Mechanical analysis of the crystalline–amorphous laminated composite based on a two-phase model

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ABSTRACT

A two-phase model was proposed to investigate the mechanical behaviors of crystalline/amorphous (C/A) laminated composite in this paper. By assuming the good bonding of crystalline and amorphous, a rate-dependent Newtonian viscous flow process was developed to describe the amorphous phase sliding behavior while a dislocation gliding behavior to crystalline phase. Based on the rule of mixture theory, the overall stress–strain kept consistent with experimental data. Due to the particular microstructures, the effects of grain size of crystalline phase and strain rate on the mechanical behaviors of C/A nanolaminate were discussed. The stress–strain relations were enhanced with the decreasing grain size and increasing strain rate. Obvious strain hardening was also observed. The strain hardening exponent was much larger than that of corresponding nanocrystalline (NC) materials and increased with the increasing strain rate and decreasing grain size.

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1. Introduction

Since Duwez et al. [1] successfully prepared amorphous $Au_{75}Si_{25}$ ribbon by rapid cooling in 1960, the great theoretical value and applied value of amorphous alloys have been gradually known. From then on, bulk metallic glasses (BMGs), as a promising class of materials for structural and functional applications; have attracted great attention owing to their excellent mechanical properties compared with crystalline materials, such as high strength, large elastic strain limit and excellent corrosion resistance [2–4]. The deformation behavior of metallic glasses (MGs) is usually classified as inhomogeneous or homogeneous deformation. Homogeneous deformation usually takes place at elevated temperatures and can be described by Newton viscous flow at low strain rates or as non-Newtonian at higher strain rates [5]. Inhomogeneous deformation occurs at temperatures well below the glass transition temperature. The current consensus for explaining the inhomogeneous deformation of MGs is the localized deformation in form of shear transformation zones (STZs) in lieu of abundant plasticity carriers-dislocations in crystals [6]. These STZs, a small cluster of closely packed atoms, create a localization of displacement in surrounding regions that trigger the evolution of highly localized shear bands during the deformation. This plastic instability in turn results in limited ductility and causes catastrophic fracture, significantly confining their structural applications [7]. Therefore, the approach to improve the ductility of MGs with little strength loss continues to be a critical issue.

Recently, with the progress of science and technology development, composite materials, made from two or more constituent materials with significantly different physical or chemical properties, are being considered as potential material systems of choice for enhancing plasticity of amorphous materials. In mechanical design applications, composites are engineered materials comprising reinforcement particles, fibers, flakes, and the like embedded in a supporting matrix of polymers, metals or ceramics [8–11]. Due to the enhancement of the reinforcement, the new materials have properties superior to those of the either original materials alone. In parallel, incorporation of crystalline and amorphous layers by adjusting their constituent has been regarded as a potential method. For instance, Alpas and Embury [12] produced laminated composite structures of amorphous $Ni_{78}Si_{10}B_{12}$–Cu by electro-deposition and diffusion bonding. The tensile strain greatly increased by reason that the constraint provided by copper layers on amorphous $Ni_{78}Si_{10}B_{12}$ layers inhibits tensile instability in the amorphous ribbons and caused a more homogeneous distribution of shear bands. Leng and Courtney [13] prepared brass (Cu–30%Zn)-nickel base MG ($Ni_{91}Si_7B_2$) composite laminates by soldering these constituents together with a Pb–Sn alloy. The laminate exhibited enhanced tensile ductility. Multiple shear bands were subsequently observed in the amorphous $Ni_{91}Si_7B_2$ ribbon with enhanced tensile ductility. Nevertheless, though having enhanced ductility of abovementioned

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laminated materials, the macroscopic strain-softening behavior, i.e. shear bands, is still obvious in tension for these composites [14]. Recently, this drawback has been successfully circumvented in some crystalline-base composites by adjusting the thickness of crystalline and amorphous. The laminated composite prepared by Li et al. [15] using the pulse electrodeposition method also exhibits good ductility below the crystallization temperature of amorphous layer. Due to the good interfacial bonding between amorphous layers and nano-Ni layers, a maximum elongation of 115.5% can be obtained when the volume fraction of nano-Ni layers was 0.77. Nieh et al. [16] synthesized NC Cu/amorphous Cu–Zr laminate with respective thickness of 35/5.7 nm by magnetron sputter deposition. The laminate possessed a very high yield and tensile strength and still retained a reasonable tensile elongation (4%) at room temperature. The Cu/CuZr C/A nanolaminate with respective thickness of 35/5 nm synthesized by Wang et al. [17] reliably showed high tensile strength (about 1.2 GPa) and large tensile elongation (about 14%) at room temperature before failure. Obviously, the abovementioned experimental results have clearly revealed that a nano-scale multilayer scheme with proper proportion of components and reasonable individual thickness is likely to suppress the shear bands at room temperature and significantly improve the deformability of MGs by forming C/A multilayer architecture.

It follows that there must be particular interactions between amorphous layers and crystalline layers. According to the Molecular Dynamic (MD) simulations and experimental results reported by Wang et al. [17], it can be seen that the shear bands formation could be suppressed by the NC layer and dislocations could be disrupted by the amorphous layer. The amorphous layers act as high-capacity sources and sinks for dislocations, enabling absorption of free volume and free energy transported by dislocations. However, most of existed research results are from experiments or MD simulations and little works have been done to describe the deformation mechanism of this special C/A laminated composite in theory. Therefore, in this paper, taking the NC Cu and amorphous CuZr as a typical C/A nanolaminate, a two phase composite model was developed to describe the deformation mechanisms of each phase and reproduce the experimentally observed behaviors. Then, the grain size effects and strain rate sensitivity were discussed to further understanding the mechanical behaviors of C/A nanolaminated composite.

2. Materials model

2.1. Materials microstructure

For Cu/CuZr C/A nanolaminates, being a typical example of C/A laminated materials, it can be idealized as a two-dimensional nanolaminate structure assembled by crystalline layers and amorphous layers as illustrated in Fig. 1. Here, the crystalline phase is assumed to be composed of an array of repeating unit columnar cells with a regular-square cross section and their grain boundaries. The individual thickness of the crystalline layers, amorphous layers and grain boundaries are represented as δ_c, δ_a and δ_{gb}, respectively. Generally, the NC Cu and nanoscale Cu/Zr amorphous nanolaminate samples are fabricated by magnetron sputter deposition of alternating layers of Cu and Zr [18]. Thus, the crystal layer thickness is approximately equal to the average grain size of NC phase which can be confirmed through the plan-view transmission electron microscopy (TEM) image in Refs. [17,18]. As a result, it can be seen that, the volume fractions of amorphous layers, crystalline layers and grain boundary phase, denoting as f_a, f_c and f_{gb}, can be obtained by their geometrical characteristics as follows:

$$f_a = \frac{d \times \delta_a}{\delta_a \times d + d \times \delta_c} = \frac{\delta_a}{\delta_a + \delta_c} \qquad (1)$$
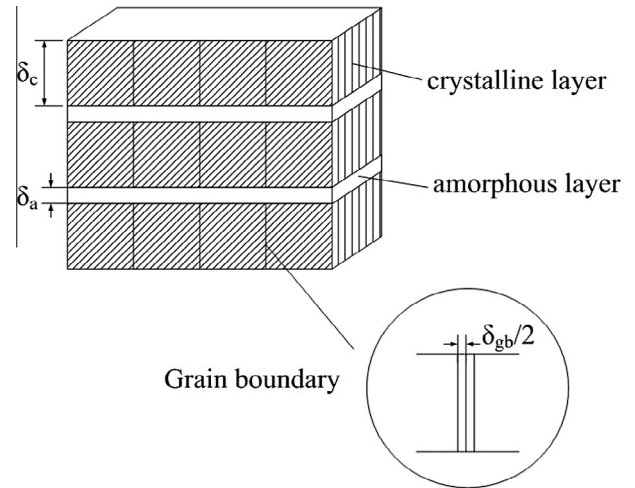

Fig. 1. The structural unit of crystalline/amorphous alternately arranged multilayer composite.

$$f_c = \frac{(\delta_c - \delta_{gb})^2}{\delta_a \times d + \delta_c \times d} \qquad (2)$$

$$f_{gb} = 1 - f_c - f_a \qquad (3)$$

In light of the results of high resolution TEM [19], the grain boundary phase with a fixed thickness of 1 nm was commonly accepted. Consequently, Fig. 2a is the variation of the volume fraction of each phase changing along with grain size with fixed amorphous phase of 5 nm and grain boundary thickness of 1 nm, (b) with fixed crystalline layer thickness of 35 nm and grain boundary thickness of 1 nm changing along with the thickness of amorphous phase.

Obviously, no matter what the thickness of crystalline phase or amorphous phase varied, the volume fraction of grain boundary phase does not exceed to 0.05, which is much little than the other two phases. As seen in Fig. 2a, the volume fraction of amorphous ranges from 15% to 40% with decreasing grain size from 40 to 10 nm, that comparable to the volume fraction of the crystalline phase. It is evident that, the amorphous phase has non-negligible volume concentration in C/A nano-laminate especially when grain size is smaller than 40 nm as seen in both Fig. 2a and b. Furthermore, high-resolution TEM examination by Wang et al. [17] also shows that the NC Cu grains/layers are nearly dislocation-free, with a {1 1 1} out-of-plane texture. Thus, it is reasonable to neglect the grain boundary thickness and their effects on the overall behaviors of the laminated composite. Therefore, the microstructure of laminated Cu/CuZr composite can be simplified with only amorphous phase and crystalline phase with their corresponding volume fraction as follows:

$$f_c = \frac{\delta_c}{\delta_c + \delta_a} \qquad (4)$$

$$f_a = 1 - f_c \qquad (5)$$

On the assumption of good bonding between crystalline phase and amorphous phase, that is, iso-strain in both of crystalline and amorphous phase, the overall stress–strain can be established by combining the mechanical behaviors of each phase based on the rule of so-called mixtures as [16,20]:

$$\sigma = f_a \sigma_a + f_c \sigma_c \qquad (6)$$

where σ_a and σ_c are stresses for amorphous CuZr layers and crystalline Cu layers. As a result of the volume fraction of grain boundaries less than 0.05, even if considering the grain boundary effects, the