MODELING OF NANOCRYSTALLINE METALS BASED ON COMPETING GRAIN BOUNDARY AND GRAIN INTERIOR DEFORMATION MECHANISMS

Ercan Gürses*a), Tamer El Sayed**
*Department of Aerospace Engineering, Middle East Technical University, Ankara, 06800, Turkey
**Computational Solid Mechanics Laboratory, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Summary Nanocrystalline (NC) materials, because of their distinct features have become the subject of intense research over the past two decades. Owing to a large volume fraction of grain boundary (GB) atoms, the deformation mechanisms in NC-metals are different from traditional coarse grained polycrystals. Indeed, there are several inelastic deformation mechanisms, e.g., GB-diffusion, GB-sliding, dislocations, grain rotation, grain growth, that can be simultaneously operative in NC-metals. In this work, a viscoplastic constitutive model that is based on competing GB and grain interior deformation mechanisms is presented. The model extends a former work with respect to four aspects: (i) the pressure dependence of the GB-diffusivity, (ii) the normal stress dependence of the GB-sliding, (iii) both the partial and full dislocation emissions from GBs and (iv) a more general lognormal grain size distributions instead of a Rayleigh distribution. The model is able to predict the inverse Hall-Petch effect, to capture the enhanced rate-sensitivity and to demonstrate the tension/compression-asymmetry.

MODEL DESCRIPTION

NC metals, because of their distinct features, e.g., high strength, low ductility, pronounced rate dependence, tension-compression asymmetry and susceptibility to plastic instability, have become the subject of intense research over the past two decades [1, 2]. Owing to a large volume fraction of grain boundary (GB) atoms, the deformation mechanisms in NC-metals are different from traditional coarse grained polycrystals. Indeed, there are several inelastic deformation mechanisms, e.g., GB-diffusion, GB-sliding, dislocations, grain rotation, grain growth and GB-migration, that can be simultaneously operative in NC-metals. In this work, a viscoplastic constitutive model that is based on competing GB and grain interior deformation mechanisms is presented. The model extends the work by Wei and Gao [3] with respect to four aspects. These are considerations of (i) the pressure dependence of the GB-diffusivity, (ii) the normal stress dependence of the GB-sliding, (iii) both the partial and full dislocation emissions from GBs and finally (iv) a more general lognormal grain size distributions instead of a Rayleigh distribution. As a result of first two points, the model proposed in this work is able to demonstrate the tension/compression-asymmetry in an agreement with experimental observations and molecular dynamics simulations.

GB-diffusion, GB-sliding, and the grain interior dislocation-mediated-plasticity are the three different types of deformation mechanisms that are assumed to be operative in this work. The first two micro-mechanisms are GB-based, whereas the last one is related with the grain interior. The inelastic strain rate due to GB-diffusion is given by the Coble creep

$$\dot{\varepsilon}_{gbd}(d,\sigma,\theta) = \frac{47\sigma\Omega_a}{k_b\theta}\frac{\delta D_{gb}(\theta,p)}{d^3} , \tag{1}$$

where Ω_a is the atomic volume, δ is the GB-thickness, $D_{gb}(\theta,p)$ is the temperature and pressure-dependent GB-diffusivity, d is the grain size, σ is the stress, θ is the temperature, p is the pressure, k_b and R are the gas constant and the Boltzmann constant, respectively. The GB-diffusivity is

$$D_{gb}(\theta,p) = D_{0,gb}\exp\left(-\frac{Q_{gb}-p\Delta V}{R\theta}\right) , \tag{2}$$

where Q_{gb} is the activation energy for the GB-diffusion, $D_{0,gb}$ is a pre-exponential multiplier and ΔV is the activation volume. The inelastic strain rate due to the collective response of GB-sliding was given by Conrad and Narayan [4] as

$$\dot{\varepsilon}_{gbs}(d,\sigma,\theta) = \frac{6b\nu_d}{d}\sinh\left(\frac{\Omega_a\tau_e(\sigma)}{k_b\theta}\right)\exp\left(\frac{-\Delta F}{k_b\theta}\right) , \tag{3}$$

where ν_d is the Debye frequency of lattice vibration, b is the Burgers vector, ΔF is the Helmholtz free energy of activation and τ_e is the effective shear stress. τ_e depends on the normal traction acting on the GB through $\tau_e = (\sigma+\lambda\sigma_n)/\sqrt{3}$, where $\sigma_n = \mathrm{sign}(\sigma)\sigma$ is the normal traction and λ is a material parameter. The plastic strain rate due to collective behavior of dislocations is given as [3]

$$\dot{\varepsilon}_{gip}(d,\sigma,\theta) = \beta_0\nu_d\,\mathrm{sign}(\sigma)\exp\left(\frac{-\Delta G^*}{k_b\theta}\right)\exp\left(\frac{\tau^\alpha(\sigma)}{\tau^f}\right) . \tag{4}$$

Here, ΔG^* is the activation energy for dislocation emission, $\tau^\alpha \approx |\sigma|/\sqrt{3}$ is the slip resistance and τ^f is the stress required to activate dislocation emission from GBs. Different from the model proposed in [3], following the work [5],

a) Corresponding author. E-mail: gurses@metu.edu.tr

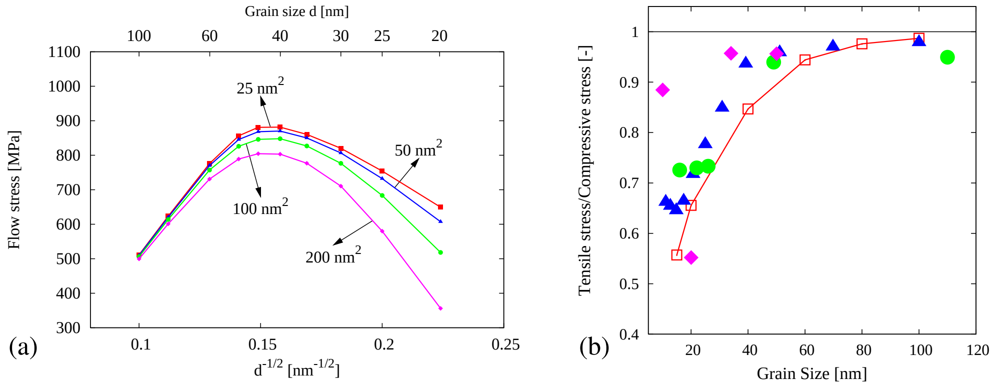

Figure 1. (a) Grain size dependence of tensile flow stress for polycrystals with different variances in their grain size distribution. (b) Ratio of tensile stress to compressive stress. Red solid line is the result of the model, whereas points are the predictions of the numerical models from the literature.

both the emission of partial and full dislocations from the GBs are considered here. Therefore, the stress required for the emission of a dislocation from the GB reads

$$\tau^f = \begin{cases} Gb/d & \text{for} \quad d > d_{cr} \\ Gb/(3d) + (d - \delta_{eq})\Gamma G/d & \text{for} \quad d < d_{cr} \end{cases} , \tag{5}$$

where G is the shear modulus and δ_{eq} is the equilibrium spacing of partial dislocations which can be approximated as $\delta_{eq} \approx \frac{1}{12\pi}\frac{b}{\Gamma}$ [5]. $\Gamma = \gamma_{sf}/Gb$ is the dimensionless reduced stacking fault energy where γ_{sf} is the intrinsic stacking fault energy. Below the critical grain size [6]

$$d_{cr} = \frac{2}{3}\frac{d}{d - \delta_{eq}}\frac{Gb^2}{\gamma_{sf}} \tag{6}$$

the emission of partial dislocations from GBs start instead of full dislocations. The macroscopic plastic strain rate is given as the sum of deformation mechanisms mentioned above, i.e., $\dot{\bar{\varepsilon}}^p(\sigma,\theta) = \dot{\bar{\varepsilon}}_{gbd}(\sigma,\theta) + \dot{\bar{\varepsilon}}_{gbs}(\sigma,\theta) + \dot{\bar{\varepsilon}}_{gip}(\sigma,\theta)$. The bar in previous equation describes an averaging of the local fields over the polycrystalline sample by using grain size distribution functions, i.e.

$$\dot{\bar{\varepsilon}}_\alpha(\sigma,\theta) = \frac{\int_0^\infty \dot{\varepsilon}_\alpha(d,\sigma,\theta)P(d)kd^3\mathrm{d}d}{\int_0^\infty P(d)kd^3\mathrm{d}d} \quad \text{where} \quad \alpha = gbd, gbs, gip \, , \tag{7}$$

where $P(d)$ denotes the grain size distribution function. A lognormal grain size distribution is employed here.

$$P_{log}(d) = \frac{1}{\sqrt{2\pi}\Sigma d}\exp\left(-\frac{1}{2}\left(\frac{\ln(d/d_0)}{\Sigma}\right)^2\right) , \tag{8}$$

where d_0 (standard deviation of $\ln(d)$) and Σ are parameters describing the shape of the distribution function. Further details of the model can be found in [7].

NUMERICAL RESULTS

Some results of the proposed model are shown in Fig. 1. The inverse Hall-Petch effect, i.e., loss of strength with grain size refinement, is successfully captured by the model as shown in Fig. 1a. The different curves in Fig. 1a correspond to lognormal grain size distributions with different variances. Furthermore, as shown in Fig. 1b, the model predicts a tension/compression-asymmetry in an agreement with experiments and molecular dynamics simulations. The red solid line is the prediction of the proposed model, while other points are results of various numerical models from the literature.

References

[1] M. Dao, L. Lu, R. J. Asaro, J. T. M. De Hosson, E. Ma: Toward a quantitative understanding of mechanical behavior of nanocrystalline metals, *Acta Materialia*, **55**:4041–4065, 2007.

[2] M. E. Meyers, A. Mishra, D. J. Benson: Mechanical properties of nanocrystalline materials, *Progress in Materials Science*, **51**:427–556, 2006.

[3] Y. Wei, H. Gao: An elastic-viscoplastic model of deformation in nanocrystalline metals based on coupled mechanisms in grain boundaries and grain interiors, *Materials Science and Engineering A*, **478**:16–25, 2008.

[4] H. Conrad, J. Narayan: On the grain size softening in nanocrystalline materials, *Scripta Materialia*, **42**:1025–1030, 2000.

[5] R. J. Asaro, P. Krysl, B. Kad: Deformation mechanism transitions in nanoscale fcc metals, *Philosophical Magazine Letters*, **83**:733–743, 2003.

[6] R. J. Asaro, S. Suresh, Mechanistic models for the activation volume and rate sensitivity in metals with nanocrystalline grains and nano-scale twins, *Acta Materialia* **53**:3369–3382, 2005.

[7] E. Gürses, T. El Sayed: A constitutive model of nanocrystalline metals based on competing grain boundary and grain interior deformation mechanisms, *Materials Letters*, **65**:3391–3395, 2011.