International Journal of Plasticity 44 (2013) 147–160

Contents lists available at SciVerse ScienceDirect

International Journal of Plasticity

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

An atomistic investigation of structural evolution in metallic glass matrix composites

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ARTICLE INFO

Article history:
Received 20 September 2012
Received in final revised form 30 December 2012
Available online 16 January 2013

Keywords:
A. Ductility
A. Microstructures
B. Metallic material
B. Particulate reinforced material
Molecular dynamics

ABSTRACT

Metallic glass matrix composites may have unique mechanical properties and potential for practical applications. Deformation mechanisms governing the structural evolution process of these mixed structures remain poorly understood. In this article, we elucidate the effect of the crystalline second phase on the tension behavior of metallic glass matrix composites by using large-scale atomistic simulations. We identify that the interaction between the crystalline second phase and the local shear bands is dominated by the cooperative activation of lattice dislocations on the glass–crystal interfaces and discrete shearing events in the neighboring glass matrix. By tailoring the morphology of the crystalline second phase, one observes deflection, bifurcation and suppression of local shear bands and succeeds in enhancing the global plasticity of the composite structure. Guiding principles aimed at designing effective crystalline second phases in metallic glasses are proposed as conclusions.

1. Introduction

The development of bulk metallic glasses (BMGs) has triggered considerable interest in their unique mechanical properties including high elastic limits (~2%) and high tensile strengths (~2 GPa) (see, for example, Greer, 1995; Schuh et al., 2007). Several BMGs even exhibit substantial fracture toughness (see Conner et al., 1997; Lowhaphandu and Lewandowski, 1998; Flores and Dauskardt, 1999; Schroers and Johnson, 2004; Xu et al., 2010). Monolithic BMGs, however, tend to fail in an apparently brittle manner in unconstrained loading geometries, restricting their applications as structural materials (see Greer, 1995; Ashby and Greer, 2006). Inhomogeneous shear banding is the typical mode of plastic deformation of BMGs at room temperature. In contrast to polycrystalline metals, where shear localization can be suppressed by work hardening (dislocation interactions) or internal barriers such as grain boundaries, monolithic BMGs do not show strain hardening and consequently fail to retain the extension of individual shear bands. It is known that disordered materials, unlike crystalline materials, suffer dilatation during plastic deformation because of the significant pressure-dependence of their yielding behavior (Schuh and Lund, 2003). To worsen the situation, shear banding events lead to strain softening and local instability of the material due to shear-induced dilatation and rapid heating inside the shear bands (see Lewandowski and Greer, 2006). As a result, the poor tensile ductility of BMGs is attributed to the catastrophic propagation of single shear bands.

MG-matrix composites have been developed in recent years to overcome the problem of limited plasticity of monolithic BMGs (see, for example, Conner et al., 1998; Hays et al., 2000; Kuhn et al., 2002; Qiu et al., 2002; Das et al., 2005; Inoue et al., 2005; Lee et al., 2005; Xu et al., 2005; Fan et al., 2006; Hofmann et al., 2008; Qiao et al., 2011; Narayan et al., 2012). A composite is essentially a heterogeneous microstructure composed of the dispersion of crystalline second phase with different

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http://dx.doi.org/10.1016/j.ijplas.2013.01.002

mechanical properties, analogous to the concept of dispersion strengthening in crystalline metals. Under external loading, the defect-like crystalline second phase suppresses the accumulation of shear strains along single shear bands and promotes the initiation of multiple shear bands nearby the glass–crystal interfaces, leading to the formation of a relatively homogeneous distribution of plastic strains in the composite.

Although MG-matrix composites exhibiting enhanced ductility have been synthesized in experiments (see Szuecs et al., 2001; Eckert et al., 2007; Hofmann et al., 2008; Wu et al., 2010; Qiao et al., 2011; Narayan et al., 2012), detailed atomistic investigation for the microstructural evolution of these crystal-reinforced composites are yet to be reported, especially for the influence of the crystalline second phase on the development of shear bands in the glass matrix. At present, the understanding of relevant topics relies mainly on post-mortem microstructure observations. In their recent experimental work, Narayan et al. (2012) showed that larger dendrite size offers higher ductility when compared with smaller ones, whereas finer interdendritic spacing results in marked improvements in both ductility and yield strength due to the confinement of shear band nucleation in the smaller volumes of the glass matrix. To study the macroscopic deformation behavior of MG-matrix composites, Lee et al. (2005) performed finite element calculations and found that particle/matrix interfaces were sources for the initiation of shear bands, whereas crystalline particles acted as effective barriers to the propagation of shear bands. Atomistic simulations can be adopted as a complement to experiments, allowing one to explore the distinct properties of MG-matrix composites that are not accessible to experiments. With a detailed record for the deformation process, one may establish a link between the mechanical properties of the materials and the underlying atomistic mechanisms. With the help of massively parallel computational power, the typical time and length scales (e.g. tens of nanoseconds and millions of atoms) of a classical MD simulation make the simulation of shear banding events in MGs tractable.

Our purpose in this paper is to investigate the effect of crystalline second phase on the structural evolution of MG-matrix composites by using large-scale molecular dynamics (MD) simulation, and to optimize the distribution of plastic strain in the composites by tailoring the geometry of the crystalline phase. To facilitate model construction, a pattern of the crystalline second phase is adopted. The shape, volume fraction, and orientation of the nanocrystal array can be easily adjusted. Uniaxial tension will be imposed on a series of composites with various crystalline patterns. Details about the simulation method are given in Section 2. Beginning from analyzing the snapshots captured during the deformation process and the corresponding stress–strain relation curves, one may reveal the controlling mechanism offered by the crystalline second phases. The simulated data given in Section 3 will shed lights on the following topics: how shear strains localize in a composite structure, especially around the second phase; how the second phase inhibits shear band propagation in the glass matrix; how the geometry of the crystalline pattern influences the distribution of plastic deformation in the loaded composite; how the atomistic mechanism governs the mechanical response of a composite, and so on. All these aspects are crucial for interpreting the mechanical behavior of MG-matrix composites. In Section 4, the paper concludes with a designing strategy for MG-matrix composites based on those observations.

2. Simulation methods

2.1. Sample preparation

Our aim is to investigate the atomistic mechanism governing the structural evolution of MG composites in the presence of crystalline second phases. The glass matrix is chosen as a typical binary MG $Cu_{64}Zr_{36}$. A number of atomistic simulations (see Duan et al., 2005; Shimizu et al., 2006; Cao et al., 2009; Murali et al., 2011) have been devoted to investigate the deformation mechanisms of Cu–Zr based systems. By inserting discontinuous Cu particles into the $Cu_{64}Zr_{36}$ glass matrix, a mixed structure can be generated and used for subsequent tension simulations. The potential given by Mendelev et al. (2007) is adopted to describe the atomic interactions. The validation of the potential can be found in the original paper. The Young's moduli for the glass matrix and the crystalline second phase are predicted to be $E_{MG} = \sim 83$ GPa and $E_{Cu\langle 100\rangle} = \sim 67$ GPa, respectively. The $Cu_{64}Zr_{36}$ glass matrix is prepared through a conventional melting-quenching procedure. Firstly, a cubic cell filled with Cu atoms arranged in an f.c.c. lattice is created. A fraction of 36% of the Cu atoms is then replaced by Zr atoms, giving rise to a solid solution alloy with a composition of $Cu_{64}Zr_{36}$. Secondly, the cubic alloy is melted at 2000 K and zero pressure for 2 ns in order to obtain homogeneity, with periodic boundary conditions applied to all three dimensions. The integration time step in our simulations is chosen as 1 fs. Finally, at a cooling rate of 100 K/ns, the alloy is gradually cooled down to 50 K over 19.5 ns. The dimension of the quenched cell is measured to be $5.6 \times 5.6 \times 5.6$ nm^3.

The as-generated cubic alloy is replicated to form larger MG samples in which various patterns of Cu particles can be added. Typical geometry of a $Cu_{64}Zr_{36}$-matrix composite structure is delineated in Fig. 1a. The second-phase particles are idealized as uniformly dispersed ellipse-shaped nanocrystals to facilitate sample construction. In view of the periodic boundary condition along the Z direction, they represent elliptic cylinders. The size of an individual Cu nanocrystal is depicted by a and b, while the interspacing of the neighboring nanocrystals along the X and Y directions are indicated by w and h.

By controlling the structural parameters (i.e. a, b, w and h) presented in Fig. 1a, various patterns of Cu nanocrystals similar to those obtained in real MG-matrix composites can be generated. Note that the crystallographic orientations of the ellipse-shaped nanocrystals are such that the [100] and [010] directions of the crystalline lattice are always parallel to their long and short axes. Firstly, three composites with various shapes of nanocrystals are created by adjusting the aspect ratio b/a, as shown in Fig. 1b. With a large aspect ratio ($b/a = 6.5$), 'Composite I' resembles those with locally parallel dendrite 'trunks'