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Gradient plasticity in gradient nano-grained metals

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ABSTRACT

Gradient nano-grained (GNG) metals are a unique class of materials with spatial gradients in grain size, typically from the surface to the bulk. Here the gradient mechanical behavior in GNG copper is studied by a crystal plasticity finite element model that accounts for grain-size-dependent yield strengths. The associated finite element simulations reveal both the gradient stress and gradient plastic strain in the cross section of GNG copper subjected to axial tension. These spatial gradients arise due to progressive yielding of gradient grains under an overall uniform deformation. They stand in stark contrast to the widely studied strain gradient plasticity induced by imposing a non-uniform deformation such as torsion, bending, and indentation. Our work suggests a new material strengthening mechanism through the introduction of plastic strain gradients via gradient microstructures.

1. Introduction

Gradient nano-grained (GNG) metals are a new class of materials with unique polycrystalline microstructures [1,2]. Their grain sizes typically change with a gradient variation between tens to hundreds of nanometers, from the surface to the bulk. GNG metals promise to achieve an unprecedented combination of strength, ductility and toughness. They have great potential in engineering applications [1–6] and also motivate exploration on various other kinds of gradient nanostructured materials [7–10].

Experiments have been performed to process the GNG metals and further study their mechanical behavior. Fang et al. [1] utilized surface mechanical grinding treatment to prepare a GNG surface layer in a bulk coarse-grained (CG) rod of face-centered cubic (FCC) Cu. The topmost layer of the GNG structure, up to a depth of 60 μm, consisted of nano-grains with an average grain size of about 20 nm. The grain size gradually increased to about 300 nm in the depth of 60 μm–150 μm. Below the depth of 150μm, the grain size continued to increase to that of coarse grains at the micrometer scale. The tensile yield strength of the GNG/CG Cu was two times that of CG Cu, and the yield strength of the free-standing GNG foil was ten times that of CG Cu. Recently, Wu et al. [5] used surface mechanical attrition treatment to prepare GNG samples of body-centered cubic (BCC) steel with a sandwich sheet structure, i.e., a CG core in between two GNG layers. The tensile tests showed that the gradient structure induced an extra strain hardening, which led to a high ductility. This extra strain hardening was attributed to the effects of the macroscopic strain gradients associated with multi-axial stress states in GNG structures.

The experiments described above have shown the enhanced mechanical properties of GNG metals. However, the detailed mechanisms underlying the observed mechanical behavior of GNG metals remain little understood [11–13]. In this letter, we employ a crystal plasticity

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finite element (CPFE) model to investigate the mechanical responses of GNG Cu. We build a GNG structure by adapting the conventional Voronoi tessellation method [14]. We also extend the classical crystal plasticity theory to incorporate the grain-size-dependent constitutive relations. The associated finite element simulations reveal a novel type of gradient stress and gradient plastic strain in the cross section of GNG samples subjected to axial tension. These spatial gradients arise due to progressive yielding of gradient grains under an overall uniform deformation. They stand in stark contrast to the widely studied strain gradient plasticity induced by imposing non-uniform deformations. Our work has important implications for material strengthening through the introduction of plastic strain gradients via gradient microstructures.

2. Modeling methods

2.1. Grain-size-dependent crystal plasticity theory

To model the constitutive response of GNG Cu, we extend the classical crystal plasticity theory by incorporating the grain size dependence of yield strength. The rate-dependent finite strain crystal plasticity theory adopted here can be traced to the work by Rice [15], Asaro and Rice [16], and Kalidindi et al. [17]. According to Kalidindi et al. [17], the plastic shearing rate on the slip system α is

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_o \left| \frac{\tau^{\alpha}}{s^{\alpha}} \right|^{1/m} \operatorname{sign}(\tau^{\alpha}) \tag{1}$$

where τ^{α} is the resolved shear stress, s^{α} is the slip resistance, $\dot{\gamma}_o$ is the reference shearing rate, and m is the strain rate sensitivity parameter. The initial value of s^{α} is denoted as s_0. During plastic deformation, the slip resistance s^{α} evolves according to

$$\dot{s} = \sum_{\beta} h^{\alpha\beta} \left| \dot{\gamma}^{\beta} \right|, \quad h^{\alpha\beta} = q^{\alpha\beta} h^{(\beta)},$$
$$h^{(\beta)} = h_0 \left(1 - s^{\beta}/s_{\text{sat}}\right)^{a} \tag{2}$$

where $q^{\alpha\beta}$ are the components of a matrix which describes the latent hardening behavior of the crystal, and h_0, a and s_{sat} are the hardening parameters taken to be identical for all slip systems.

Our crystal plasticity model is dependent on grain size. For each grain, the slip resistance parameters, including $\{s_0,\ h_0,\ a,\ s_{\text{sat}},\ m\}$, are taken as functions of grain size [18,19]. According to the classical Hall–Petch relation, the overall yield strength is inversely proportional to the square root of grain size [20,21]; such a relation is valid for grain sizes greater than ~20 nm [22,23]. In this work, we assume that all the slip resistance parameters at the single crystal level are inversely proportional to the square root of the size of the local grain D,

$$\{s_0(D), h_0(D), a(D), s_{\text{sat}}(D), m(D)\} \sim D^{-1/2}. \tag{3}$$

The numerical values of grain-size-dependent s_0 are readily estimated from the available experimental data in the literature, but the determination of the strain hardening related parameters $\{h_0,\ a,\ s_{\text{sat}}\}$ requires certain assumptions. Specifically, the values of s_0 are determined based on the experimentally measured yield stresses of nanocrystalline Cu with uniform grain size, i.e., from 860 MPa to 400 MPa for D from 20 nm to 110 nm [24–26]. Dividing these macroscopic yield stresses by Taylor's factor of 3, we estimate s_0 in between 286 MPa and 133 MPa. Nanocrystalline Cu exhibits little hardening in experiments. However, we assign small values of $\{h_0,\ a,\ s_{\text{sat}}\}$, so as to produce a weak hardening for ensuring numerical stability in CPFE simulations. For the 20 nm grain, we take $h_0 = 102$ MPa, $a = 2.0$, $s_{\text{sat}} = 600$ MPa; and for the 110 nm grain, $h_0 = 48$ MPa, $a = 1.8$, $s_{\text{sat}} = 287$ MPa. Furthermore, experiments show that the strain rate sensitivity exponent m of nanocrystalline Cu with uniform grain size varies from 0.04 to 0.022 for D from 20 nm to 110 nm [27,28]. To evaluate s_0 for intermediate grain sizes, we use the above bounding values to fit the formula of $s_0 = B + C \cdot D^{-1/2}$ where B and C are the fitting constants. Along the same line, we also fit other slip resistance parameters of $\{h_0,\ a,\ s_{\text{sat}},\ m\}$ for intermediate grain sizes. The following fitting formulas are obtained:

$$\begin{aligned} s_0(\text{MPa}) &= 19.3 + 1196 \cdot D^{-1/2}, \\ h_0(\text{MPa}) &= 8.68 + 415.8 \cdot D^{-1/2}, \\ a &= 1.65 + 1.56 \cdot D^{-1/2}, \\ s_{\text{sat}}(\text{MPa}) &= 53.7 + 2443 \cdot D^{-1/2}, \\ m &= 0.0086 + 0.1403 \cdot D^{-1/2}. \end{aligned} \tag{4}$$

Other material properties, including elastic constants $(C_{11},\ C_{12},\ C_{44})$, twelve $\{111\}\langle 110\rangle$ slip systems, and the latent hardening matrix $\left\{q^{\alpha\beta}\right\}$, are assumed to be independent of grain size. For FCC Cu, we take $C_{11} = 170$ GPa, $C_{12} = 124$ GPa and $C_{44} = 75$ GPa; $q^{\alpha\beta} = 1.0$ if the slip systems α and β are coplanar and $q^{\alpha\beta} = 1.4$ if they are non-coplanar [17].

2.2. Finite element model

We construct a two-dimensional GNG structure with columnar grains by adapting the Voronoi tessellation method in Matlab. The geometrical information of the GNG structure is then used to develop the corresponding finite element model in ABAQUS/CAE with a Python script. Fig. 1 shows an example of the GNG structure generated in ABAQUS/CAE. In this case, the grain size D increases linearly from ~20 nm in the top/bottom surface layer to ~110 nm in the central region. The overall sample geometry is 640 nm in length and 1120 nm in width. As such, the spatial gradient in grain size, $|dD/dy|$, is about 0.1. The orientation of grains is assigned randomly in terms of three Euler angles, $\{\theta,\ \varphi,\ \Omega\}$, representing rotations from the crystal basis to the global basis [17]. The sample is meshed with the non-structured plane strain elements. As a result, most elements have four nodes (CPE4R) and a small fraction three nodes (CPE3). Displacements and tractions are continuous at grain boundaries, meaning no separation or sliding between every pair of adjoining grains. A user material subroutine VUMAT [29] is developed in ABAQUS/EXPLICIT to implement the grain-size-dependent crystal plasticity model described above. All the slip

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