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Atomistic deformation mechanisms of amorphous/polycrystalline metallic nanolaminates

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ABSTRACT

A series of multilayer amorphous $Cu_{50}Zr_{50}$/Cu nanolaminates with consideration of grain boundary characteristics in the Cu layers were constructed and compressed to investigate the atomistic mechanisms of yielding and plastic deformation behavior using large-scale atomistic simulations. The results revealed that yielding occurs initially in the Cu layers through lattice dislocations, while plastic deformation in the amorphous layers is induced by the transfer of dislocation plasticity from the Cu layers, mainly at the intersections of the crystalline-amorphous interfaces and grain boundaries. Similar to the roles of defects-like secondary phases, the Cu layers serve as sites for heterogeneous nucleation of embryonic shear bands, as well as barriers to their propagation into mature ones. The coupled interplay between the crystal plasticity and the glassy plasticity in the nanolaminates promotes a more homogeneous redistribution of plastic deformation, providing a kind of hardening mechanism. In addition, our simulations also demonstrate a transition of the deformation mode from localized to homogeneous-like deformation by tailoring the relative volume fraction of the Cu layers. The findings provide more detailed atomistic information for understanding the underlying deformation mechanisms that are difficult to obtain by post-mortem observations and are useful for optimizing the structure of amorphous/crystalline metallic nanolaminates.

1. Introduction

Metallic glasses (MGs) have many attractive mechanical and physical properties that include high strength and elasticity, high hardness combined with excellent corrosion resistance [1–3]. However, one major impediment in utilizing MGs is the lack of ductility in comparison with their crystalline counterparts [4–6]. In the absence of microstructures that induces strain hardening and internal barriers such as grains boundaries as observed in crystalline metals, plastic deformation of most MGs at room temperature is usually localized into individual shear bands (SBs), which propagate unhindered to the extent that negligible macroscopic plasticity is experienced before catastrophic failure [7–9]. One promising route to alleviate this problem is to incorporate alternating crystalline metal layers to form periodically modulated multilayer nanostructures, i.e., amorphous/crystalline (a/c) nanolaminates, where the “defect-like” crystalline layers promote strain delocalization [10,11]. Recently, numerous a/c nanolaminates, such as CuZr/Cu [12–15], PdSi/Cu [16,17], CuNb/Cu [18], have been experimentally synthesized and their mechanical properties have been extensively probed [12–14,16–20]. Through micropillar compression on CuZr/Cu nanolaminates with varied Cu layer thickness (10–100 nm), Guo et al. [20] found that the 100 nm-CuZr/50 nm-Cu nanolaminate exhibited a flow stress comparable to the strength of monolithic MGs while achieving a fracture strain exceeding 40%. Zhang et al. [13] compressed a series of micropillars laminated with equal layer thickness (5–50 nm) and revealed a transition of the deformation mode from pronounced shear banding to homogeneous-like co-deformation with increasing layer thickness. Knorr et al. [16] also revealed that the deformation morphologies of the multilayered architectures can be controlled by tuning the layer thickness as well as the relative volume fractions. These results have demonstrated great potential for tailoring a/c nanolaminates with a sought-after combination of improved plasticity and high strength. Although many previous reports pointed out that the plasticity improvement is greatly contributed to the cooperative deformation between amorphous layers and crystalline layers, the mechanistic insights were mainly based on speculation from post-mortem microstructure observations on post-deformed samples. The dilemma behind experimentation is that the details of the deformation process are tough to unravel since the plasticity carriers, such as the shear transformation zones (STZs), SBs and dislocations in the

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composites, are confined within narrow regions generally no more than 5–20 nm, and the transient synergistic interactions among them could hardly be captured [11,21]. All these make it difficult to fully understand the deformation behavior of the a/c nanolaminates.

On the other hand, atomistic modeling which allows one to directly investigate the detailed deformation behavior as a function of the tailored architectures from atomic-scale level and to effectively establish links between the underlying atomistic deformation mechanisms and corresponding mechanical properties, are a useful tool to supplement the experiments [22–25]. So far, certain researchers have applied large-scale molecular dynamics (MD) simulations to investigate the deformation behavior of a/c nanolaminates. In tensile simulation of CuZr/Cu nanolaminate that contains a single crystal Cu layer, Wang et al. [11] found that crystalline-amorphous interfaces (CAIs) act as sources for nucleation of dislocations, and also demonstrate unique inelastic shear transfer characteristics that can induce STZs when impinged on by dislocations from the neighboring layer. This finding was also verified in simulation on compressing an a/c bilayer structure conducted by Arman et al. [26], who found that dislocations emitted near CAIs could directly induce a correlated SB pattern in amorphous layers across CAIs, thus resulting in a more stable shear banding process. The results of these pioneering simulation studies are instructive for understanding the deformation behavior of a/c nanolaminates. However, these adopted atomistic models were simplified either to be bilayer a/c structures or single crystal for the polycrystalline layers (without the presence of intrinsic GBs) [27,28], so that the simulated deformation physics may not be fully bridged with actual experiments. Up to now, detailed atomistic investigation on the deformation behavior of multilayer amorphous/polycrystalline metal nanolaminates is yet to be undertaken.

In this study, a series of multilayer amorphous $Cu_{50}Zr_{50}$/polycrystalline Cu nanolaminates were constructed by tailoring the relative volume fractions of the Cu phases with consideration of GB characteristics to more closely resemble experimentally synthesized structures. Uniaxial compressive deformations were accomplished using MD simulations to investigate the deformation behavior, the underlying atomistic mechanisms of yielding and plasticity improvement, and the transition of the deformation mode from localized to homogeneous-like deformation in the multilayer nanostructures. Research emphasis was placed on the unique interplay between crystal plasticity and glassy plasticity in the two kinds of layers at the nanoscale. The findings provide a more detailed atomistic understanding of tailorable deformation behavior and mechanical properties in the a/c nanolaminates.

2. Methods

MD simulations were performed utilizing LAMMPS [29]. Binary $Cu_{50}Zr_{50}$ MG and pure Cu, were chosen as the amorphous layers and crystalline layers, respectively. The interatomic interactions were described by the embedded-atom-method (EAM) potential developed by Sheng et al. [30]. To construct a monolithic MG, a primitive $Cu_{50}Zr_{50}$ amorphous configuration, composed of 30000 atoms, was first prepared by quenching its melting liquid (2000 K) to the glassy state (100 K) at a cooling rate of 1×10^{10} K/s. The constant-pressure-temperature ensemble (*NPT*) and three-dimensional periodic boundary conditions (PBCs) and a time step of 2 fs were applied. The MG sample was then generated by replicating the as-cast configuration, followed by sub-T_g annealing at 600 K for 0.5 ns ($T_g \sim 715$ K for $Cu_{50}Zr_{50}$ MG), and further brought back to 100 K. The final obtained monolithic MG, of dimensions $\sim 58.7 \times 5.3 \times 117.4$ nm^3, corresponds to a total atomic number of ~3 million. In constructing the a/c nanolaminates, the polycrystalline Cu layers, treated as a series of columnar grains with arbitrary crystallographic orientations, were generated by employing the Voronoi-tessellation method [31] using a single crystal Cu as the source of material. Then, $Cu_{50}Zr_{50}$/Cu nanolaminates were constructed by incorporating these polycrystalline Cu layers into the monolithic MG. Atoms near the CAIs and GBs that overlapped with separation distances less than 2.0 Å were removed. The in-plane grain sizes of polycrystalline Cu approximate to the thickness of Cu layers to better represent the experimentally synthesized nanolaminates [32]. The nanograins are infinitely long columnar shapes along the Y-direction in view of the applied PBCs. The constructed nanolaminates were further annealed at 600 K for 0.5 ns by applying an external hydrostatic pressure of 1.5 GPa to generate more realistic interfaces and eliminate voids which may be generated during sample construction.

Uniaxial compressive simulations were conducted along the Z-direction via scaling the corresponding cell length at 100 K and a strain rate of 1×10^8 s^{-1}. Note that the effect of different deformation strain rates (1×10^8 s^{-1}, 2×10^8 s^{-1} and 5×10^8 s^{-1}) was examined and found that the strain rate mildly affects the peak strength and flow stress of the nanolaminates, but has no apparent influence on the deformation mechanism of the nanolaminates. A low temperature of 100 K was chosen to eliminate the effect of thermodynamic fluctuation and promote SBs formation under loading, highlighting the responses upon mechanical activation in the superfast quenched MD samples [33,34]. PBCs were imposed in three dimensions to mimic a bulk size and wipe off the free surface effects which may add complications on the deformation of the nanoscale samples [22,26]. In addition, the normal stresses in the X-axis and Y-axis were relaxed to zero to allow lateral contraction during compression. The resultant stress was extracted from the normal tensor component of the virial stress along the loading direction [22].

To monitor the deformation process of the samples, the atomic-level deformation was monitored by local atomic shear strain, η^{Mises}, proposed by Shimizu [35]. Generally, regions mapped with relatively large η^{Mises} (i.e., $\eta^{Mises} > 0.2$) indicate a collective inelastic shearing of local clusters of atoms in response to the applied strain and can be viewed as volumes of atoms involved in plastic deformation [22,36]. To quantify the deformation degree, $\psi = N^{\eta > 0.2}/N$, $\psi_g = N_g^{\eta > 0.2}/N$ and $\psi_c = N_c^{\eta > 0.2}/N$ was defined to quantify the fractions of atoms participating in the plastic deformation in the whole samples (ψ), in the amorphous layers (ψ_a) and Cu layers (ψ_c), where $N^{\eta > 0.2}$, $N_g^{\eta > 0.2}$, $N_c^{\eta > 0.2}$and N represents the number of atoms with $\eta^{Mises} > 0.2$ in the whole samples, the amorphous layers, Cu layers and the total atoms in the samples. To evaluate the deformation inhomogeneity of the nanolaminates, the strain localization parameter proposed by Cheng et al. [37], was introduced, $\delta = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\eta_i - \bar{\eta})^2}$, where $\bar{\eta}$ is the average atomic shear strain over all atoms in the samples. The δ value quantifies the overall deviation of the atomic strain distribution of the samples from homogeneous deformation in which case δ approaches 0. The local structural orders and dislocations in the Cu layers were distinguished by the common neighbor analysis method (CNA) [38,39] and the so-called dislocation extraction algorithm (DXA) [40], respectively. The visualization was realized using OVITO [41].

3. Results and discussion

3.1. The structure of nanolaminates

In this study, we fabricated three a/c nanolaminates (hereafter labeled as sample "2L", "4L", "6L"), in which the corresponding numbers of polycrystalline Cu layers were embedded in the monolithic $Cu_{50}Zr_{50}$ MG, respectively. More specifically, the 2L, 4L and 6L nanolaminates have alternating stacks of CuZr(47 nm)/Cu(10 nm), CuZr (18 nm)/C(10 nm) and CuZr(9 nm)/Cu(10 nm) bilayers, which corresponds to a volume fraction of 17.5%, 35.7% and 52.6% for the polycrystalline Cu phases, respectively. The final sub-T_g annealed a/c nanolaminates shown in Fig. 1 reveal that almost all the nanograins (average grain size ~10 nm) in the polycrystalline Cu layers are in perfect face-centered cubic (FCC) structure. Only trace amounts of