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On tension–compression asymmetry in ultrafine-grained and nanocrystalline metals

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ABSTRACT

We present a physically motivated computational study explaining the tension/compression (T/C) asymmetry phenomenon in nanocrystalline (nc) and ultrafine-grained (ufg) face centered cubic (fcc) metals utilizing a variational constitutive model where the nc-metal is modeled as a two-phase material consisting of a grain interior phase and a grain boundary affected zone (GBAZ). We show that the existence of voids and their growth in GBAZ renders the material pressure sensitivity due to porous plasticity and that the utilized model provides a physically sound mechanism to capture the experimentally observed T/C asymmetry in nc- and ufg-metals.

1. Introduction

Nanocrystalline (nc) and ultrafine-grained (ufg) face centered cubic (fcc) metals have normally average grain sizes $d < 100$ nm and 100 nm $< d <$ 1 μm, respectively. Owing to a large volume fraction of grain boundary atoms, these metals are known to posses several distinct features when compared to traditional coarse-grained polycrystals. These include high strength and fatigue resistance, low ductility, pronounced rate dependence, tension–compression asymmetry and susceptibility to plastic instability. Therefore, these materials have become the subject of intense research over the past two decades (see recent review articles [9,17,18,23,40]). Despite these extensive research efforts, there are still some points of debate about their properties and operative deformation mechanisms due to the fact that alternative synthesis techniques may produce substantially different microstructures with unique processing-induced defects [9,21,34,43]. Furthermore, extremely small grain sizes result in additional experimental difficulties that are absent in coarse-grained polycrystals [36]. However, the following aspects of nc- and ufg-fcc metals seem to be well agreed upon [7,9,18,23,40]: (i) Dislocation mediated crystal plasticity in the grain interiors and inelastic deformation mechanisms, i.e., atomic shuffling, grain boundary diffusion and sliding, in the GBAZ are two competing deformation mechanisms. (ii) Dislocations are emitted from grain boundaries which act also as sinks for dislocations. (iii) As the grain size decreases, strain rate dependence and tension/compression (T/C) asymmetry increase.

T/C asymmetry in strength, i.e., having higher strength undergoing compression in comparison to tension, is not observed in coarse grained metals. However, nc- and ufg-single phase metals [30,31,42] and alloys [4,5,12,14] exhibit this behavior. Carsley et al. [4,5] investigated the mechanical behavior of a bulk ufg-Fe–10%Cu alloy (for grain sizes ranging from 45 nm to 1.7 μm) prepared by ball milling of powders followed by hot isostatic pressing. They observed a pressure-sensitive yielding behavior where the compressive yield strength is 30% higher than the tensile one. Almost an ideal plastic behavior that leads to localized shear banding was reported under both loadings. As a result of the pressure dependence of the yield strength, the orientation of shear band planes under compression and tension were different and neither of them coincided with the plane of maximum shear stress. Hayes et al. [14] studied the mechanical behavior of ufg-Al–10Ti–2Cu (bimodal grain size distribution with $d \sim 150$ nm) prepared by cryomilling at temperatures from room temperature up to 798 K. The room temperature compressive yield strength was quoted as 22% higher than the tensile yield strength. Yu et al. [42] conducted tests on ufg-Al ($d \sim 350$–750 nm) produced by an equal channel angular extrusion at room temperature and 77 K. It was reported that the yield strength is about 20% higher in compression than in tension for 350 nm $< d <$ 750 nm, and the T/C asymmetry disappears as the grain size further increases. Schuster et al. [31] conducted micro-compression tests on electrodeposited nc-Ni ($d \sim 29$ nm). The compressive flow stress value was found to be 16% higher than

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the tensile value reported in [35] for the same batch of material. Fan et al. [12] tested Ni–18%Fe alloys ($d \sim 23$ nm) and reported ultimate strength that is 25% higher in compression than in tension.

In addition to experimental observations, molecular dynamics simulations [19,20,25] predict a similar T/C asymmetry of the flow stress as well. Lund at al. [19] performed static atomistic simulations of nc-Ni for extremely small grain sizes of 2 nm < d < 4 nm (near the amorphous limit), where the nc-material exhibits the inverse Hall–Petch (H–P) behavior, i.e., loss of strength with grain size refinement. The T/C strength differential was found to be in the order of 30%. The authors found similarities between the deformation behavior of the GBs and shear transformation zones observed in pressure sensitive amorphous metallic glasses. Thus, the T/C asymmetry was associated to the pressure-dependent deformation mechanisms in the GBs, e.g. atomic shuffling, grain boundary sliding and void growth. Lund and Schuh [20] extended their previous work in [19] and performed static molecular simulations of biaxial deformations of nc-Ni in addition to uniaxial tests. It was shown that the macroscopic yield surfaces of purely deviatoric phenomenological von Mises and Tresca models cannot capture the biaxial yield surface generated by the molecular dynamics simulations. Dongare et al. [11] used large-scale molecular dynamics simulations to understand macroscopic yielding mechanisms in nc-Cu (d = 6 nm) at very high strain rates. Molecular dynamics simulations predicted an asymmetry around 6–8% in the tensile and compressive flow stress values. The strength of the T/C asymmetry was found to increase with increasing loading rate. Biaxial loading cases suggested that the yield surface can be represented by a von Misses ellipse, however, the center of the ellipse deviates slightly from the origin due to the T/C asymmetry. Monk and Farkas [25] investigated size effects in nc-Ni nanowires using molecular dynamics at very high loading rates. Tensile and compressive tests were performed for nanowires having radii in the range of 5–18 nm, and a grain size of 10 nm. The T/C asymmetry was found to be dependent on the wire radius such that the wires are stronger in compression than in tension and the difference decreases for wires having smaller radii. It was observed that grain boundary sliding is easier and therefore there are less dislocations emitted in tension than in compression. For the smallest radius tested, a reversal in the T/C asymmetry was observed, i.e., the tensile strength of nc-wire was stronger than the compressive one. In other words, as the wire radius gets very small the effect of free surfaces increases and the behavior becomes similar to single crystalline nanowires, see e.g. Diao et al. [10] for T/C asymmetry in single crystalline gold nanowires. Apart from atomistic simulations, there have been continuum scale models [7,15,37,38,44] that are able to describe the T/C asymmetry. Cheng et al. [7] proposed a simple model that predicts the strength as a function of grain size and captures the T/C asymmetry. They assumed that the main plastic deformation mechanism is the dislocation emission from the GBs and employed the pressure-dependent dislocation self-energy of Jung [16] during bow-out of dislocations from a GB. Jiang and Weng [15] developed a composite model based on a generalized self-consistent scheme for nc-materials. They employed a grain size dependent plasticity model for grain interiors and a pressure-dependent Drucker-type plasticity model for the GB phase. The model was able to capture the T/C asymmetry through the pressure dependence of the GB phase. Wei et al. [38] developed a rate-dependent amorphous plasticity model, which accounts for cavitation and related failure phenomena, to represent the GB response. The grain interiors were simulated by using a continuum crystal-plasticity model in which the slip system resistances were assumed to be inversely proportional to the grain size. The employed crystal-plasticity model was based on [1,45], which accounted for the transition from partial to complete dislocations depending on a critical grain size. Also, the inverse Hall–Petch behavior, a marked rate dependency and a T/C asymmetry were predicted. Zhou et al. [44] proposed a constitutive model in which, different from two-phase approaches, nc-materials were treated as an integral object sustaining dislocation movements, diffusion and GB sliding. The T/C asymmetry was modeled by assuming different phenomenological evolution laws for the total defect area in tension and compression. Wei and Anand [37] formulated an isotropic, rate-dependent elastoplastic model for powder-consolidated nc-materials in which the plastic flow was taken to be pressure-dependent. The plastic flow was assumed to arise from shear- and cavitation-dominated contributions. It was shown that the proposed model was able to predict the T/C asymmetry in nc-Mg-based alloys.

In this article we briefly outline the model proposed by Gürses and El Sayed [13] and study the T/C asymmetry in nc- and ufg-Cu. In this model, the nc-material is treated as a two-phase material consisting of a grain interior phase and a grain boundary affected zone (GBAZ). A crystal-plasticity model which accounts for the transition from partial dislocation to full dislocation mediated plasticity is employed for the grain interior, whereas an isotropic porous plasticity model is employed to describe the GBAZ. The porous plasticity model responds to volumetric expansion and compression differently as a consequence of the void growth mechanism. It is shown that the pressure sensitivity of the porous plasticity model provides a physically sound mechanism to capture the experimentally observed T/C asymmetry.

2. Model description

Let $\mathbf{F}$ with $J = \det \mathbf{F} > 0$ be the deformation gradient and the Jacobian, respectively. In what follows we consider the classical multiplicative decomposition of the deformation gradient $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$ into an elastic part $\mathbf{F}^e$ and a plastic part $\mathbf{F}^p$. Treating a particular grain as a composite material consisting of a grain interior phase and a GBAZ [32], the free energy function can be written in a simple volume average form

$$W = \xi W_{gi} + (1-\xi) W_{gb}, \tag{1}$$

where ξ is the volume fraction of the grain core region, W_{gi} and W_{gb} denote the free energies of the grain interior and boundary phases, respectively. The average first Piola–Kirchhoff stress $\mathbf{P}$ reads similarly $\mathbf{P} = \xi\mathbf{P}_{gi} + (1-\xi)\,\mathbf{P}_{gb}$. The volume average stress $\mathbf{P}$, the grain interior stress $\mathbf{P}_{gi}$ and the grain boundary stress $\mathbf{P}_{gb}$ are computed from Coleman's relations by evaluating the partial derivatives of W, W_{gi} and W_{gb} with respect to $\mathbf{F}$. Assuming cubical grains [6] and a constant thickness d_{gb} of GBAZ, the volume fraction is computed as

$$\xi = (d - d_{gb})^3/d^3. \tag{2}$$

Following Weinberg et al. [39] the plastic deformation rate for GBAZ is assumed to be

$$\dot{\mathbf{F}}^p_{gb}\mathbf{F}^{p-1}_{gb} = \dot{\epsilon}^p\mathbf{M} + \dot{\theta}^p\mathbf{N}, \tag{3}$$

where multipliers $\dot{\epsilon}^p$ and $\dot{\theta}^p$ are subject to irreversibility constraints. $\mathbf{M}$ and $\mathbf{N}$ are the directions of the deviatoric and volumetric plastic deformation rates, respectively. The free energy is assumed to have an additive structure

$$W_{gb}(\mathbf{F}, \mathbf{F}^p_{gb}, \epsilon^p, \theta^p) = W^e_{gb}(\mathbf{F}^e_{gb}) + W^p_{gb}(\epsilon^p, \theta^p), \tag{4}$$

where $W^e_{gb}(\mathbf{F}^e_{gb})$ and $W^p_{gb}(\epsilon^p, \theta^p)$ are the elastic and plastic stored energy densities, respectively. Material frame indifference requires that W^e_{gb} has to depend on $\mathbf{F}^e_{gb} = \mathbf{F}\mathbf{F}^{p-1}_{gb}$ through the elastic right Cauchy–Green tensor $\mathbf{C}^e_{gb} = \mathbf{F}^{eT}_{gb}\mathbf{F}^e_{gb}$. In order to incorporate a logarithmic