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MODELING THE HALL-PETCH EFFECT WITH A GRADIENT CRYSTAL PLASTICITY THEORY INCLUDING A GRAIN BOUNDARY YIELD CRITERION

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Abstract. A strain gradient crystal plasticity theory including the gradient of the equivalent plastic strain $\nabla\gamma_{eq}$ is discussed. A grain boundary yield condition is proposed in order to account for the influence of the grain boundaries. Periodic tensile test simulations show the mechanical predictions of the numerical model.

1 INTRODUCTION

Modern products, like mechanical components for cars or airplanes, must be small, light-weight, robust and cheap. Product optimization requires, amongst other things, high-performance materials. There is a significant industrial need for new strategies concerning material design and the development of new materials. Nowadays, many materials are developed by microstructural design. Simulations play an important role in this context, since they are cheaper and often faster than experiments. Moreover, the ongoing miniaturization of high performance products requires micromechanical models. These are in many cases inadequate and computationally expensive. For example, their ability to reproduce size effects, interface behavior or damage is limited. Therefore, models for metallic microstructures with grain boundaries are reviewed.

2 MODELING OF AGGREGATES OF CRYSTALS

The microscopic properties which determine the macroscopic mechanical response are reviewed in the following. Excellent continuum models exist for the elastic properties, which are in general anisotropic. The slip system kinematics are also very well represented in crystal plasticity theories. However, the modelling of size effects is still a field of ongoing research. The same holds for modeling grain boundaries within a continuum mechanical

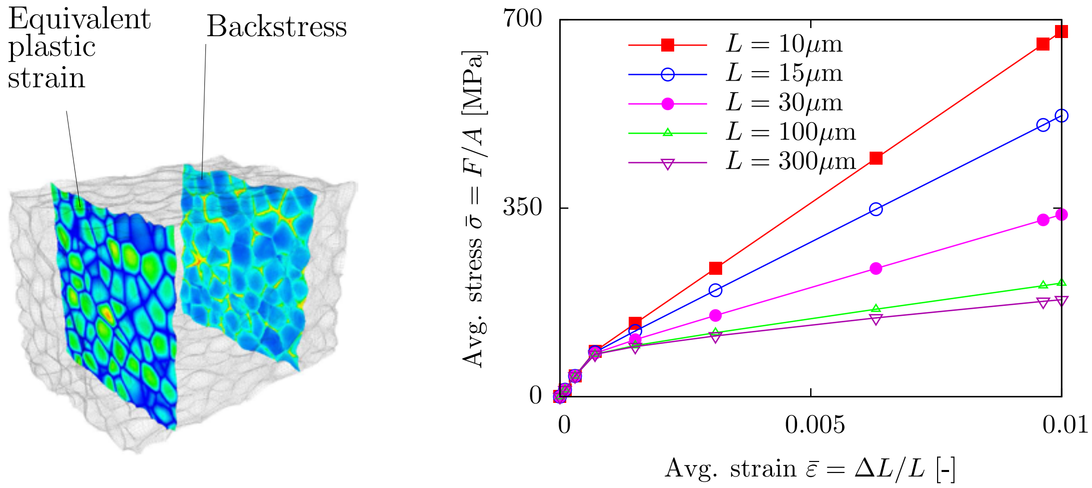

Figure 1: Simulations results based on micro-hard grain boundaries (left). The macroscopic hardening is size-dependent (right) in contrast to the yield stress. This kind of behavior contradicts with experiments.

setting. The contribution at hand focusses on the description of grain boundaries in the context of gradient plasticity. Grain boundaries (GBs) are obstacles for dislocations, mainly due to the grain misorientation. Consequently, dislocation pile ups emerge at the GBs. At the beginning of the deformation process, the GBs can in most cases be assumed impenetrable for dislocations. Only when the loading reaches a critical value, the grain boundary yields. Before a model for this effect is introduced, a review of a gradient theory for impenetrable so-called micro-hard GBs is considered.

3 REVIEW OF GRADIENT THEORIES WITH MICRO-HARD GRAIN BOUNDARIES

For simplicity, a geometrically linear single-slip theory is reviewed. A model including micro-hard GBs is considered in Table 1. The model can be considered a special version of Gurtin's theory [1]. Besides the traction vector $\boldsymbol{t} = \boldsymbol{\sigma n}$, a microtraction $\Xi = \boldsymbol{\xi} \cdot \boldsymbol{n}$ is introduced. The linear momentum balance and the microforce balance represent the field equations. Micro-hard boundary conditions are introduced as Dirichlet conditions $\gamma = 0$. The simulations illustrated in Fig. 3 show the mechanical response of this class of models with micro-hard boundaries and a quadratic ansatz for the defect energy (the model is described in detail in [5]).
The boundary conditions lead to vanishing plastic slip at the GBs. Consequently, pile-ups and backstresses emerge close to the boundaries. The size-effect is, in this case, the macroscopically observed hardening. However, the yield stress is size-independent. This behavior is different from the real material behavior observed in experiments where the yield stress is size-dependent. Barely any dependence of the hardening on the grain size is observed in experiments. This unphysical model behavior is mainly due to the boundary

conditions. In the following, a model for the transition from micro-hard to penetrable grain boundaries is shortly summarized and motivated physically.

Additive decomposition	$\text{grad}\,(\boldsymbol{u}) = \boldsymbol{H} = \boldsymbol{H}^e + \boldsymbol{H}^p$	
Plastic distorsion	$\boldsymbol{H}^p = \gamma \boldsymbol{d} \otimes \boldsymbol{n} = \gamma \boldsymbol{M}$	
Elastic strain	$\boldsymbol{\varepsilon}^e = \text{sym}(\boldsymbol{H}^e)$	
GND-densities	$\rho_\vdash = -\boldsymbol{d} \cdot \nabla\gamma; \quad \rho_\odot = \boldsymbol{l} \cdot \nabla\gamma$	
Stored energy	$W = W_e(\boldsymbol{\varepsilon}^e)$	$+ \quad W_g(\rho_\vdash, \rho_\odot)$
Stresses	$\boldsymbol{\sigma} = \partial_{\boldsymbol{\varepsilon}} W$	$\boldsymbol{\xi} = \partial_{\rho_\odot} W\, \boldsymbol{l} - \partial_{\rho_\vdash} W\, \boldsymbol{d}$
Tractions	$\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n}$	$\Xi = \boldsymbol{\xi} \cdot \boldsymbol{n}$
Balance equations	$\boldsymbol{0} = \text{div}\,(\boldsymbol{\sigma})$	$0 = \tau + \text{div}\,(\boldsymbol{\xi}) - \tau^d,\ \tau^d = \tau^d(\dot{\gamma})$
Dirichlet BCs	$\boldsymbol{u} = \bar{\boldsymbol{u}}$ on $\partial\mathcal{B}_u$	$\gamma = 0$ on GBs (impenetrable)

Table 1: A theory with micro-hard boundary conditions.

4 AN EXPLANATION APPROACH FOR THE HALL-PETCH EFFECT

In the following, it is assumed that the Hall-Petch effect can be motivated by slip bands leading to high stress concentrations at the grain boundaries. This assumption is outlined, e.g., in the works of Eshelby et al. (1951) and Armstrong et al. (1962) ([2], [3]). Large grains imply high stress concentrations which can activate dislocation sources in the vicinity of the GBs. This mechanism can propagate a slip band from one to another grain. Macroscopically, this effect is assumed to be observable as the elasto-plastic transition. As a consequence, fine-grained metals are assumed to exhibit high yield stresses.

5 A GRAIN BOUNDARY YIELD THEORY

A possible gradient extension of a crystal plasticity without internal length scale is given as follows

$$W_e(\boldsymbol{\varepsilon}_e) + W_h(\gamma_{eq}) + W_g(\nabla\gamma_1,\ \nabla\gamma_2,\ \ldots,\ \nabla\gamma_N). \tag{1}$$

Here, W_h models isotropic hardening. In most cases, the energy W_g represents a phenomenological approach to account for size effects. This class of models implies generally many degrees of freedom (DOFs) of the numerical model. As an example, a face centered cubic (FCC) metal can have 15 degrees of freedom per node. Consequently, the gradient extension implies a massive increase of DOFs. Wulfinghoff and Böhlke (2012) proposed an approach which is based on a simplified kinematical framework

$$W_e(\boldsymbol{\varepsilon}_e) + W_h(\gamma_{eq}) + W_g(\nabla\gamma_{eq}). \tag{2}$$

Instead of GND-measures like Nye's tensor $\boldsymbol{\alpha}$ [4] this approach introduces a simplified purely phenomenological gradient measure $\nabla\gamma_{eq}$. This idea is mainly motivated by the desire to simulate multi-grain aggregates. The numerical treatment otherwise is usually computationally very expensive. Therefore, hardly any three-dimensional gradient crystal plasticity simulations can be found in the literature. The model (2) implies only four degrees of freedom per node. Table 2 summarizes the model equations.

Additive decomposition	$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p$	
Plastic distorsion	$\boldsymbol{\varepsilon}^p = \sum_\alpha \lambda_\alpha \boldsymbol{M}^S\alpha$	
GND-measure	$\nabla\gamma_{eq}, \quad \gamma_{eq} = \sum_\alpha \lambda_\alpha$	
Stored energy	$W = W_e(\boldsymbol{\varepsilon}^e) + W_h(\gamma_{eq}) + W_g(\nabla\gamma_{eq})$	
Stresses	$\boldsymbol{\sigma} = \partial_{\boldsymbol{\varepsilon}} W$	$\boldsymbol{\xi} = \partial_{\nabla\gamma_{eq}} W$
Tractions	$\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n}$	$\Xi = \boldsymbol{\xi} \cdot \boldsymbol{n}$
Balance equations	$\boldsymbol{0} = \mathrm{div}\,(\boldsymbol{\sigma})$	$0 = \tau_\alpha + \mathrm{div}\,(\boldsymbol{\xi}) - \tau_\alpha^d$
Dirichlet BCs	$\boldsymbol{u} = \bar{\boldsymbol{u}}$ on $\partial\mathcal{B}_u$	Kuhn-Tucker conds. on GBs
Isotropic Voce hardening	$W_h = \tau_\infty^C \gamma_{eq} + \frac{1}{\Theta_0}(\tau_\infty^C - \tau_0^C)^2 \exp\left(-\frac{\Theta_0\gamma_{eq}}{\tau_\infty^C - \tau_0^C}\right)$	
Defect energy	$W_g = \frac{1}{2} K_G \nabla\gamma_{eq} \cdot \nabla\gamma_{eq}$	

Table 2: Equivalent plastic strain theory including a grain boundary model.

The model equations include thermodynamically consistent flow rules for the bulk and the grain boundary behavior. The bulk flow rule reads

$$\dot{\lambda}_\alpha = \dot{\gamma}_0 \left\langle \frac{\tau_\alpha - \tau_b - (\tau_0^C + \beta)}{\tau^D} \right\rangle^p \tag{3}$$

including the following stresses

- backstress $\tau_b = -\mathrm{div}\,(\boldsymbol{\xi}) = -K_G \Delta\gamma_{eq}$
- isotropic hardening stress $\beta = \partial_{\gamma_{eq}} W_h$

The grain boundary flow rule is incorporated by a yield condition and the Kuhn-Tucker conditions. The model has two additional material constants compared to its counterpart

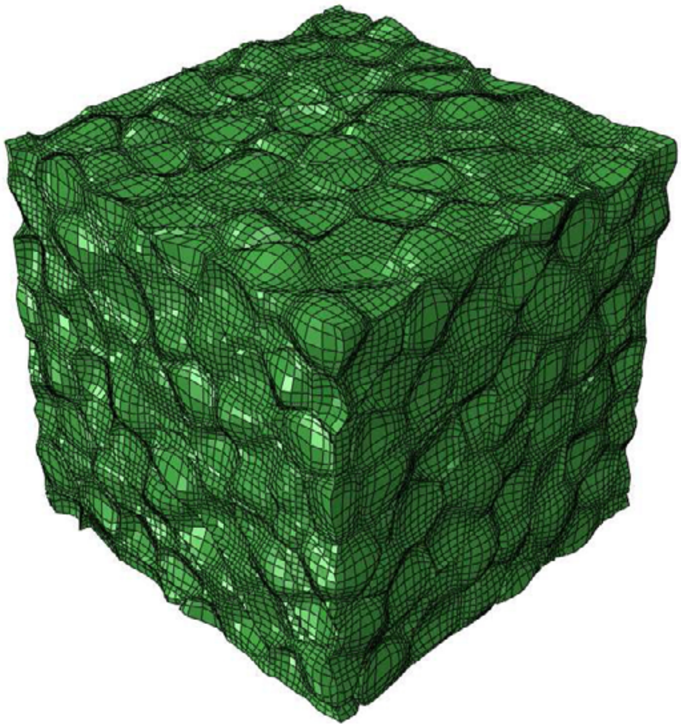

Figure 2: The figure shows a periodic mesh. The mesh has been deformed starting from a perfectly cube-shaped mesh in order improve the resolution at the grain boundaries.

without internal length scale. The defect energy parameter K_G controls the influence of the gradient while the grain boundary yield strength controls the resistance of the grain boundaries.

6 IMPLEMENTATION

The model has been implemented in an in-house FE-code. A micromorphic approximation of the theory is used including four DOFs per node (for $\boldsymbol{u}$ and γ_{eq}). A standard active set search accounts for the transition from impenetrable to penetrable GBs. The integration point routine is documented in [6]. The solution is fully periodic. The meshes have a high resolution close to the GBs, Fig. 2. The mesh creation has been done by deforming of a perfectly cube shaped mesh. Fig. 3 compares two simulation results of 80 grains with different mesh resolutions. The first mesh has $\sim$1 Mio. DOFs. The second mesh is much coarser (30000 DOFs, i.e. only 3% of DOFs of the first mesh). The simulation results show that for two RVE sizes with edge lengths $L = 30\mu$m and $L = 100\mu$m the macroscopic yield stress is indeed grain-size-dependent, as desired. The hardening behavior barely shows any size-effect.

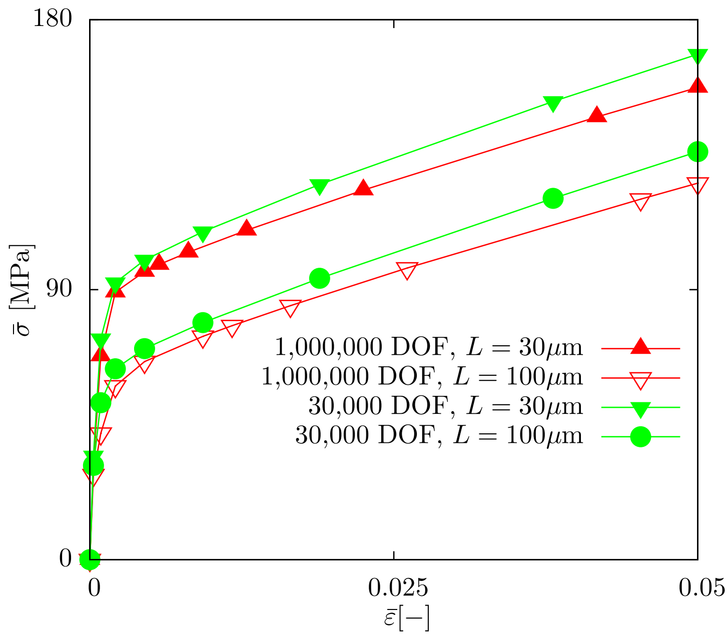

Figure 3: Comparison of the simulation results of 80 grains, discretized by ∼1 Mio. DOFs and a DOF-reduction by 97% (30000 DOFs).

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