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Molecular dynamic simulations of the mechanical properties of crystalline/crystalline and crystalline/amorphous nanolayered pillars

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ABSTRACT

By properly introducing interfaces and boundaries to nanomaterials, good plasticity can be obtained without sacrificing the strength. Nanolayered crystalline/crystalline (C/C) Cu/Zr and crystalline/amorphous (C/A) Cu/CuZr with and without twin boundaries (TBs) are investigated by large scale molecular dynamic simulations. By characterizing the plastic deformation on atomic scale, the simulation results show that the C/C interfaces, C/A interfaces, grain boundaries (GBs) and TBs have different effects on the deformation behaviors of nanolayered pillars. In C/C pillars, partial dislocations slip in the columnar nano-crystals of Cu layers and diffusion and motion of GBs take place in Zr layers. The dislocations entrapped within the C/C interfaces and the diffusion and motion of GBs in Zr layers lead to strain softening. TBs can effectively improve the yield stress of C/C pillars but not that of C/A pillars. The dominant deformation mechanisms in C/A pillars are the activations of the shear transformation zones (STZs) and the interplay of dislocations and STZs at the interfaces, which, in conjunction with the strain compatibility of the amorphous layers, contribute the less strain softening responses in C/A pillars.

1. Introduction

Traditional grain refinement can improve the strength of metallic materials due to dislocation pileup at grain boundaries (GBs). However, it usually decreases the ductility dramatically because both nucleation and motion of dislocations are confined in nanoscale crystals. Consequently, nanocrystalline (NC) materials are usually strong but brittle [1,2]. Bulk metallic glasses (MGs) with amorphous structures possess high elastic limit and strength, but nearly no tensile plasticity because of the shear localization which is through shear transformation zones (STZs) at catastrophic failure [3]. The brittleness of NC and MG materials largely limit their applications.

In recent years, new methods have been developed to improve the ductility of NC and MG materials by properly applying interfaces and boundaries, such as crystalline/crystalline (C/C) interfaces [4–6], crystalline/amorphous (C/A) interfaces [7–9], and twin boundaries (TBs) [10–13]. These methods were found to be able to improve the plasticity of the nanomaterials without sacrificing their strength. Nanolayered materials can offer additional interfaces to tune the strength and ductility of materials and hence they have attracted a growing interest in recent years. Such materials include C/C and C/A nanolaminates. For instance, Sun and his co-workers [14,15] discussed the length scale dependent mechanical behaviors of crystalline Cu/crystalline Zr pillars and found that deformation modes transited from dislocation dominated symmetric slip to localized shear induced by asymmetric slip and GB motion as layer thickness decreasing. Liu et al. [16,17] studied stacking fault and partial dislocation dominated strengthening mechanisms in highly textured C/C multilayered materials and discussed the interfaces and TB effects. Taken the nanocolumn size, interface barriers and twins into account, Chen et al. [18] investigated the strengthening mechanisms of C/C materials with different layer thicknesses. Misra and co-workers [19–21] investigated the length scale dependent strengths and mechanisms in multilayered C/C composites by both experiment and multiscale modeling. They found the dominant mechanisms are dislocation pile-up, single dislocation confined in individual layer and interface crossing with the layer thickness decreasing from sub-micro meters to a few nanometers. Deformation instability and localized shear bands have been observed in samples consisting of thin layers by Zhang and his co-workers [22–24]. Formation of the shear bands is due to grain rotation and grain boundary sliding. As to C/A materials, they are found to have the capacity of sustaining good ductility and high strength [7–9,25]. Wang et al. [8] observed an exceptional tensile ductility of 13.8% in crystalline Cu/amorphous CuZr nanolaminates. Kim et al. [7] utilized size dependent homogeneous

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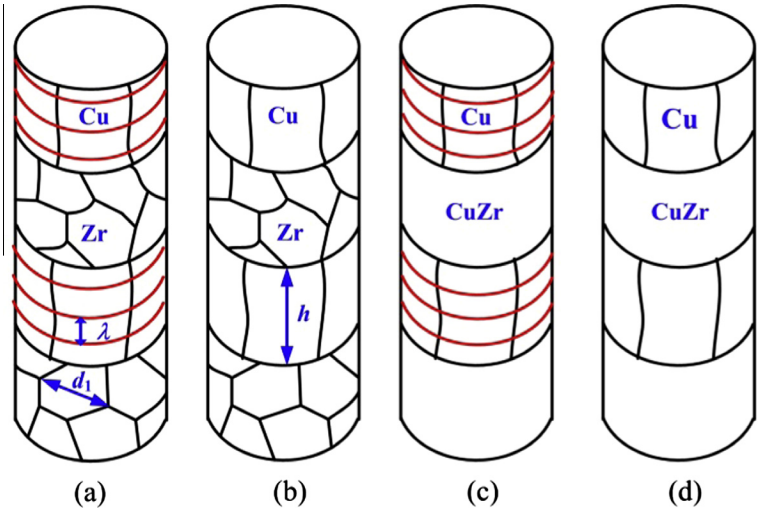

Fig. 1. Schematic illustrations of (a) nanotwinned Cu/crystalline Zr (NTCu/Zr) and (b) nanocrystalline Cu/crystalline Zr (NCCu/Zr) pillars; (c) nanotwinned Cu/amorphous CuZr (NTCu/CuZr) and (d) nanocrystalline Cu/amorphous CuZr (NCCu/CuZr) pillars.

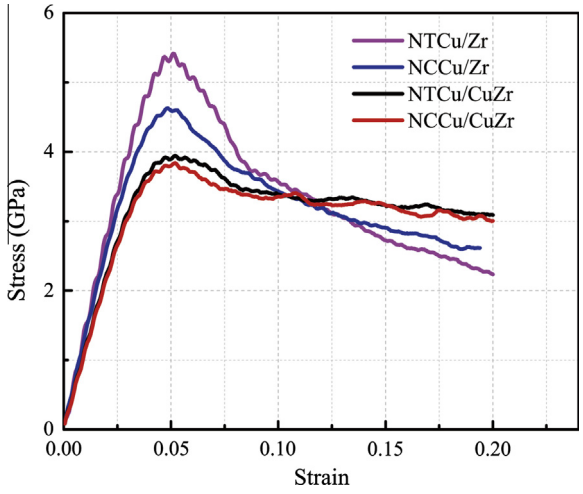

Fig. 2. Compressive stress-strain curves for nanolayered pillars in Fig. 1.

plasticity of MGs to obtain high strength and good plasticity C/A nanolayered materials. Zhang et al. [9] claimed that superhigh homogeneous deformation (more than 30% strain) rather than localized shear banding can be achieved in crystalline Cu/amorphous CuZr micropillars. It was also found that deformation-induced devitrification via absorption/annihilation of abundant dislocations, triggering the cooperative shearing of STZs in glassy layers contribute to this extraordinary plasticity. Liu et al. [25,26] studied the microscale deformation behaviors and the interfacial strength of C/A materials. Zhang et al. [27] compared the homogeneous boundaries and heterophase interfaces in plastic deformation of nanostructured micropillars and discussed the different roles of boundaries and interfaces in the rate-limiting process of nanomaterials.

In addition to experimental and theoretical studies, atomistic simulations were employed to uncover the underlying deformation mechanisms of the nanolayered materials. Molecular dynamic (MD) simulation has been shown to be an effective method to study the nanoscale mechanisms, especially with the development of high performance computing. Dislocation interacting with coherent and incoherent interfaces have been studied in details by MD simulations [6,28–33]. For the coherent interfaces, the same crystal structures and small lattice mismatch induce large coherent stress which can strengthen the composites. Dislocations can transmit form one layer to another due to the continuous slip systems [29,31,32]. The incoherent interfaces [6,28,33] act as barriers for slip transmission and shear easily due to the lower shear strength comparing to the layers. Dislocations can be attracted to spreading cores within the interfaces and entrapped to create steps at the interfaces. Abdolrahim et al. [34] studied the strengthening mechanisms of nanolayered Cu/Nb with incoherent interfaces and found competitive deformation mechanisms in nanolayered C/C materials. Arman et al. [35] and Brandl et al. [36] used MD simulations to study the compression and shear deformation of C/A interfaces. Wang et al. [8] showed that C/A interfaces can acts as both sources and sinks for dislocations. However, in nanolayered materials, majority of factors as TBs, GBs, C/C interfaces and C/A interfaces can influence the interactions between dislocation and interface and hence affect the mechanical properties. Different roles of the boundaries and interfaces in nanolayered materials need to be further studied. Here, large scale MD simulations are performed for nanolayered pillars involving million atoms. The plastic strain transmission through the C/C and C/A interfaces as well as effects of TBs and GBs on the strength and deformation mechanisms of nanolayered pillars are discussed in view of the obtained numerical results.

2. Simulation method

As mention above, Zhang et al. [27] conducted compression experiments of different types of micropillars to study the effects of homogeneous boundaries and heterophase interfaces on plastic deformation. To further understanding the different roles of boundaries and interfaces in nanolayered materials, MD simulations are employed to explore the deformation mechanisms for two types of nanostructures: (i) C/C (Cu/Zr), and (ii) C/A (Cu/CuZr) pillars. Models with and without TBs for each type of the nanopillars are generated. All the models have similar structures but smaller size comparing to the experiment models in [27].

As shown in Fig. 1, columnar Cu structures with (1,1,1) textured in Z direction are adopted in the simulations, with their in-plane average grain size of being 10 nm. In addition, uniform nanotwins of spacing $\lambda = 1.88$ nm are also introduced into the columnar Cu structures in Fig. 1(a) and (c). In the models for nanotwinned Cu/crystalline Zr (NTCu/Zr) and nanocrystalline