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Strengthening mechanisms of the nanolayered polycrystalline metallic multilayers assisted by twins

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ABSTRACT

To study the assistance of growth twin in nano-layered polycrystalline metallic multilayers to their strength, a series of uniaxial tensile modeling of nano-twinned Cu//Ag and Cu//Ni multilayers is performed via molecular dynamics method, with especial attentions to the influence of the twin lamella thickness and its spatial distribution on the strengthening mechanism. The results indicate that the strengths of nano-twinned multilayers can be enhanced significantly by introducing nano-twin lamellae into them and show strong twin thickness effect. By checking the atomic details, it is found there exists a critical twin lamella thickness above which the deformation mechanism of metallic multilayers is the hairpin-like partial dislocation gliding dominated and below which it becomes the necklace-like multiple jogged dislocation gliding dominated, however. The formation and transition of different deformation mechanisms are discussed in detail and analyzed theoretically, and the effect of the distinct deformation mechanisms on the strength of multilayers is also depicted quantitatively. In addition, the strengths and deformation mechanisms of two type nano-twinned Cu//Ag multilayers with non-uniform twin lamellae distribution are also discussed. The results show that the necklace-like dislocation mechanism and the hairpin-like dislocation mechanism can coexist in those non-uniform twinned multilayers and the necklace-like multi-jogged extended dislocations are unexpectedly observed in thicker twin lamellae. Although there are synergetic interactions between two mechanisms, the strengths of multilayers with non-uniform nano-twin lamella thickness can be well predicted by the rule of mixture.

1. Introduction

With rapid progress in micro/nano manufacture technology, multilayered metallic films (MMFs) have been extensively used in integrated circuit chip, various coating materials (PalDey and Deevi, 2003; Stueber et al., 2009), micro/nano sensors (Kleinfeld and Ferguson, 1995) and structural or functional modules of the Micro–Electro-Mechanical Systems (MEMS) (Bhushan, 2007; Spearing, 2000). Increasing application of the MMFs in these fields benefits from their excellent hardness (Hoagland et al., 2004; Lu et al., 2014; Yan et al., 2012), ultra-high tensile strength (Lu et al., 2014) and radiation damage resistance (Misra et al., 2007; Yu et al., 2013) which are attributed to massive phase interfaces in MMFs. In the past decade, a series of experiments (Liu et al., 2013b; Lu et al., 2014; Misra et al., 2005; Zhang et al., 2010) and simulations

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(Abdolrahim et al., 2014; Salehinia et al., 2014; Shao et al., 2012; Wang et al., 2014a, 2014b; Zbib et al., 2011) have been performed, which indicated convincingly that with individual layer thickness λ decreasing from hundreds of nanometers to several nanometers, the strength of multilayer increases to one third or even half of its theoretical strength limit (Clemens et al., 1999). Increasing strength of MMFs with decreasing layer thickness λ is usually ascribed to three mechanisms, including the pile-up of dislocations at the phase interfaces when λ is above dozens of nanometers, the propagation of a single hairpin-shaped dislocation loop parallel to interfaces when λ is in the range of dozens of nanometers to several nanometers, and the interface crossing of single dislocation when λ is at several nanometers (Misra et al., 2005; Zhu et al., 2014). In material science, a well-known dilemma is the strength–ductility trade-off (Koch et al., 2005; Lu et al., 2009; Sanders et al., 1997; Wei et al., 2014). In other words, the strength of metallic multilayers is enhanced usually at the expense of their ductility (Li and Zhang, 2010; Zhang et al., 2011). With the layer thickness decreasing from hundreds of nanometers to several nanometers, fracture mode in multilayers transits gradually from ductile necking to brittle shear (Zhang et al., 2011), which renders the nano-layered metallic multilayers to crack abruptly at very low strain. In addition, within the multilayers with individual layer thickness of several nanometers, the interface instability due to highly localized shear bands is frequently observed, which limits severally the deformability of nano-layered metallic multilayers (Bhattacharyya et al., 2009; Li et al., 2008; Mara et al., 2010). All these fatal disadvantages can trigger the multilayers to fracture prematurely, which extremely limit the extensive application of the multilayers in NEMS/MEMS devices. How to enhance the strength of nanostructured materials without sacrificing ductility comes into focus recently in academic circles and industry (Lu, 2014; Wei et al., 2014).

In recent years, many efforts have been made to evade the strength-ductility trade-off dilemma of nano-structured materials. By means of a particular thermo mechanical treatment, Wang et al. (2002) prepared a bimodal bulk Cu with micrometer sized grains embedded inside a matrix of nanocrystalline and ultrafine grains. Due to cooperating contributions of larger grains to strain hardening rate and smaller grains to high strength, this bimodal bulk Cu achieves a marked improvement in ductility, without sacrificing much of the strength. Zhao et al. (2006) engineered very small second-phase particles into nanostructured Al alloy matrix. Due to greatly increased dislocation accumulation and resistance to dislocation-slip by the second-phase particles, the ductility and strength of bulk nanostructured materials are increased simultaneously. Lu et al. (2009) employed the pulsed electrodeposition to synthesize high-purity Cu foils with the nano-twinned lamellae embedded in submicrometer sized grains, achieving striking strength and considerable ductility relative to coarse grained (CG) Cu. By high pressure torsion (HPT) processing, Liddicoat et al. (2010) engineered hierarchically nanostructured aluminum alloys with nanoscaled grains and sub-granular solutes, which exhibits nearly twice the strength of the T6 treated alloy but only little decrease in tensile elongation. Adopting the surface mechanical grinding treatment (SMGT) technology, Fang et al. (2011) prepared a nano-grained Cu film with a spatial gradient in grain size on a bulk CG Cu substrate, achieving a 10 times higher yield strength and a tensile plasticity comparable to that of the CG film. By the same technology, various gradient microstructures with the grain size increasing from nanometer scale at the surface to micron scale in the core is produced, which shows a superior ductility–strength synergy that is inaccessible to homogeneous microstructures (Lu et al., 2014; Wu et al., 2014a, 2014b). By means of a molecular-level liquid–liquid mixing/doping technique, Liu et al. (2013a) manufactured a hierarchically microstructured molybdenum alloys with nanosized oxide particles dispersed in the sub-micrometer grain interior, reaching a strength of 800 MPa and a total elongation to failure of 40%. Recently, by applying torsion to cylindrical steel samples, a gradient hierarchical nano-twinned structure was generated along the radial direction (Wei et al., 2014). Due to synergistic interaction of gradient twin structures, the yielding strength of the material is doubled without reduction in ductility. Obviously, all these efficient ways, which succeed in simultaneously improving the strength and ductility, have one thing in common: the hierarchical nanostructure is specially designed and successfully introduced into materials as nature does (Wegst et al., 2014). A similar strategy is expected to be also effective for the present interested nanolayered polycrystalline metallic multilayers (NPMMs) with ultrahigh strength but very low ductility. In order to mediate the strength and the ductility of NPMMs, a possible strategy is to replace the conventional crystalline/crystalline layered structure which is strong but brittle by the crystalline/amorphous structure. For example, Wang et al. (2007) found the tensile elongation to failure of Cu_3Zr/Cu (5 nm/35 nm layered) nano-laminates is six or more times higher than that typically observed in conventional crystalline/crystalline laminates; Liu et al. (2012a) found the homogeneous compression strain of the metallic ZrCu-amorphous/Cu-crystalline nano-layered micropillars could reach as high as 100%; Zhang et al. (2013) found that with the individual layer thickness of nano-layered Cu-crystalline/CuZr-amorphous micropillars decreasing from 100 nm to 20 nm, their strength increased from 1.5 to 2.3 GPa but the fracture strain could maintain at about 25%. These experiments showed that the layered crystalline/amorphous structure indeed could improve significantly the ductility of multilayers. Different from them, here we pay our attention to another strategy, i.e. introducing nano-twinned lamellae into NPMMs, which is expected to have potential to enhance simultaneously the strength and the ductility of the NPMMs.

During recent decade, nano-twinned metals with a high density of nanoscale twins have attracted a lot of attention (Jang et al., 2012; Li et al., 2010; Shen et al., 2005; Wang et al., 2012). A series of experiments and atomic simulations have repeatedly showed that the growth twin in metals could efficiently evade the trade-off between strength and ductility of metallic materials (Anderoglu et al., 2010; Cao et al., 2007; Lu et al., 2009; Shen et al., 2005; Wei et al., 2014; Zhou and Qu, 2010). In these nano-twinned metals, the low energy coherent twin boundaries are as effective as conventional grain boundaries in strengthening materials. On the other hand, with the decrease of the twin thickness, the dislocation-TB interactions become more facilitative and more rooms are afforded for storage and accumulating of dislocations, which contributes to pronounced strain hardening and high ductility in the nano-twinned polycrystalline metals (Lu et al., 2009).