

A Micromechanical Study of the Effect of Grain Size and Strain Rate on the Yield Strength of Nanostructured Materials

Ricardo A. Lebensohn¹, Eduardo M. Bringa² and Alfredo Caro²

¹**Materials Science and Technology Division, MS G755, Los Alamos National Laboratory, MS 755, NM 87545, USA (lebenso@lanl.gov).**

²**Computational Material Sciences, P.O. Box 808, L-367, Lawrence Livermore National Laboratory, CA 94550, USA (ebringa@llnl.gov, caro2@llnl.gov).**

ABSTRACT

We present a micromechanical approach based on Fast Fourier Transforms to study the role played by dislocation glide and grain boundary (GB) accommodation in the determination of the plastic behavior of nanostructured materials. Under quasi-static conditions, assuming diffusion-controlled mechanisms at GB, the model predicts a strain-rate sensitivity increase in nanocrystalline samples with respect to the coarse-grained material of the same order as in recently published experiments.

1. Introduction

The yield strength of polycrystalline materials depends strongly on their grain size. For aggregates with grains in the micron range and above, the yield stress increases inversely with the square root of the grain size. At these grain sizes, the highly disordered GB regions represent only a negligible volume fraction of the material. On the contrary, when the grain dimensions approach nanometer sizes, the volume fraction of GBs become significant and the GB regions start to play an active role in accommodating deformation (e.g. [1]). Given the highly disordered character of the GB regions, the microscopic mechanisms associated with GB activity are intrinsically different from the ones associated with plastic deformation by dislocation motion that takes place in the bulk of the grains. A sound constitutive equation of GB deformation would not involve directionality, as it is indeed the case of the usual constitutive description of crystal plasticity. Also, due to the short range of the interactions involved in GB accommodation, the stress required to activate this mechanism should be essentially independent of the grain size of the aggregate [2]. Furthermore, the constitutive equations that describe dislocation glide in the bulk of the grains and accommodation at GBs will have, in general, different sensitivities to temperature and strain rate. A constitutive micromechanical model incorporating such sensitivities would be able to capture the interplay and competition between bulk and GB mechanisms for a particular topology of these nanostructured aggregates. Such a model could be used as a predictive tool to obtain the mechanical behavior of the aggregate, and its sensitivity to different deformation conditions and/or microstructural changes.

2- Model

In this work we report a new micromechanical formulation to study the effect of grain size, pressure and strain rate on the yield strength of fcc nanocrystalline materials. The proposed model is a full-field approximation that takes into account the actual topology of the aggregate consisting in bulk crystalline regions surrounded by a GB percolating phase. Both regions co-deform plastically according the following constitutive behaviors: a) for grain interiors: crystal viscoplasticity, with Hall-Petch grain size dependence; b) for grain boundaries: isotropic viscoplasticity with flow stress independent of grain size. The length-scale of the problem is given by the GB thickness, taken to be 1 nm. A very efficient approach based on the Fast Fourier Transform (FFT) algorithm is used to solve the mechanical problem (e.g. [3]). This FFT-based solution of a unit cell problem for a representative volume element (RVE) gives the local mechanical fields that develop inside heterogeneous materials in great detail. Periodic boundary conditions, required for this type of spectral approximation, are sufficient for the kind of parametric study that we want to perform. In the present case, the unit cell represents an aggregate of single crystal grains with prescribed orientations, surrounded by outer layers of percolating grain boundary regions. The particular orientation of each single crystal determines different anisotropic plastic properties from grain to grain, while, due to its intrinsic disordered character, the GBs are assumed to have a homogeneous isotropic behavior throughout the interconnected “GB phase”. A 3-D implementation of the FFT-based method requires to discretize a cubic unit cell using a regular grid of $N \times N \times N$ Fourier points (FPs). In this work we adopted $N=128$, resulting in 2097152 discretization points. Each FP belongs either to a grain interior, or to the GB phase. The dimensions of such Fourier grid are large enough such that each grain and the GB phase are represented by a large number of Fourier points. The length-scale associated with the RVE is determined by the GB thickness, taken to be 1 nm. In order to study the effect of grain size without interference of other microstructural characteristics (like crystallographic texture, or any particular orientation correlation between neighbor grains) four self-similar RVEs were generated of grain sizes 29, 15, 7 and 5 nm (for details, see [4]).

The local constitutive equation for a Fourier point \mathbf{x} belonging to a grain interior is given by the following power law for single crystal viscoplasticity:

$$\dot{\boldsymbol{\varepsilon}}(\mathbf{x}) = \dot{\gamma}_0 \sum_s \boldsymbol{\mu}^s(\mathbf{x}) \left(\frac{|\boldsymbol{\mu}^s(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x})|}{\tau_0^s} \right)^{n_{GI}} \times \text{sign} \left[\boldsymbol{\mu}^s(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x}) \right] \quad (1)$$

where $\dot{\boldsymbol{\varepsilon}}(\mathbf{x})$ and $\boldsymbol{\sigma}(\mathbf{x})$ are the local strain rate and stress tensors; $\boldsymbol{\mu}^s(\mathbf{x})$, $\dot{\gamma}^s(\mathbf{x})$, $\tau^s(\mathbf{x})$ and τ_0^s are, respectively, the orientation-dependent Schmid tensor, the shear rate, the resolved shear stress, and a reference shear stress, of slip system (s). The pre-factor $\dot{\gamma}_0$ is a reference shear rate, and n_{GI} is an exponent, which can be associated with the inverse of the rate-sensitivity of the coarse-grained material. The local constitutive behavior for a Fourier point \mathbf{x} belonging GB phase is here assumed to be given by the following J_2 -isotropic power law for nonlinear isotropic materials:

$$\dot{\boldsymbol{\varepsilon}}(\mathbf{x}) = \frac{3\dot{\varepsilon}_0}{2\sigma_{\text{eq}}(\mathbf{x})} \left(\frac{\sigma_{\text{eq}}(\mathbf{x})}{\sigma_0} \right)^{n_{\text{GB}}} \boldsymbol{\sigma}(\mathbf{x}) \quad (2)$$

where $\sigma_{\text{eq}}(\mathbf{x})$ and σ_0 are the von Mises equivalent of the stress and a reference equivalent stress, respectively, $\dot{\varepsilon}_0$ is a reference strain rate, and n_{GB} is an exponent, which can be identified as the inverse of the rate-sensitivity associated with the deformation mechanisms of GB accommodation. For the grain-size dependent value of τ_0^S and the grain-size independent value of σ_0 , we followed the work of Bringa et al [5] and references therein (see [4] for details). Moreover, we adopted $n_{\text{GI}} = 50$ and $n_{\text{GB}} = 1$. This value of n_{GI} corresponds to a rate-sensitivity of the coarse-grained (CG) material $m_{\text{CG}} = 1/n_{\text{GI}} = 0.02$. The latter is compatible with warm deformation of fcc materials (e.g. $m = 0.025$ for CG Al deformed at 250 °C [6]).

3- Results

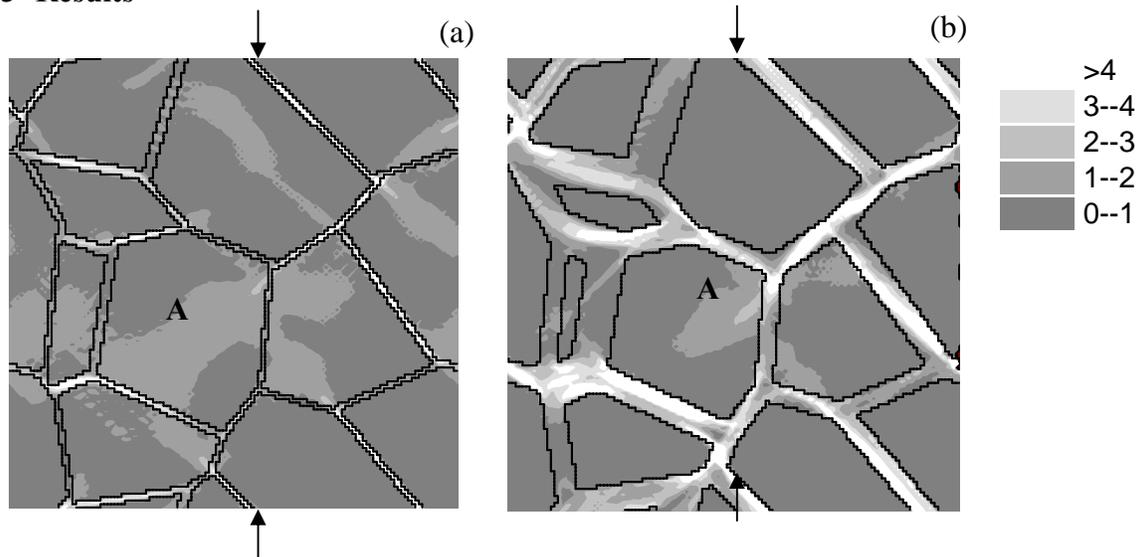


Figure 1: Predicted 2-D section maps (YZ plane at X=64) of local von Mises equivalent strains, relative to the applied macroscopic von Mises equivalent strain, for axisymmetric compression along the z-axis, for RVEs with grain sizes: a) 29 nm and b) 7 nm.

Fig. 1 shows the 2-D section maps of local von Mises equivalent strain for two (29 and 7 nm) of the four self-similar RVEs considered, relative to the applied macroscopic von Mises equivalent strain, for the case of nanocrystalline Cu deformed in quasi-static axisymmetric compression along the z-axis. The main observation is that the strain is concentrated at GBs, reaching 10 times the macroscopic strain, while significant portions of the grain interiors undergo local strains which are less than the applied macrostrain. Another interesting observation is that the grains that deform the most are not necessarily the softest but the ones best located to link favorable oriented GBs (e.g. grain "A").

Fig. 2a shows the relative activities (strain partition) in the grain interiors and the GB phase, along with the corresponding volume fractions, as a function of grain size.

Consistent with the results of Fig. 1, the relative activity at GB exceeds the corresponding GB volume fraction. This trend is more marked as the grain size decreases. At 5 nm, the grain interiors contribute only with 10% to the overall strain, while they still represent almost half of the volume.

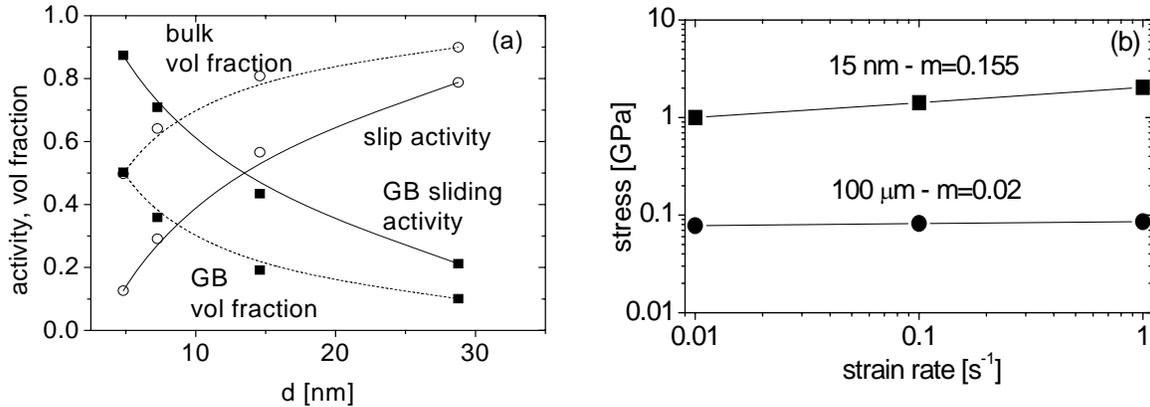


Figure 2: a) Strain and volume fraction partition as a function of grain size. b) Predicted log-log plot of yield strength vs. strain rate for the 15 nm grain and the CG material.

Fig. 2b shows the yield strength variations in the strain rate range 10^{-2} - $10^0 s^{-1}$, for axisymmetric compression, as predicted for the 15 nm RVE. For comparison, we have included the strain-rate dependence of the coarse-grained material (100 μm). The resulting effective strain-rate sensitivity of the 15 nm material is $m=0.155$ (representing roughly an eight-fold increase with respect to the CG value of 0.02). This increase is comparable with the seven-fold increase with respect to the coarse-grained rate-sensitivity value reported by Lu et al [7] for the case of Cu containing nano-sized twins of ~ 20 nm width, deformed at room temperature and also with the ten-fold increase reported by May et al. [6] in ECAP-deformed Al with grain size of ~ 300 nm deformed at 250 $^{\circ}C$.

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