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PREDICTING SIZE EFFECTS USING MECHANISM BASED GRADIENT CRYSTAL PLASTICITY

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Summary. *A strain gradient crystal plasticity model is used to predict size effects for an FCC cube oriented block subjected to simple-shear loading conditions. A feature of the model is inclusion of the geometrically necessary dislocation densities necessary to satisfy the lattice compatibility and both short and long range dislocation interactions. The long range interactions define a back stress which introduces an internal length scale suitable for predicting material size effects.*

1 INTRODUCTION

Microstructural and geometrical dimensions have been shown to influence the macroscopic response, leading to so-called size effects. These effects become increasingly apparent if the dimensions decrease towards an internal length scale of the material i.e. the grain size. This condition can occur in micro-forming of ultra-thin sheet where the sheet thickness ranges between 50 to 500 μm.

2 MATERIAL MODEL

Evers [1, 2] developed a mechanism based strain gradient crystal plasticity model that includes dislocation hardening arising from both short and long range dislocation interactions. Short range interactions include those between statistically stored (ρ_{SSD}) and geometrically necessary (ρ_{GND}) dislocations densities and give rise to the slip system resistance, while long range interactions arise from the repulsive nature of the dislocation induced stress fields. The geometrically necessary dislocations ensure compatibility of the crystal lattice in the presence of slip gradients, where the slip rates on a slip system α ($\alpha = 1, 2, 3 \cdots, 12$) for an FCC lattice, are defined by:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\frac{\tau^{\alpha} - \tau_b^{\alpha}}{s^{\alpha}} \right) \left(\frac{|\tau^{\alpha} - \tau_b^{\alpha}|}{s^{\alpha}} \right)^{1/m-1} \quad (1)$$

with:

$$s^{\alpha} = Gb \sqrt{\sum_{\xi} \mathsf{A}^{\alpha\xi} |\rho_{GND}| + \sum_{\xi} \mathsf{A}^{\alpha\xi} |\rho_{SSD}|} \quad (2)$$

with τ^{α} and τ_b^{α} the resolved shear and resolved back stresses, respectively, G the shear modulus, b the Burgers vector, and $\dot{\gamma}_0^{\alpha}$ and m are material constants. The resolved stress (τ^{α}) and resolved back stress (τ_b^{α}) are computed from:

$$\tau^{\alpha} = \boldsymbol{s}_0^{\boldsymbol{\alpha}} \cdot \mathsf{P} \cdot \boldsymbol{n}_0^{\boldsymbol{\alpha}} \quad (3)$$

$$\tau_b^{\alpha} = -\boldsymbol{s}_0^{\boldsymbol{\alpha}} \cdot \left(\sigma_{\mathsf{e}}^{\mathsf{int}} + \sigma_{\mathsf{s}}^{\mathsf{int}} \right) \cdot \boldsymbol{n}_0^{\boldsymbol{\alpha}} \quad (4)$$

where $\boldsymbol{s}_0^{\boldsymbol{\alpha}}$ and $\boldsymbol{n}_0^{\boldsymbol{\alpha}}$ are the slip direction and slip system normal, respectively, where the subscript 0 refers to the undeformed reference state and P is the second Piola-Kirchhoff stress. The tensors $\sigma_{\mathsf{e}}^{\mathsf{int}}$ and $\sigma_{\mathsf{s}}^{\mathsf{int}}$ are the dislocation induced internal stresses determined by integrating the elastic stress fields associated with individual edge and screw dislocations over an area defined by the radius R according to:

$$\sigma_{\mathsf{e}}^{\mathsf{int}} = \frac{GbR^2}{8(1-\nu)} \sum_{\xi} \nabla_0 \rho_{GND}^{\xi} \cdot \left[3\boldsymbol{n}_0^{\xi}\boldsymbol{s}_0^{\xi}\boldsymbol{s}_0^{\xi} - \boldsymbol{s}_0^{\xi}\boldsymbol{s}_0^{\xi}\boldsymbol{n}_0^{\xi} - \boldsymbol{s}_0^{\xi}\boldsymbol{n}_0^{\xi}\boldsymbol{s}_0^{\xi} + \boldsymbol{n}_0^{\xi}\boldsymbol{n}_0^{\xi}\boldsymbol{n}_0^{\xi} + 4\nu\boldsymbol{n}_0^{\xi}\boldsymbol{p}_0^{\xi}\boldsymbol{p}_0^{\xi} \right] \quad (5)$$

$$\sigma_{\mathsf{s}}^{\mathsf{int}} = \frac{GbR^2}{4} \sum_{\xi} \nabla_0 \rho_{GND}^{\xi} \cdot \left[-\boldsymbol{n}_0^{\xi}\boldsymbol{s}_0^{\xi}\boldsymbol{p}_0^{\xi} - \boldsymbol{n}_0^{\xi}\boldsymbol{p}_0^{\xi}\boldsymbol{s}_0^{\xi} + \boldsymbol{p}_0^{\xi}\boldsymbol{s}_0^{\xi}\boldsymbol{n}_0^{\xi} + \boldsymbol{p}_0^{\xi}\boldsymbol{n}_0^{\xi}\boldsymbol{s}_0^{\xi} \right] \quad (6)$$

Lattice incompatibility resulting from gradients in the crystallographic slip is restored through the geometrically necessary dislocations as follows:

$$\rho_{GND} = -\frac{1}{b} \sum_{\alpha} \nabla_0 \gamma^{\alpha} \cdot \boldsymbol{s}_0^{\alpha} \quad (7)$$

for an edge dislocation while a similar equation can be derived for a screw dislocation. As can be seen from Equation 2, both ρ_{GND} and ρ_{SSD} contribute to the slip system resistance (s^{α}), while gradients of ρ_{GND} define an internal stress field which is used to compute the back stress.

3 APPLICATION TO SIMPLE-SHEAR

The influence of the sample height is shown for the case of simple-shear of a semi-infinite block of material as shown in Figure 1. The block represents an FCC cube oriented material with 12 unique slip systems. Four sample heights ranging from $0.22 \leq H \leq 2.2$ mm are modeled using a single column of 50 four noded plane-strain elements with selectively reduced integration. Along the upper and lower surfaces, crystallographic slip

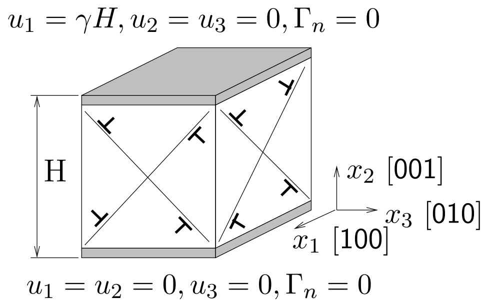

Figure 1: Geometry and boundary conditions for the simple-shear test. Periodic boundary conditions are applied to nodes in the x_1 direction while plane-strain exist in the x_3 direction.

in the surface normal direction (Γ_n) is prohibited, representative of a slip obstructing grain boundary. Figure 2 plots the through-thickness crystallographic slip rates and ρ_{GND} distributions for the case when H=0.22 mm and after an applied shear of $\gamma = 0.01$. In Figure 2 slip systems pairs develop with identical slip rates to maintain lattice symmetry and compatibility in response to the applied load and boundary conditions. A net crystallographic shape change results from the contribution of slip systems with opposing slip directions and defines the crystallographic origin of the shear plotted in Figure 3. No crystallographic slip develops along the {001} plane as a result of the imposed plane-strain and periodic boundary conditions. Approaching the upper and lower surfaces, where the crystallographic slip vanishes, the ρ_{GND}'s develop in order to enable a gradient in the slip rates according to Equation 7. Along the {100} planes edge dislocations are formed while screw dislocations accumulate on the {010} planes. The

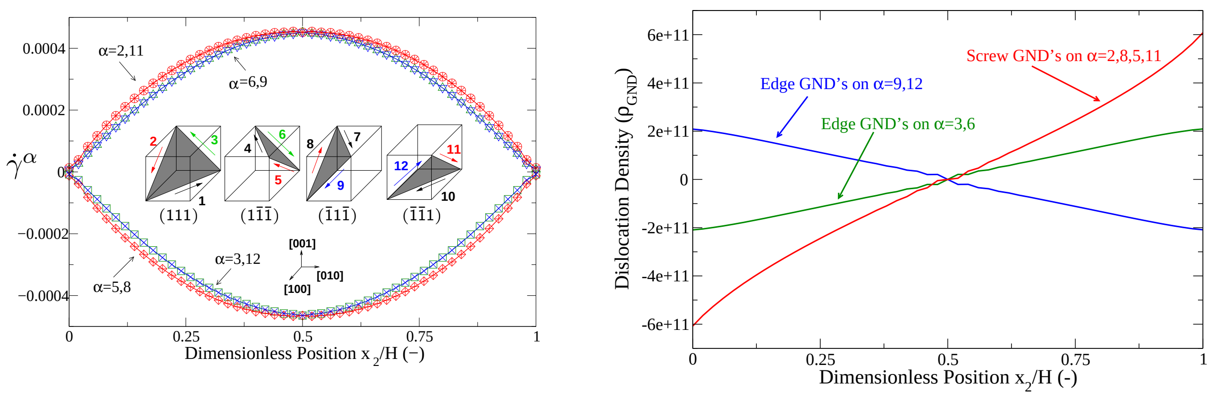

Figure 2: Through-thickness slip rates and ρ_{GND} distributions for H=0.22 mm at $\gamma = 0.01$. The four unit cubes sketch the 12 FCC slip systems oriented such that [100], [001], and [010] are in the x_1, x_2, and x_3 directions, respectively, and where α indexes the 12 slip systems.

influence of the sample dimension H is evident in the applied force and through-thickness shear profiles plotted in Figure 3. With decreasing sample dimension, the shear profiles deviate from the homogeneous solution obtained by prescribing ρ^{ξ}_{GND}=0.0 along the upper and lower surfaces. In the former case, a boundary layer develops in which there is an increased dislocation density (Figure 2) and an associated internal stress field arising from Equations 5 and 6. With H=0.22 mm, the depth of the boundary layer extends to the mid-plane of the specimen. Due to the presence of this boundary layer, the results are size dependent, with decreased sample dimension H associated with increased hardening i.e. smaller is stronger.

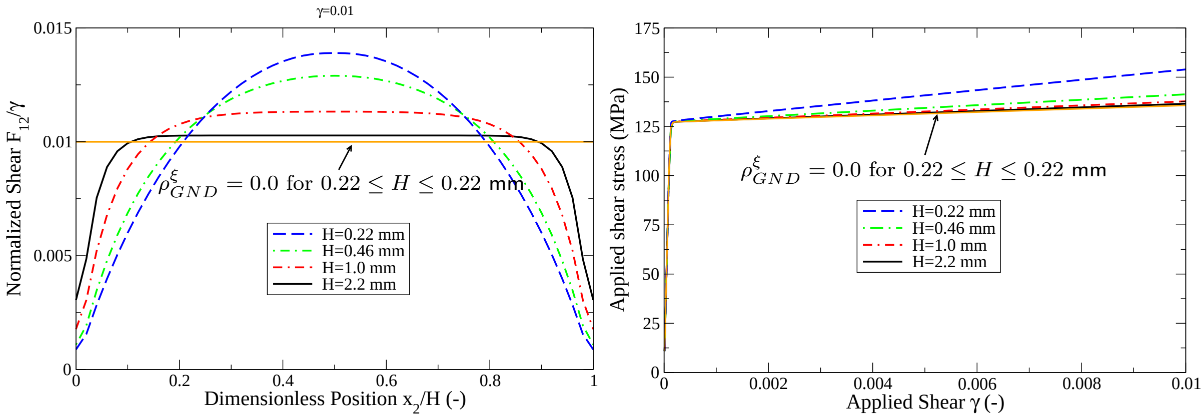

Figure 3: Comparison of the through-thickness normalized shear profiles and applied external stress for $2.2 \leq H \leq 0.22$ mm. The homogeneous solution is obtained by prescribing ρ^{ξ}_{GND}=0.0 along the upper and lower surfaces which has the effect of permitting unrestricted surface normal crystallographic slip.

4 CONCLUSIONS

- Material size effects can be introduced with a crystal plasticity model by including internal stress fields associated with the gradient of the geometrically necessary dislocation density.
- For the case of simple shear in which surface normal crystallographic slip is restricted, boundary layers develop in which there is a heterogeneous deformation gradient. In order to satisfy the gradients in the crystallographic slip rates, geometrically necessary dislocations are introduced which contribute to the size-dependent behaviour of the results.

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