



# Plastic deformation due to interfacial sliding in amorphous/crystalline nanolaminates



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## ABSTRACT

Molecular dynamics simulation was used to study the properties of the amorphous  $\text{Cu}_{46}\text{Zr}_{54}$ /crystalline interface and their effects on mechanical responses. Structural heterogeneity was observed in the  $\text{Cu}_{46}\text{Zr}_{54}$  layer in both an as-quenched and a separately quenched sample. Based on the simulation results, a new multi-yielding scenario for the formation of shear transformation zones (STZs), interfacial sliding, thickening of micro-sliding bands and lattice dislocation is proposed. During shear deformation, both samples first yielded due to the formation of STZs in the amorphous layers. After the formation of the STZs, micro-sliding bands with highly localized atomic shear strain formed in both samples via different interfacial mechanisms: via the growth of STZs at the amorphous/crystalline interfaces (ACIs) in the separately quenched sample, and via the spreading of the dislocation loop at the ACIs in the as-quenched sample. The thickening of micro-sliding bands on an amorphous layer via internal friction is identified as a new plastic deformation mechanism under appropriate loading conditions. The thickening rate in the as-quenched sample was higher than that in the separately quenched sample. The crystalline layer finally yielded due to partial dislocation slip. An analytical model suggests that this new multi-yielding scenario should be expected to operate in bulk metallic glass-based composites.

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## 1. Introduction

“The smaller, the stronger” is a well-accepted concept in the materials scientific community [1–3]. Recent promising developments in the manipulation of metal structures at the nano scale offer diverse approaches for achieving ultrahigh-strength materials [3]. An interesting approach is to create interfaces with nano-scale spacing in metals [4,5]. Such interfaces can limit dislocation motion to the nano-scale volume, thus exerting ultrahigh resistance to dislocation slip and inducing ultrahigh strength. Examples of such bulk metallic materials include nanocrystalline [3] and nanotwinned metals [4] and metallic nanolaminates [6]. The mechanical properties, most importantly the ductility/brittleness, of such materials strongly depend not only on the size of their microstructural features but also on the properties of their interfaces [7–13]. Molecular dynamics (MD) has revealed preliminary dislocation structures in the grain boundaries of nanocrystalline

metals [3] and bimetal interfaces in nanolaminates [10,14–16]. Dislocation always nucleates at the interfaces in both nanocrystalline metals and nanolaminates via delocalization of interfacial dislocation [14–16]. However, the grain boundaries and bimetal interfaces of the two materials are dissimilar. The grain boundary (GB) in nanocrystalline materials can carry considerable plastic deformation via GB sliding, dislocation nucleation and annihilation [3,17–19]. In contrast, while metallic nanolaminates are always high in strength, they are quite brittle because the bimetal interfaces with no coherency are unable to transmit dislocations at low stress levels. This induces high-density dislocation pile-ups, which inhibit further plastic deformation and result in fractures at these interfaces [7,11]. Twin boundaries are another example of interfaces that possess high strength and considerable ductility. They not only exert a repulsive force on moving dislocations but also allow them to penetrate or slide on the boundaries if the conditions are suitable [20–22]. It can be concluded, therefore, that the ability of an interface to release concentrated local stress via interfacial sliding or the transmission of plastic events is crucial to maintain ductility.

A recent study showed that a macroscopic-sized nanolaminate with alternating 5-nm amorphous  $\text{Cu}_{\approx 3}\text{Zr}$  layers and 35-nm

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nanocrystalline copper layers had high strength of about 1 GPa and almost ideal plasticity [23]. The MD simulations in that study revealed that amorphous/crystal interfaces (ACIs) play a significant role during deformation: in bulk metallic glass (BMG), dislocations in the crystal are transformed into shear transformation zones (STZs) at the ACIs, which accounts for the ideal plasticity [23]. It has been reported that ultimate tensile strength decreases as the thickness of the amorphous layer decreases below about 100 nm [24], due to the size dependence of the suppression of shear localization. However, another MD simulation showed that a shear band can form in extremely thin amorphous layers under uniaxial compression [25]. The role of ACIs in this size dependence of shear localization remains unclear. Unlike other interfaces, the ACIs in such materials should have some unique features because the structures on the two sides of the interface are different: one side has an ordered structure and the other an amorphous structure. MD simulation identified similar complex interface dislocation structures at the ACI with a bimetal interface, which were confirmed to be closely linked to interfacial shear [26]. It was also reported that the composition gradient of the ACI extended from the amorphous layer across the interface into the crystalline layer [26]. As the structural features of the amorphous layer are identical to those of BMG, the ACI should be a common interface in BMG-based composites containing nanocrystals. Investigation of the ACI may help to understand the mechanical properties of BMG-based composites. A deformation map of the dislocation emission and annihilation at the ACI and the transformation from dislocation to STZ was preliminarily illustrated by Wang et al. [23] and further elaborated by others [25,27,28]. However, the structural change of the amorphous layer induced by the presence of an ACI has not been fully studied, and the effect of such a change on the deformation of the amorphous layer remains unclear.

In this study, we investigated the ACI and its response to pure shear deformation using MD simulations. The results confirm that interfacial sliding at the ACI is an important plastic deformation mechanism. In addition, a new mechanism, the thickening of a micro-sliding band, is presented, and atomistic insights into the BMG deformation mechanism are developed. The remainder of the paper is organized as follows. Section 2 describes the simulation details, Section 3 discusses the results of the simulations in detail and Section 4 provides the conclusions.

## 2. Methodology

The simulations were performed in the LAMMPS [29] MD simulator. The atomic interactions between Cu and Zr atoms are described according to the embedded atom method potential, as developed by Cheng et al. [30], which was optimized for varieties of Cu–Zr–Al BMGs and intermetallic systems. Two samples were prepared following two distinct thermodynamic treatments with periodic boundary conditions in all directions. The first sample (S1) was separately quenched and prepared by thermal relaxing from an original configuration of alternating layers of crystal copper and nanoglass. Nanoglass layers were formed by combining several well-quenched small samples of  $\text{Cu}_{46}\text{Zr}_{54}$  BMG. A small BMG piece was prepared using the melt quench procedure. First, we randomly replaced Zr atoms with a probability of 54% in a copper crystal, with periodic boundary conditions set for all directions. This small system was rapidly quenched from 1600 to 0 K in 16 ns at a cooling rate of  $10^{11}$  K/s. The thicknesses of the crystal layer and nanoglass layer were 16 nm and 10 nm, respectively, along the  $z$  direction. The other dimensions were all 20 nm, which was sufficient to eliminate size effects on both the crystalline and the amorphous layer along the  $x$  and  $y$  directions. The crystalline directions of the copper layer were  $[\bar{1}\bar{1}2]$ ,  $[1\bar{1}0]$  and  $[111]$  along the  $x$ ,  $y$  and  $z$

directions, respectively. The sample geometry is illustrated in Fig. 1. A relaxation of S1 at 550 K was conducted for 50 ps after static energy minimization, which induced significant diffusion of the Zr atoms to the crystalline copper. S1 was finally quenched to 1 K in 50 ps for further simulations.

The second sample (S2), an as-quenched sample, had the same initial atomic configuration as S1 but was prepared using a different thermodynamic treatment. Consistent with the argument that Zr atoms should diffuse into the copper layer, the entire S2 was thermally relaxed at 800 K (above the glass transition temperature) for 1 ns, after being quenched from 1200 to 800 K in 4 ns while the copper layer was only fixed when the temperature was higher than 800 K. S2 was finally quenched from 800 to 0 K in 8 ns for further deformation. The overall cooling rate of the amorphous layer in S2 was the same as that of the small BMGs in S1. Pair distribution functions confirming amorphous structures of  $\text{Cu}_{46}\text{Zr}_{54}$  layers in both S1 and S2 are provided in the Supplementary Material. S2 was assured to have a more realistic interface than S1 [26] because it has been verified experimentally that the amorphous layer can be formed by the fast diffusion of Zr atoms into crystalline copper substrate [23]. However, the structure of S1 could also be possible because interfaces between glassy particles and crystal grains may be unstable in some mechanically annealed BMG-based composites.

Pure shear deformations were applied to S1 and S2 by directly changing the tilt factor of the supercells. The time steps during all deformations were set to be 1 fs, and the tilt factor changed every 200 time steps to obtain a constant engineering shear strain rate,  $\dot{\gamma}_{xz}(t)$ . Shear deformations with different strain rates of  $5 \times 10^9/\text{s}$  and  $5 \times 10^8/\text{s}$  were applied to S1 and S2. The boundary conditions were set to be periodic for all deformations. A constant pressure and temperature ensemble was used to maintain the system temperature at 1 K, and the other five stress tensor components were set to be traction free. Atomic shear strain analysis [31] and the common neighbor analysis (CNA) method [32] were used to display the deformation process. For convenience, in this work, atomic shear strain refers to von Mises atomic shear strain. Visualization of the simulations was performed by the software package OVITO [33].

## 3. Results and discussion

### 3.1. Interface characterization

Reference energy must be introduced to obtain the interfacial energy. A piece of BMG the same size as the amorphous layer and a crystal the same size as the crystalline layer were separately relaxed following the above procedures. The sum of the potential energies of the separately thermally relaxed BMG and the crystal was treated as the energy benchmark,  $E_{\text{benchmark}}$ . The interfacial energy of an ACI is defined as  $(E_{\text{potential}} - E_{\text{benchmark}})/2\Delta S$ , in which  $E_{\text{potential}}$  and  $\Delta S$  are the potential energy and cross-sectional area of nanolaminates S1 and S2 at a temperature of 1 K, respectively. Note that the interfacial energy definition is not based on the energy change in the affected zone of the interface alone but on the energy change of the whole sample. The ACI changes the chemical composition distribution of the entire nano-sized amorphous layer, not just the zone near the interface; hence, the energy distribution changes across the whole amorphous layer. The interfacial energy values for S1 and S2 were determined to be 72.60 and  $-133.1$  mJ/m<sup>2</sup>, respectively. The lower energy value for S2 than S1 implies that more zirconium diffused into the crystal in S2 than in S1, inducing more Cu–Zr bonding at the interface. Most importantly, the negative interfacial energy of S2 indicates that the distortion energy induced by the ACI was smaller than the energy

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