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Strong and ductile nanolaminate composites combining metallic glasses and nanoglasses

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ABSTRACT

The proven superior ductility of nanoglasses (NGs) makes them a promising second phase for metallic glass (MG) matrix composites. Here we evaluate the mechanical properties of MG-NG nanolaminate composites by performing molecular dynamics simulations of tensile loading. We focus on the effects of NG layer thickness and separation as well as the loading direction on the predicted strength and inelastic deformation profile. Our results reveal that nanolaminates with NG layers separated by more than 50 nm fail by shear banding. Meanwhile, the predicted nanolaminate strength versus MG volume fraction follows an inverse Hall-Petch relationship rather than the linear rule-of-mixtures. In contrast, by closely packing NG layers to 4.8 or 6.5 nm, the nanolaminates exhibit enhanced tensile ductility for tensile loading perpendicular or parallel to the MG-NG interfaces, respectively. Our results further reveal that the change in the loading direction causes the differences not only in the location of SB initiation but also the critical distance between NG layers for failure mode transition. Finally, the MG-NG nanolaminate structure with NG layers closely packed and interfaces oriented parallel to the loading direction is identified as the most effective heterostructure, which preserves superplasticity while producing a maximum strength of 2.35 GPa, a value 15% greater than that of monolithic NG with a grain size of 5 nm. Our work demonstrates that a nanolaminate combining MG and NG layers of suitable thicknesses is able to withstand large plastic deformations while maintaining the structural stability, and we expect that these results will inspire the development of novel strong and superplastic MG matrix composites that will broaden the possible applications of MGs.

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1. Introduction

Over the past few decades, metallic glasses (MGs) have attracted tremendous attention due to their superior mechanical properties such as large elastic limit, high strength, and high fracture toughness, compared with crystalline metals and alloys (Dudina et al., 2009; Greer and Ma, 2007; Greer and De Hosson, 2011; Li et al., 2008; Maass and Loffler, 2015; Schuh et al., 2007; Wang et al., 2004, 2013; Wang, 2012; Zhong et al., 2016). However, despite all of these desirable features, MGs are not being widely utilized due to their propensity for catastrophic failure by propagation of shear bands (SBs) (Chen et al., 2008, 2014; Jang et al., 2011; Şopu et al., 2016). As a consequence, considerable efforts have been applied towards enhancing tensile ductility of MGs at room temperature (Chen et al., 2011; Huang et al., 2014; Jang and Greer, 2010; Kuzmin et al., 2012a, 2012b; Magagnosc et al., 2013; Sarac and Schroers, 2013; Sun et al., 2016; Tonnies et al., 2014; Zhao et al., 2010). One of the most promising strategies is to develop a heterogeneous microstructure, e.g. by combing a MG matrix with crystalline second phase particles (Chen et al., 2013; Hays et al., 2000; Hofmann et al., 2008; Kim et al., 2011, 2012; Tong et al., 2016; Zhou et al., 2013). This approach enables multiplication, branching, and restriction of SBs by their interaction with the ductile crystalline particles. For example, the failure strain of 13.1% was observed in the Zr-Ti-Cu-Nb-Be MG matrix composites containing ductile dendrites (Hofmann et al., 2008). This enhanced tensile ductility, however, came at the expense of decreased ultimate tensile strength (UTS) due to the soft dendritic phase relative to the MG matrix. More recently, the tensile behavior of nanolaminates with alternating layers of 16–900 nm thick $Cu_{50}Zr_{50}$ MG and 16 nm thick nanocrystalline Cu was reported (Kim et al., 2011). When the critical MG layer thickness falls below 120 nm, a marginal fracture strain enhancement of 4% was achieved, without any sacrifice of UTS. Therefore, given the strength-ductility tradeoff, the challenge remains to develop MG matrix composites, which would exhibit UTSs close to that of monolithic MGs while still possessing high ductility such as that typically observed for crystalline metals (Kim et al., 2012).

There are several criteria for the selection of the second phase for constructing MG matrix composites. Firstly, the second phase should be ductile, such as crystalline Cu (Donohue et al., 2007; Wang et al., 2007a), nanocrystalline Cu (Kim et al., 2011), and polyisoprene (Kim et al., 2012). It should be emphasized that these second phases chosen previously are elastically soft inclusions relative to the MG matrix. Secondly, the chemical composition of the second phase should be compatible with the MG matrix for fabrication processing. Recently, nanoglasss (NG), a new class of engineering material composed of nanometer-sized glassy grains separated by glass-glass interfaces, is attracting significant technological interest (Adibi et al., 2013, 2016; Gleiter, 2008; Sha et al., 2015a; Singh et al., 2014; Şopu and Albe, 2015; Şopu et al., 2011). By inert gas condensation, as opposed to casting of MGs, a variety of NGs with various chemical compositions, such as Au–Si, Au–La, Fe–Si, Fe–Cu, La–Si, Pd–Si, Ni–Ti, Ni–Zr, and Ti–P, have been synthesized (Gleiter, 2008). NGs combine a considerable fraction of the MG strength with enhanced global plasticity when compared to that of monolithic MG, due to the soft glass-glass interfaces, hence, they have been proposed to have the potential to tune the properties of MGs (Adibi et al., 2013, 2016; Gleiter, 2008; Sha et al., 2015a; Singh et al., 2014; Şopu and Albe, 2015; Şopu et al., 2011). Previous investigations on $Cu_{50}Zr_{50}$ NG revealed a transition in the deformation mechanism from a single SB to homogeneous superplastic flow with a decrease in the glassy grain size to 5 nm (Adibi et al., 2013). More importantly, compared to crystalline metals and alloys, NGs have higher UTSs. Moreover, the NGs have the same chemical compositions as the MGs. Therefore, NGs are deemed to be great candidates for the second phase, providing a new approach to construct strong and ductile MG matrix composites. For instance, a preliminary investigation showed that a nanolaminate nanopillar composed of 5 nm thick layers of $Cu_{64}Zr_{36}$ MG and NG show exceptional plasticity and failure by necking (Adibi et al., 2016).

In the present work, motivated by the development of NGs, we comprehensively evaluate the mechanical properties of nanolaminates of $Cu_{50}Zr_{50}$ MGs and NGs with a grain size of 5 nm. We employ the molecular dynamics (MD) simulations of tensile loading to characterize the deformation and failure mechanics of MG-NG nanolaminates as a function of NG layer thickness, distance between NG layers, and direction of loading. Finally, our study identifies the most effective heterostructure that shows superplasticity together with improved strength, and provides significant insights into the deformation and failure mechanisms of MG matrix composites.

2. Computational method

The MD simulations are performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) (Plimpton, 1995). Both the $Cu_{50}Zr_{50}$ MG and $Cu_{50}Zr_{50}$ NG with a grain size of 5 nm are slabs of dimensions of 99.1 (x) × 49.5 (y) × 6.23 (z) nm^3. The sample dimensions we chose are consistent with those of monolithic MGs and NGs samples of our previous MD simulations (Adibi et al., 2013), for comparison purposes. The atomic interactions are modeled using an embedded atom method (EAM) potential fitted to CuZr properties (Cheng and Ma, 2011). A constant integration time step of 2 fs is used in all simulations. In constructing the $Cu_{50}Zr_{50}$ NG sample, a $Cu_{50}Zr_{50}$ MG sample is built first as follows. A small cube (~13,000 atoms) with periodic boundary conditions (PBCs) along all three independent directions is first equilibrated at 2000 K for 2 ns, then cooled at a quenching rate of 10^9 K/s to 50 K, at zero external pressure. The large $Cu_{50}Zr_{50}$ MG sample is then constructed by replications of this small cube, annealed for 0.5 ns at 800 K, and finally brought back to 50 K (Cao et al., 2009; Sha et al., 2013). $Cu_{50}Zr_{50}$ NG is generated using the Poisson-Voronoi tessellation method by employing the $Cu_{50}Zr_{50}$ MG structure as a source material for the glassy grains (Adibi et al., 2013; Şopu and Albe, 2015; Şopu et al., 2011). $Cu_{50}Zr_{50}$ NG is then sintered by applying an external hydrostatic pressure of 3 GPa at 50 K in order to relax the atomic structure of the interfaces and eliminate voids (Adibi et al., 2013; Şopu et al., 2011), which may appear during the NG

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