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Grain rotations during uniaxial deformation of gradient nano-grained metals using crystal plasticity finite element simulations

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ABSTRACT

Gradient nano-grained (GNG) metals have great application potential due to its outstanding performance in both strength and ductility. In this paper, we investigate the uniaxial deformation response of GNG Cu utilizing the developed size-dependent crystal plasticity model with random initial grain lattice orientation implemented by the user-material subroutine of ABAQUS. The results show that the grain size gradient leads to gradient distribution of stress and strain, consistent with the results in the literature. In addition, the Lode parameter also shows a gradient distribution with the value closer to zero at the small-grained surface regions. Importantly, we discover that the magnitude of grain rotation strongly depends on the initial lattice orientation of the grain, but does not depend on the grain size in the current crystal plasticity finite element framework. Furthermore, we gave a reasonable explanation for the distribution of grain rotation magnitudes. Our study provides insights into the outstanding mechanical properties of GNG metals and the evolution of texture.

1. Introduction

Gradient nano-grained materials are defined by the spatially distributed grain size that varies gradually from tens of nanometers in the top layer to micrometers in the bulk. GNG metals can be prepared by introducing significant plastic deformation to the surface which produces a large number of staggered dislocations to divide coarse grains (CGs) into fine grains. Such methods include but are not limited to grinding or rolling the surface [1,2] and impacting the surface by severe shot peening [3–5]. GNG metals possess advanced mechanical properties combining high strength with satisfactory ductility [6–9] which manifest its great application prospects. According to Fang et al. [6], introducing a GNG coating to CG Cu can double its yield strength, while at the same time does not compromise its tensile plasticity. This advantage just distinguished GNG metals from the classic nanocrystalline metals which are very strong but brittle. Other remarkable material properties of GNG metals, including significant hardness and excellent fatigue resistance, have also been revealed in many experiments [10,11].

A number of efforts have been devoted to exploring the mechanisms underlying the peculiar properties of GNG metals. On the basis of the experiment, Fang et al. [6] advocated that the outstanding tensile plasticity of GNG materials was attributed to mechanically driven grain boundary migration. Wu et al. [9] proposed that the extra strain hardening resulting from enhanced dislocation activities could explain why the GNG structures possess high ductility. He also pointed out that the gradient grain size distribution could give rise to a macroscopic strain gradient. Some researchers investigate the mechanical responses of the GNG metals utilizing the crystal plasticity finite element method (CPFEM) [12] which is effective over a wide range of length scales. There are two approaches of CPFEM in terms of the constitutive description of strain hardening, i.e., physics-based approach and phenomenological approach. Physics-based constitutive models [13] investigate grain size dependence by introducing geometrically necessary dislocations [14–16] which are necessary in describing the non-uniform plastic deformation [17]. Ma et al. [18] succeeded in implementing the physics-based model into the finite element codes to simultaneously simulate the geometrically necessary dislocations and statistically stored dislocations and therein demonstrate the size dependence. Li and Soh [19] also studied the mechanical response of the GNG/CG materials based on the evolution of dislocation density. The advantage of their model is that it takes into account the grain growth [6] and the decreasing hardening with grain refinement [20]. The above physics-based constitutive models describe work hardening of the crystal based on dislocation evolution (Lin et al. [21]; Sluys and Estrin [22]), while the phenomenological constitutive models [13] describe the hardening laws from the viewpoint of the resolved shear stress. Efforts in phenomenological CPFEM approach include the work by Peirce et al. [23], Bassani and Wu [24], Kalidindi et al. [25], etc. To investigate the effect of grain size gradient on the stress and strain distribution [9], some authors

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(e.g., Gürses and Sayed [26], Zeng et al. [27]) try to incorporate the grain size dependence into the hardening laws. They successfully predict the non-uniform distribution of the stress and strain in GNG metals.

In addition, the change of grain lattice orientation can be calculated using CPFEM. Bearing in mind that the mechanical properties of the crystalline metals are also dependent on the grain lattice orientations, it is important to study how the grains of GNG structures rotate under uniaxial stretching. Several authors have investigated the grain rotation during the plastic deformation of metals. For example, Wroński and Wierzbanowski [28] predicted the texture formation from the change of lattice orientation which was attributed to the gliding on slip systems. Chen et al. [29] developed a finite element algorithm to simulate the texture evolution during metal rolling. The lattice rotation in their work was described by three Euler angles. In fact, the driving force for grain rotation comes from several mechanisms, e.g., mass diffusion through lattice, mass diffusion along grain boundary, grain boundary sliding, grain boundary migration, etc. The crystal plasticity based on dislocation slip is one of the major reasons that cause grain rotation. In spite of the existing work in the literature, research on grain rotation due to crystal plasticity is not sufficient, especially for the GNG materials.

In this paper, we first incorporate the grain size dependence into the hardening law, and simulate the tensile response of the GNG Cu using the finite element code ABAQUS/standard via a user material subroutine UMAT [30]. Specifically, the lattice orientations are introduced as state variables, and are updated every time the subroutine UMAT is called. We investigate the grain rotations and propose a reasonable grain rotation law, which well explains the distribution of grain rotation magnitudes in the CPFEM simulations.

2. Model description

2.1. Size-dependent crystal plasticity theory

According to the classic crystal plasticity theory [23], a simple power law was used to describe the relationship between the shearing rate $\dot{\gamma}^{(\alpha)}$ and the resolved shear stress $\tau^{(\alpha)}$ on αth slip system.

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^{\frac{1}{m}} sign\left(\tau^{(\alpha)}\right) \tag{1}$$

Where $\dot{\gamma}_0$ is the reference strain rate, m is the rate sensitivity exponent, and $g^{(\alpha)}$ is the current strength on slip system α, which has the evolution law:

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta}\ \dot{\gamma}^{(\beta)} \tag{2}$$

$$h_{\alpha\alpha} = h(\gamma) = h_0 \sec h^2 \left| \frac{h_0}{\tau_s - \tau_0}\gamma \right| \quad (no\ sum\ on\ \alpha) \tag{3}$$

$$\gamma = \sum_{\alpha} \int_0^t \left|\dot{\gamma}^{(\alpha)}\right|\ dt \tag{4}$$

$$h_{\alpha\beta} = qh(\gamma) \qquad (\alpha \neq \beta) \tag{5}$$

Where, $h_{\alpha\beta}$ $(\alpha, \beta = 1, 2, \ldots, 12)$ are the slip hardening moduli. h_0, τ_s *and* τ_0 are the initial hardening modulus, the saturation value of resolved shear stress and the yield stress, respectively. q is the latent hardening coefficient.

According to the work by Kim and Estrin [31], and Iyer et al. [32], the hardening rate of nc-materials increases with increasing grain size, which means that slip hardening moduli increases with increasing grain size. Considering the Hall–Petch relationship [33,34], and following literature [26], we incorporate the grain size dependence into crystal plasticity by modifying Eq. (3) as:

$$h_{\alpha\alpha} = h(\gamma, D) = h_0 \left(\frac{D}{d_0}\right)^{\frac{1}{2}} \sec h^2 \left| \frac{h_0 \left(\frac{D}{d_0}\right)^{\frac{1}{2}}}{\tau_s - \tau_0}\gamma \right| \tag{6}$$

Where D is the grain size, d_0 is its reference value.

Furthermore, we assume that parameters related to hardening, i.e., h_0, τ_s , τ_0, m, are subjected to Hall–Petch relationship, namely that these parameters are inversely proportional to square-root of grain size. The detailed relation between rate sensitivity exponent m and grain size D is determined by experimental data in literature [35] which indicate m varying from 0.046 to 0.0223 as D varying from 20 nm to 120 nm. The fitted function is given as:

$$m = 0.006 + 0.1788D^{-0.5} \tag{7}$$

According to [27], the yield stress varies from 860 MPa to 392 MPa as grain size increases from 20 nm to 120 nm. Dividing the Taylor's factor by 3, we can therefore obtain:

$$\tau_0 = 23.7 + 1173D^{-0.5} \tag{8}$$

For simplicity, here we assume that h_0 and τ_s are proportional to the yield stress τ_0:

$$h_0 = \xi\tau_0, \quad \tau_s = \eta\tau_0 \tag{9}$$

Where ξ and η are constant coefficients. Following literature [23], ξ is set to 8.9, and η is equal to 1.8 for different grain sizes.

2.2. Finite element model

Fig. 1 shows the two-dimensional computational sample of the gradient nano-grained (GNG) structure with columnar grains. It was constructed by utilizing the Voronoi tessellation function in software MATLAB. Then, the finite element (FE) model was established by developing a PYTHON script and incorporating it into the generalized FE codes ABAQUS using ABAQUS/PYTHON interface. As shown in Fig. 1, the grain size gradually increases from 20 nm at the upper and bottom surfaces to 120 nm in the middle along y direction. The overall finite element model contains 811 grains. It is worth noting that the thickness of grain boundary is assumed as

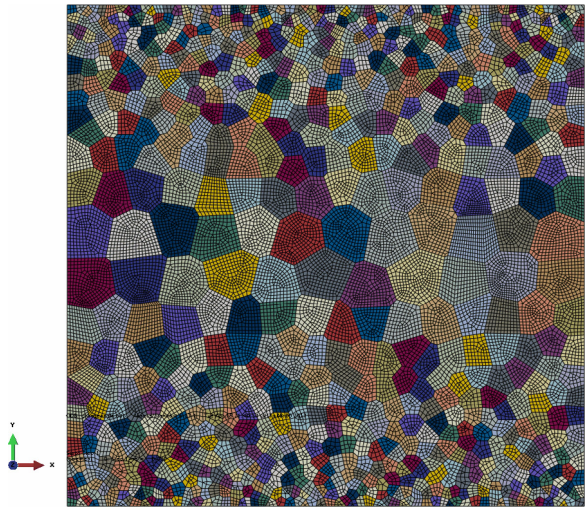

Fig. 1. Finite element model of GNG Cu.