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Deformation mode transitions in $Cu_{50}Zr_{50}$ amorphous/Cu crystalline nanomultilayer: A molecular dynamics study

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ABSTRACT

The amorphous/crystalline (A/C) nanomultilayers have been aroused great interest in people due to its first-class mechanical properties. The effects of the thickness of crystalline and amorphous on the deformation mechanism of A/C CuZr/Cu nanomultilayers under tension loading here are investigated by molecular dynamics method. The results indicate that the mechanical behavior of nanomultilayer strongly depends on the bidirectional synergistic deformation mechanism between crystal phase and amorphous phase. The deformation behavior of nanomultilayers can be controlled by integrating the thickness of different phases to achieve high strength and superplastic multilayer materials. For the nanomultilayers with constant crystal layer, the plastic deformation changes from shear band propagation to a pronounced interface slip-accommodation mechanism, and ultimately to crack propagation mode with decreasing amorphous thickness. For the nanomultilayers with fixed amorphous layer thickness, the mechanical behavior changes from localization to plastic co-deformation mode with the crystalline thickness decreases. This study proposes an approach for achieving a good balance between strength and ductility, which is useful for the synthesis of A/C nanomultilayer with high strength and predominant ductility.

1. Introduction

Metallic glasses (MGs), possessing unique microscopic structures being short of long-range order, have been studied far and wide over the past few decades to comprehend the underlying physics underpinning their high strength [1–3] and other distinctive properties, including high hardness, good corrosion resistance, large elastic strain limit, and so on [3–6]. However, MGs are not being widely used due to their propensity for disastrous failure by development of shear bands (SBs) [7]. As is known to all, the development of SBs is the main reason for the failure of monolithic MG, which is induced by the aggregation of shear transformation zones (STZs). STZs are defined as the large atomic strain cluster bearing local events of cooperative shearing and realigning to a more astable state [8,9]. It is considerable that the deformation progress of MG should go hand in hand with the development of STZs. Hence, STZs can carry plasticity and induce the formation of SBs with the increasing loading. For the purpose of ameliorating the plasticity of MGs, one of the most prospective strategies are to create multiple SBs and hinder SB propagation, leading to homogeneous non-localized deformation [10–13]. Previous studies have confirmed that the crystalline phase can impede the propagation of SBs [14–17]. When crystalline phases are incorporated into the amorphous matrix, these phases can slow down the catastrophic SBs behavior. The main reason for this is that the crystalline phase inlaying in monolithic MGs is considered to be an absorber for deformation localization. Because crystalline phases can restrain the propagation of SBs and assimilate the remainder strain, either by diffusionless solid-state phase transformation or dislocation slip. These results imply that the plasticity of MGs can be enhanced by integrating MGs components or microstructures.

So far many studies find that tuning crystalline and amorphous layer to constitute amorphous-crystalline (A/C) nanomultilayers (ACNMs) are in a position to inhibit the development of SBs achieving potentially good ductility and high-impact strength in both experiments and simulations [15,16,18]. These findings indicate that the plastic deformation ability of A/C multilayers could be result of not only dislocation nucleation and absorption at the amorphous-crystalline interfaces (ACIs) but also activation of STZs triggered by dislocation activities in adjacent crystal layers. Wang et al. [19] propose that the ACI serves as the source and sink of the dislocations, so that it plays a non-negligible role in the plastic deformation behavior of

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nanomultilayers. Moreover, the deformation mechanisms of A/C nanocomposite show a strong size dependence, because relevant dislocation motion in crystalline layer and the formation and propagation of SBs in amorphous layer are both size-dependent [15,20]. For instance, a transition from a brittle to a ductile behavior is found in Cu/CuNb crystalline/amorphous nanomultilayers when the bilayer thickness is reduced to dozens of nanometers [21]. However, some research [22,23] have found that the mechanical property of nanocomposites shows a relatively weak dependence on layer thickness. Therefore, the influence of ACIs and related size effect on the deformation mechanism of A/C nanlominates still remained not yet clear. In addition, previous studies on size effect have focused on those multilayers with equal modulation ratio or the situation that only one-layer thickness is changing, but the optimal size matching relationship between different phases is still unclear. In order to improve the performance better, it is necessary to reveal the deformation mechanisms of C/A nanomultilayers on the atomic level. In reference to the experimental achievement in the manufacture of ACNMs, basic understanding of the microcosmic details of ACNM deformation mechanism lags far behind and is still open to study. Molecular dynamics (MD) simulation, possessing several merits over experimental research, acts as an effective method for exploring the microscopic properties of materials, in especial when the observations of mechanical properties in experiment are ambiguous [24]. Notably, the plastic deformation mechanism of ACNM depends on the coordination interaction between the crystalline and amorphous phases, and this synergistic effect is closely related to the properties of the crystalline phase. At present, most of studies on ACNM focus on the effects of soft crystalline phase on nanolaminates. However, the research on nanomultilayer comprised by the hard crystal phase and soft amorphous phase is still exiguous. Here, to reveal how plasticity transforms/interchanges between the soft MG and hard crystal phase, the deformation mechanism of A/C (CuZr/Cu) nanomultilayers are investigated by using MD methods.

To the end, the remaining part of the paper is organized as follows: The simulation models and methodology for MD method are determined in Section 2. In addition, the simulation results are analyzed in Section 3. Finally, Section 4 exhibits some conclusions of this study.

2. Simulation models and method

In the interest of obtaining the appropriate amorphous structures, a conventional “melt-quench-duplicate” approach is adopted. In order to ensure chemical stability, the fcc Cu50Zr50 alloys (the initial Cu50Zr50 alloys, owning three-dimensional size of nearly 2.2 nm (X)-5.6 nm (Y)-5.6 nm (Z), a number of 4056 atoms including 2028 Zr and 2028 Cu atoms, are arranged in a cubic in order) with periodic boundary conditions (PBCs) along all three independent directions are first relaxed at 2000 K, then cooled down rapidly to 50 K at a cooling rate of 10^{12} K/s. The monolithic Cu50Zr50 (labelled as CuZr) amorphous with different dimensions ($2.2 \times 15 \times 50\ nm^3$) are then obtained by replications of the initial CuZr amorphous, as shown in Fig. 1. The monolithic CuZr MGs are heated to 600 K at 10^{12} K/s, aged at 600 K for 0.5 ns, and then quenched at a quenching rate of 10^{12} K/s to 50 K in order to release the stress and eliminate voids. Subsequently, the resultant MG is then merged with crystalline Cu to construct the ACNM, in which the orientations of Cu layer are built as the $X-[\bar{1}\bar{1}2]$, $Y-[\bar{1}10]$ and $Z-[111]$, respectively. The MD simulations involve two different types of models corresponding to this study. For model I, the total superposed height of the A/C (CuZr/Cu) multilayers in the Z direction is ~50 nm with diverse amorphous layer height in the range between 1.55 and 21 nm while the thickness of crystalline layers are always fixed at 4 nm. Meanwhile, the width and the thickness of the nanomultilayers in the Y and X directions are 15 nm and 2.2 nm, respectively. For model II, the multilayers have fixed amorphous layer thickness of 6 nm. By changing the thickness of crystalline layer from 1 nm to 4 nm, and the total thickness of multilayers are about 50, 45, 40 and 35 nm, respectively, other conditions remain unchanged. As a matter of convenience, the subsequent notation is utilized to refer to each nanomultilayer: Cu (A)/CuZr (B), where A and B represent the thickness of crystalline layer and the CuZr amorphous layer, respectively. In order to allow shear offset on the free surfaces to occur, the free surface is exerted along the Y axis, while PBCs are imposed on the X and Z directions to eliminate the influence of boundary effect. During loading, the tensile strain is imposed along *Z*-direction with the applied strain rate of $1.25 \times 10^8\ s^{-1}$. Here, the MD simulations apply a 2.0 fs time step. All of simulations are conducted at a fixed temperature of 50 K and all microstructural analysis and visualization of atomic configurations are performed using the open-source visualization tool OVITO [25].

In addition, the quality of the potential function essentially determines the accuracy of the simulation. Here, the interatomic interactions can be described by the embedded atom method (EAM) potential proposed by Mendeley for the Cu-Zr binary system [26]. This potential function has been successfully proven by many instances [27–29]. It is also necessary to point out that the average stress in current study is calculated by using the Virial theorem [30], which is expressed by:

$$\Pi^{\alpha\beta} = \frac{1}{\Omega}\left\{-\sum_{i} m_i v_i^{\alpha} v_i^{\beta} + \frac{1}{2}\sum_{i}\sum_{j\neq i} F_{ij}^{\alpha} r_{ij}^{\beta}\right\} \quad (1)$$

where the Ω and $\Pi^{\alpha\beta}$ represent the system volume and the mean stress, respectively. The first part of in the right side of Eq. (1) stands for a kinetic energy component for atom i, while the second part is produced due to the inner-atom force. m_i and v_i^{α} (or v_i^{β}) are the mass and velocity of atom i, and F_{ij}^{α} is the force between atom i and atom j, where the indices α, β denote the Cartesian components. r_{ij}^{β} is the distance vector between atom i and atom j along coordinate β.

3. Simulation results and discussion

3.1. Effects of amorphous layer thickness on the mechanical behavior of nanomultilayers

3.1.1. The stress-strain relationship of nanomultilayers

To study the effect of amorphous layer thickness on the mechanical behavior of A/C (CuZr/Cu) nanomultilayers under the tensile loading, the emblematical stress-applied strain behavior of samples with various amorphous thickness ranging from 1.55 to 21 nm are given in Fig. 2(a). Here, the crystalline Cu layer thickness is fixed at 4 nm. In order to clearly comprehend the difference of deformation mechanism, just six representative curves are given. For comparison purpose, the stress-strain curves of CuZr MG and single crystal Cu are also displayed, and the peak stresses of monolithic CuZr and Cu [111] are 3.56 GPa and 22.14 GPa, respectively, as shown in Fig. 2. It can be seen in Fig. 2(a) that the yield stress (peak stress) of nanomultilayers spans from 3.81 GPa to 6.29 GPa, which lies in between that of single crystal Cu and monolithic amorphous. Upon inspecting the yield stress and the elastic modulus, it is found they change distinctly with altering the MG layers thickness, showing significant size effect. It is clear that the single crystal Cu exhibits a much higher elastic modulus than that of monolithic amorphous. And the curve of single crystal Cu suffers a sudden drop (for simplicity, it doesn't show up in the graph) due to the dislocation sliding mechanism. Besides, it is quite obvious that the yield stress of A/C (CuZr/Cu) nanocomposites is strongly influenced by the amorphous layer thickness. Fig. 2(b) shows the simulation results of yield stress for nanomultilayers as functions of inverse square root of amorphous layer thickness. When the CuZr MG thickness is reduced gradually, the existing outcomes indicate that the yield stress of nanomultilayers gradually increases, which is in accordance with the Hall-Petch relationship [31]. The change in yield stress is likely to result from the strengthening effect of the ACIs when the CuZr amorphous thickness is < 20 nm [32]. Several momentous conclusions could be