due to the stress redistribution and f_v evolution, which is solved using finite element method (FEM). The commercial finite element package ABAQUS is employed as the FEM solver and the kMC algorithm is coded in its user subroutines. The procedure is detailed in [19].

Fig. 1a and b show the two-dimensional (2D), plane-strain FEM model setup to simulate the nanoindentation. The simulated sample has the width and height of 100 nm and 35 nm, respectively. Periodic boundary conditions are applied along the *X* direction, while the sample top surface is free and the bottom is fixed. The radius of indenter is 40 nm, and the indentation rate is set at 1 nm/s along the *Y* direction, which is close to the experimental values (~4-50 nm/s) [15]. Our simulated glass samples take the material properties of Vitreloy 1 ($Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$), with the shear modulus 35.8 GPa, Poisson's ratio 0.352, the Debye temperature 327 K, and the STZ volume 0.8 nm^3 [25]. The samples are processed by cooling down from a fully relaxed structure at 650 K ($>T_g$ = 623 K) at a cooling rate of 10 K/s to 300 K. The preexisting STZ strain and f_v of one obtained structure are shown in Fig. 1a and b, respectively. To address the statistical feature of the MG yielding at the nanoscale, 10 variants of the simulation cell are produced, and thus 10 different local glass structures are indented. We first conduct monotonic loading, followed by various cyclic nanoindentation simulations. An example of the applied triangular loading function of 5 cycles is shown in Fig. 1c. In our simulations, the number of cycles take 1, 3, or 5, and the cyclic depth is 0.5 nm, 0.7 nm or 0.9 nm, which are in the nominal elastic regime. Large loads that cause global yielding are applied afterwards. It is noteworthy that the simulations use a model glass, geometry and test conditions that are different from the experiments (e.g., plane strain versus axisymmetric, displacement- versus load-controlled), and thus the comparison is only qualitative. But the simulated indentation rate is on the same order of magnitude of experiments. In terms of the nanomechanics and kinetics of STZ and free volume activities, we expect to provide valuable information which cannot be obtained from atomistic simulations.

3. Results and discussion

Fig. 2a displays a typical load as a function of displacement under various loading conditions. To set a baseline, the simulated, fully elastic

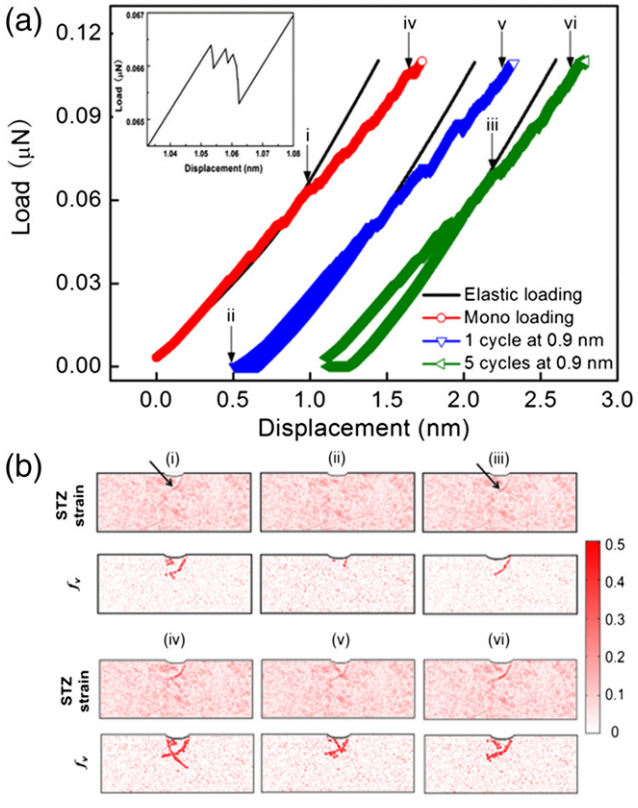

Fig. 2. (a) Load–displacement curves for the monotonic loading, 1-cycle and 5-cycle loading with cyclic depth of 0.9 nm. Vertical arrows indicate the points: (i) at yield of the monotonic loading; (ii) at reload after the 1st cycle. (iii) at yield after the 5-cycle loading; and (iv), (v) and (vi) at a post-yield load of 0.1 μN for the three loading conditions. The origin of the 1-cycle and 5-cycle loading curves are shifted for a clear view. The inset shows an enlarged view of load drops around (i). (b) The snapshots display the spatial distribution of STZ strain and f_v at points (i)–(vi). Black arrows denote the STZ strain accumulation at (i) and (iii).