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Analysis of the twin spacing and grain size effects on mechanical properties in hierarchically nanotwinned face-centered cubic metals based on a mechanism-based plasticity model

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ABSTRACT

Hierarchical twin lamellae in polycrystalline face-centered cubic (fcc) metals possess a possibility to achieve higher strength with keeping an acceptable elongation. The present work is concerned with the analysis of twin spacing and grain size-dependent plastic performance in hierarchically nanotwinned fcc metals using a generalized strain-gradient plasticity model. The dislocation density-based physical model for constitutive description of nanotwinned fcc metals is expanded for the hierarchical structures of nanotwins. The strengthening mechanism and the failure behavior in these hierarchical nanostructures are studied to evaluate the strength and ductility. Moreover, the transition twin spacing between the strengthening and softening is obtained in different order of twin lamellae. A dislocation-based model on nucleating deformation twins is presented to predict the critical twin spacing in the lowest twin lamellae for generating the subordinate twin lamellae. Our simulation results demonstrate that the existence of the hierarchical nanotwins gives rise to a significant enhancement in the strength, and the resulting global flow stresses are sensitive to the twin spacings of the hierarchical twin lamellae and the grain size. Two softening stages are observed with variation of twin spacing, and the relevant transition twin spacing depends on the microstructural size in hierarchically nanotwinned metals. We further find that the predicted failure strain decreases with decreasing the twin spacing, which is quite different from the case of the individually nanotwinned fcc metals. The critical twin spacing for generating subordinate twins also depends on the twin spacing of superordinate twin lamellae and the grain size. These findings suggest that the high yield strength and good ductility can be achieved by optimizing the grain size and the twin spacings in the hierarchical twins.

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1. Introduction

The simultaneous high strength and good ductility in nanostructured metallic materials is expected in applications of metals and alloys in modern technologies. This expectation can be realized through various approaches, such as mixing various sizes of microstructures in nanostructured materials (Wang et al., 2002; Zhao et al., 2008; Dirras et al., 2010; Ramtani et al., 2010; Li and Soh, 2012) and generating internal boundaries in polycrystalline metals (Lu et al., 2004, 2005, 2009a, 2009b, 2009c; Shen et al., 2006). Nanotwinned metals have been proved to possess a good combination of strength and ductility (Lu et al., 2009a, 2009b, 2009c) and considered to be suitable for the applications where both factors are important. Such metals derive their reinforced mechanical performance from the intrinsic properties of twin lamellae, which includes the inner twin boundaries acting as obstacles to move the dislocations and the increasing twinning partials benefiting to the pronounced strain hardening. A major issue here is on the hierarchical nanotwins in polycrystalline fcc metal, as its presence can give rise to the significant change of the mechanical performance in comparison to one of individually-nanotwinned fcc metals. This is especially pertinent to the use of the high strength metals where the nanotwins can been formed conveniently, such as in nanotwinned fcc metals and the twinning induced plasticity (TWIP) steels.

The nanostructural hierarchy has been clarified as an alternative approach to achieve the high strength in metals and alloys. Such hierarchy consists of the subnanometer intragranular solute cluster, two geometries of nanometer-scale solute structures as well as the nanograins, all of which contribute to mechanical properties in aluminum alloys together (Liddicoat et al., 2010). During martensitic transformation, the hierarchically twinned structures are often observed in experiments (Saburi et al., 1980; Müllner et al., 2003). In these structures, the secondary twins appear in the primary twins and the tertiary twins are generated in the secondary ones. These hierarchical twins are identified to play a key role in mechanical behaviors of the materials (Müllner and King, 2010). For example, through the surface mechanical attrition treatment (SMAT) or equal-channel angular pressing (ECAP), the primary and secondary nanoscale twin lamellae have been observed in the ultrafine/nanocrystalline Cu (Tao and Lu, 2009) and Cu–Al alloy (Qu et al., 2009). These hierarchical nanotwins are beneficial to enhance simultaneously the strength and ductility in the fcc polycrystalline metals. Interestingly, the secondary and tertiary nanotwins have been observed in TWIP steels during the process of SMATs and tensile test. These hierarchical nanotwins are supposed to be the essential factor for the achievement of high strength in TWIP steels (Kou, 2011). More recently, Wei et al. (2014) observed the gradient hierarchical nanotwins during tensile testing in pre-torsioned TWIP steel, and they demonstrated that such kind graded nanotwinned structures can lead to a pronounced improvement of strength with no reduction of ductility. From this perspective, understanding the relationship between the hierarchical twins and the mechanical properties becomes significantly important in achieving high strength and high ductility by designing the microstructures of the hierarchically nanotwinned fcc metals.

The deformation mechanism in nanotwinned fcc metals has been well studied in the recent years. The molecular dynamic (MD) simulations offer the possibility, through the theoretical analysis in the atomic scale, to quantify the contributions to the strength, strain hardening, and toughness of the twin boundaries (TBs). The dislocation–TB interactions have been confirmed initially via MD simulations (Jin et al., 2006; Wang and Huang, 2006) to be the underling mechanism for the reinforced mechanical properties in nanotwinned fcc metal. The pinning effect of TBs on dislocations, for example, the slip arresting in the form of Lomer–Cottrell locking at the twin boundaries, induces the increasing yield stress in nanotwinned copper (Afanasyev and Sansoz, 2007; Zheng et al., 2009). The TBs, acting as the additional sources under further deformation, could also lead to an increase in strain hardening (Froseth et al., 2004, 2005; Cao et al., 2007; Jin et al., 2008). For the high ductility in nanocrystalline copper, Zhu et al. (2007) indicated that the gradual loss of coherence of TBs during deformation gives rise to the high ductility of nanotwinned copper. For experimental observations of softening and detwinning in nanotwinned metals (Lu et al., 2009a, 2009b, 2009c; Li et al., 2011a, 2011b), the large-scale MD simulations have been performed to demonstrate that the activities of twinning partial dislocations dominate the softening and detwinning behaviors (Wang et al., 2010; Li et al., 2010), and the nucleation of these partials at TB–GB intersections could lead to the reduction in yield strength. The plastic anisotropy and associated deformation mechanism are also investigated by MD simulations in columnar-grained copper with nanoscale twins (You et al., 2013). More recently, MD simulations have been performed to provide the evidence for forming V-shaped and T-shaped double twins: GB-mediated intersecting mechanism and self-partial-multiplication twinning mechanism (Yuan and Wu, 2013a). Moreover, a series of large-scale MD simulations also have been carried out to investigate size effects and corresponding deformation mechanisms in hierarchically nanotwinned fcc metals as well as the atomistic scale fracture behaviors (Yuan and Wu, 2013b, 2013c).

Besides the atomic simulations, the mechanism-based theoretical models with a continuum description have been presented to describe the mechanical behaviors in the nanotwinned metal. Two- and three-dimensional crystal plasticity models for nanotwinned copper were developed to simulate the stress–strain response by finite element method as well as to estimate the tensile ductility through a failure criterion (Dao et al., 2006; Jerusalem et al., 2008). These models account for the strong plastic anisotropy and rate-sensitivity anisotropy originated from the presence of the TBs, but the softening behavior has not been considered in their simulations. Through incorporating the softening mechanism, a discrete twin crystal plasticity model was established with a focus on modeling the strengthening–softening yield transition in nanotwinned copper (Mirkhani and Joshi, 2011). This model could qualitatively capture the experimental results in the transition of yield strength with decreasing the twin spacing of nanotwinned copper. As pointed out by the large scale MD simulations (Li et al., 2010), the critical twin spacing for the transition of yield strength is sensitive to the grain size. With the aid of analyzing the competitive plastic deformation mechanism between the strengthening mechanism by inclined