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Tensile and nanoindentation deformation of amorphous/crystalline nanolaminates: Effects of layer thickness and interface type

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ABSTRACT

We perform molecular dynamics simulations to investigate plastic deformation of alternative $Cu_{64}Zr_{36}$/Cu amorphous-crystalline nanolaminates (ACNLs) with different layer thicknesses and interface types under uniaxial tension and nanoindentation. Plastic deformation is characterized by shear transformation zones (STZs) or shear bands in amorphous layers and dislocations in crystalline layers, respectively. Nucleation of STZs or shear bands in an amorphous layer can be triggered at glass-glass interfaces (GGIs) in the same layer or at the intersections of amorphous-crystalline interfaces (ACIs) and dislocations from the neighboring Cu layers. Decreasing layer thickness and introducing grain boundaries (GBs) or GGIs into ACNLs are effective methods to improve ductility and facilitate the transition from inhomogeneous deformation to homogeneous deformation or co-deformation. With the decrease of layer thickness, more ACIs are introduced and behave as nucleation sites of STZs and dislocation. These STZs at the adjacent interfaces can interact with each other directly, promoting the deformation transition. Additionally, the introduction of GBs and GGIs facilitates crystal plasticity and glass plasticity in corresponding layers, which again boosts the plasticity of nearby layers and contributes to homogeneous strain distribution and co-deformation. However, the improved ductility of ACNLs is at the price of strength and hardness. Thus, keeping a balance among them can be useful for the synthesis of novel nanolaminate with superior ductility, high strength and high hardness.

1. Introduction

Bulk metallic glasses (BMGs) are fabricated by cooling high-temperature alloy melts rapidly and retaining their disordered atomic arrangement [1–4]. Due to their amorphous atomic structure, BMGs have some unique mechanical and physical properties, such as high strength, high elastic limit and the absence of dislocation [5–7]. Unfortunately, the industrial application of BMGs is largely limited by their lack of tensile ductility, manifested as catastrophic failure via the propagation of deformation localization or shear bands [2,8]. Such a problem is often dealt with through introducing a crystalline phase into the BMG matrix to synthesize metallic glass/crystalline composites [4,9,10]. Although the second, crystalline, phases have different shapes, such as particle solution [11], dendrites [12] and fibres [13], they play similar roles in improving the ductility of BMGs, i.e., diffusing and homogenizing strain and deformation localization.

Nanolaminated materials are attracting more and more attention [14,15]. Recently, amorphous/crystalline nanolaminates (ACNLs), as novel BMG composites, were synthesized via magnetron sputter deposition of alternating layers of nanocrystalline and metallic glass [16–21]. Such laminate composites can achieve much higher tensile ductility than BMGs, mainly due to size effect on the deformation mode of glass layer [16,17] and co-deformation of glass layers and crystalline layers at the nanoscale [19,22]. When the thickness of glass layer is reduced to nanoscale, its deformation mode can transform from highly localized plasticity to homogeneous deformation. At the nanoscale, the co-deformation of glass layers and crystalline layers occurs as well, impeding catastrophic and localized shear banding. However, the detailed mechanisms of the layer-thickness-dependent transition are not fully understood, due to the difficulties associated with *in situ* techniques to probe atomic-level structural changes. Herein, molecular dynamic (MD) simulations can serve as a good complement to address this problem.

Currently, there are two types of interfaces in synthesized ACNLs,

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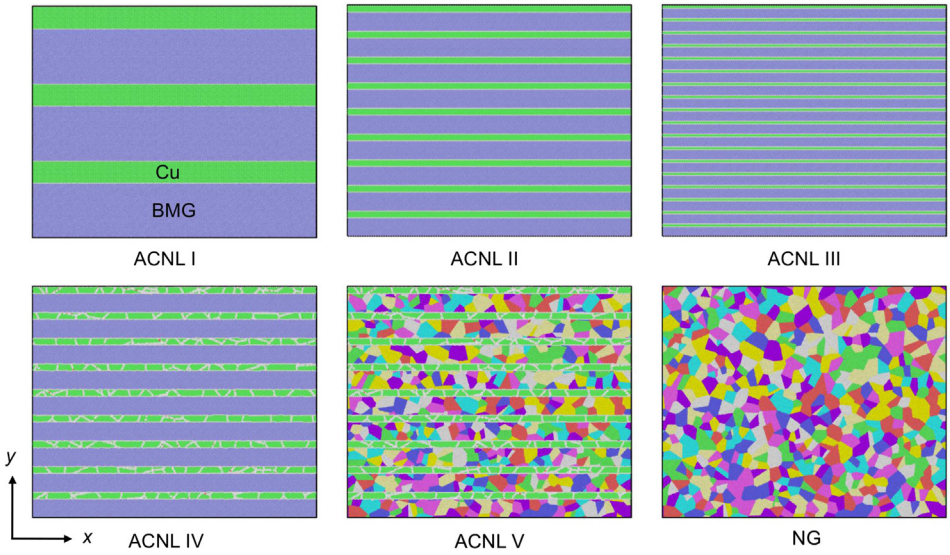

Fig. 1. Initial atomic configurations of $Cu_{64}Zr_{36}$/Cu ACNLs I−V and $Cu_{64}Zr_{36}$ NG with a grain size of 3 nm. Atoms in amorphous layers of ACNLs I−IV are colored blue. Individual grains in NG and amorphous layers of ACNL V are shown in different colors. FCC Cu atoms and GB atoms in crystalline layers of ACNLs I−V are colored green and grey, respectively. ACNL: amorphous-crystalline nanolaminate; NG: nanoglass; BMG: bulk metallic glass. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

i.e., amorphous/crystalline interfaces (ACIs) and grain boundaries (GBs). Previous MD simulations elucidated the dual role of ACI as the nucleation source and the barrier to shear transformation zones (STZs) and dislocations [23–25]. By emitting, impeding, absorbing and then re-emitting STZs or dislocations, ACIs can dissipate strain localization into larger region, resulting in more homogeneous strain distribution. In the MD simulations mentioned above, crystalline layers of ACNLs are made of single crystals and ACNLs have only one kind of interface, i.e., ACI. However, GBs, acting as sources and sinks for dislocations, can influence the dislocation motion significantly, especially in nanocrystalline metals [26]. A recent study [27] revealed that GBs in the crystalline phase of metallic glass/crystalline interpenetrating phase nanocomposites can enhance crystal plasticity drastically and then eliminate the formation of localized mature shear bands from ACIs. Although GBs exist commonly in the synthesized ACNLs, their effects on the plastic deformation of ACNLs have rarely been examined. In addition to ACIs and GBs, glass−glass interfaces (GGIs) in nanoglasses (NGs) or nanograined metallic glasses have been of increasing interest. Herein, NGs are synthesized by severe plastic deformation [28], magnetron sputtering [29] and inert gas condensation [30]. Experiments [31,32] and MD simulations [33–37] have revealed that GGIs can facilitate the nucleation of STZs, whose random distribution can accommodate localized shear localization, leading to homogeneous strain field and enhanced ductility. In view of the important roles of ACI, GB and GGI in improving ductility of BMGs and their composites, we further postulate that a novel ACNL, consisted of alternative nanocrystalline and NG layers, may achieve better ductility. From the viewpoint of material synthesis, alternately depositing nanocrystalline and NG layers during magnetron sputtering provides a feasible method for the synthesis of such laminate composites. Therefore, investigating their plastic deformation behaviors with MD simulations is of significant interest for their potential applications and to understand the effects of different interfaces.

In this work, we utilize large-scale MD simulations to investigate tensile and indentation behaviors of $Cu_{64}Zr_{36}$/Cu ACNLs with different layer thicknesses and different interfaces, e.g., ACI, GB or GGI. Although decreasing layer thickness and introducing GBs or GGIs into ACNL layers can improve effectively the ductility of ACNLs, their strength and hardness are reduced. Choosing proper layer thickness and controlling the fraction of GBs and GGIs carefully can achieve a desired combination of ductility, strength and hardness. Section 2 addresses the methodology related to MD simulations and atomic-level structural analysis, followed by results and discussion in Section 3, and conclusions in Section 4.

2. Methodology

The Large-scale atomic/molecular massively parallel simulator (LAMMPS) is utilized for MD simulations [38]. To describe atomic interactions in the Cu-Zr system, we employ the Finnis-Sinclair potential developed by Mendelev et al. [39], which has been widely applied to investigate plastic deformation of metallic glass composites [27,40,41]. The initial $Cu_{64}Zr_{36}$ glass is obtained by melting single crystal $Cu_{64}Zr_{36}$ alloy at 2000 K and then cooling the melt to 50 K at a rate of 0.01 K/ps. Such a glass model (consisting of 5148 atoms) is replicated and annealed at 800 K for another 500 ps to eliminate possible artifacts from replication. Finally, the whole system is cooled to 50 K again and a larger glass configuration forms ($758 \times 618 \times 52$ Å^3, or ~1.51 million atoms).

We use the Poisson−Voronoi tessellation method [42–44] to construct $Cu_{64}Zr_{36}$ nanograined glass (or simply nanoglass) and nanocrystalline Cu, where columnar glass grains and crystal grains with an average grain size of 3 nm are generated from the $Cu_{64}Zr_{36}$ monolithic glass and Cu single crystal, respectively. Herein, $Cu_{64}Zr_{36}$ monolithic glass, $Cu_{64}Zr_{36}$ nanoglass, Cu single crystal and nanocrystalline Cu are identical to one another in the super-cell dimensions. To construct $Cu_{64}Zr_{36}$/Cu ACNLs, 30 vol.% of the configuration is occupied by Cu slabs (single crystal or nanocrystalline) and the rest, amorphous $Cu_{64}Zr_{36}$ slabs (monolithic glass or nanoglass). According to specified layer thicknesses, $Cu_{64}Zr_{36}$ monolithic glass, $Cu_{64}Zr_{36}$ nanoglass, Cu single crystal and nanocrystalline Cu are cut and assembled in pairs to form ACNL I−V. In particular, the crystalline layers in ACNLs IV and V are made of nanocrystalline Cu slabs and the amorphous layers in ACNL V are made of $Cu_{64}Zr_{36}$ nanoglass. In this way, we introduce GBs and GGIs into ACNLs. All the ACNLs have the same dimensions as the $Cu_{64}Zr_{36}$ monolithic glass configuration mentioned above. Fig. 1 compares the configurations of ACNLs I−V and NG, and the details on ACNL configurations (I−V) are also listed in Table 1. To separate the effects of layer thickness and interface type on plastic deformation of ACNLs, we divide ACNL I−V and NG into two groups. The first group includes