Three Dimensional Grain Boundary Modeling in Polycrystalline Plasticity

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Abstract. At grain scale, polycrystalline materials develop heterogeneous plastic deformation fields, localizations and stress concentrations due to variation of grain orientations, geometries and defects. Development of inter-granular stresses due to misorientation are crucial for a range of grain boundary (GB) related failure mechanisms, such as stress corrosion cracking (SCC) and fatigue cracking. Local crystal plasticity finite element modelling of polycrystalline metals at micron scale results in stress jumps at the grain boundaries. Moreover, the concepts such as the transmission of dislocations between grains and strength of the grain boundaries are not included in the modelling. The higher order strain gradient crystal plasticity modelling approaches offer the possibility of defining grain boundary conditions. However, these conditions are mostly not dependent on misorientation of grains and can define only extreme cases. For a proper definition of grain boundary behavior in plasticity, a model for grain boundary behavior should be incorporated into the plasticity framework. In this context, a particular grain boundary model ([1]) is incorporated into a strain gradient crystal plasticity framework ([2]). In a 3-D setting, both bulk and grain boundary models are implemented as user-defined elements in Abaqus. The strain gradient crystal plasticity model works in the bulk elements and considers displacements and plastic slips as degree of freedoms. Interface elements model the plastic slip behavior, yet they do not possess any kind of mechanical cohesive behavior. The physical aspects of grain boundaries and the performance of the model are addressed through numerical examples.

INTRODUCTION

At meso scale, isotropic material models no longer apply since they are not capable of predicting inherent plastic and elastic anisotropy of crystals, which results in stress concentrations at grain boundaries due to lattice misorientations. In stress corrosion cracking and fatigue conditions the stress concentrations might initiate small cracks leading to failure of materials. Another important phenomenon due to grain boundaries is the Hall-Petch effect, namely the grain size effect on plasticity, resulting from the deformation heterogeneity occurring around the grain boundaries. The materials with small grain structure would have more possibilities for interactions between dislocations and grain boundaries leading to more dislocation accumulation and further hardening. Therefore, it is quite crucial to study the underlying physical mechanisms of grain boundary mechanics through micromechanically motivated models. In this context higher order strain gradient crystal plasticity models allow a smooth implementation of recent grain boundary models due to the fact that plastic fields are incorporated as additional degree of freedom and they constitute the GB models degrees of freedom as well.

[1] presents a theoretical framework including the effect of both the misorientation between the neighboring grains and the orientation of the grain boundaries in a free energy expression which could potentially be used for continuum description of dislocationgrain boundary interactions within a thermodynamically consistent crystal plasticity framework. Later in [3] the GB model is incorporated into strain gradient crystal plasticity in 2D through interface elements describing the behavior of plastic slip at the boundaries and the numerical examples are presented. The model is extended to 3D and bi-crystal examples are studied in a simple setting in [4]. In the current work the model

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is extended to 3D and implemented into Abaqus software as user bulk and interface element for polycrystalline simulations which bring a lot of technical difficulties. The procedure is automated through a number of scripts preparing 3D grain structures, automatically inserting interface elements between grains, converting the data into an Abaqus input file and post-processing the results. While the strain gradient crystal plasticity model could only supply (soft and hard) boundary conditions for the grain boundaries the incorporation of the grain boundary model enables us to capture cases in between these two limiting cases. The numerical examples clearly illustrate this effect.

STRAIN GRADIENT CRYSTAL PLASTICITY AND GB MODEL

For the modelling of the grain boundary behavior two types of user finite element subroutine have been developed and implemented in Abaqus software. The simulation of the size dependent bulk material behavior is conducted through a rate dependent, higher order, plastic slip based, strain gradient crystal plasticity model taking into account plastic slips and displacement as coupled degree of freedom ([5], [2], [4]). The model is based on the additive decomposition of the strain into elastic and plastic components and the plastic slip field evolution is governed by $\dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha \left(|\tau^\alpha + \nabla \cdot \xi^\alpha| / s^\alpha\right)^{\frac{1}{m}} \operatorname{sign}(\tau^\alpha + \nabla \cdot \xi^\alpha)$ where $\tau^\alpha = \sigma : \mathbf{P}^\alpha$ is the resolved Schmid stress on the slip systems with $\mathbf{P}^\alpha = \frac{1}{2}(\mathbf{s}^\alpha \otimes \mathbf{n}^\alpha + \mathbf{n}^\alpha \otimes \mathbf{s}^\alpha)$, the symmetrized Schmid tensor, where $\mathbf{s}^\alpha$ and $\mathbf{n}^\alpha$ are the unit slip direction vector and unit normal vector on slip system α, respectively and ξ^α is the micro-stress vector $\xi^\alpha = \partial \psi_{\nabla\gamma} / \partial \nabla\gamma^\alpha = A \nabla\gamma^\alpha$ bringing the plastic slip gradients into the plasticity formulation. A is a scalar quantity, which includes an internal length scale parameter, and in this work it is defined as $A = ER^2/(16(1-\nu^2))$ where R is a typical length scale for dislocation interactions.

The simulation of the grain boundary behavior is conducted through the Gurtin GB model (see e.g. [1]) which considers the effect of the grain boundary orientation and the orientation mismatch between neighboring grains. The slip incompatibility of the neighboring grains is described in terms of the grain boundary Burgers tensor defined as, $\boldsymbol{G} = \sum_\alpha [\gamma_B^\alpha \boldsymbol{s}_B^\alpha \otimes \boldsymbol{n}_B^\alpha - \gamma_A^\alpha \boldsymbol{s}_A^\alpha \otimes \boldsymbol{n}_A^\alpha](\boldsymbol{N}\times)$ where for any vector $\boldsymbol{N}$, $\boldsymbol{N}\times$ is the tensor with components $(\boldsymbol{N}\times)_{ij} = \varepsilon_{ikj} N_k$. In this relation, the relative misorientation of grains is reflected by the difference term and the grain boundary orientation is accounted for by the tensor $\boldsymbol{N}\times$. $C_{AA}^{\alpha\beta}$ and $C_{BB}^{\alpha\beta}$ represent interactions between slip systems within grain A and grain B respectively, whereas $C_{AB}^{\alpha\beta}$ represent the interaction between slip systems of the two grains and called inter-grain interaction moduli. Ignoring the dissipative effects, a simple potential energy in the form $\psi_{GB} = \frac{1}{2}\kappa |\boldsymbol{G}|^2$ is used where κ is a positive constant modulus and it represents the strength of the grain boundary. Principal of virtual power is followed for both bulk and grain boundary parts, where the rate of free energy expressions are used. Then dissipation inequalities are obtained for both parts. Obtained balance equations and grain boundary relations are solved through the finite element method.

TABLE 1: Material properties of the strain gradient crystal plasticity model.

Young modulus E [MPa]	Poisson ratio ν [/]	Reference slip rate $\dot{\gamma}_0$ [s^{-1}]	Slip resistance s [MPa]	Orientations [°]	Material length scale R [μm]
70000.0	0.33	0.115	25.0	Random	0.4

NUMERICAL EXAMPLES

A mixed finite element formulation is used for the solution of the strain gradient crystal plasticity problem inside each grain. The displacement and plastic slips are taken as primary variables and these fields are determined within the problem domain by solving simultaneously the linear momentum balance and the microscopic force balance. The discretization is conducted by 10-node tetrahedra elements with quadratic interpolation for the displacement field and linear interpolation for the slips. To facilitate the integration of the grain boundary contributions, 12-node zero thickness interface elements are developed and inserted along the grain boundaries. By means of these elements, one has the access to the slip values along the grain boundary as approached from grain A and grain B. The interface

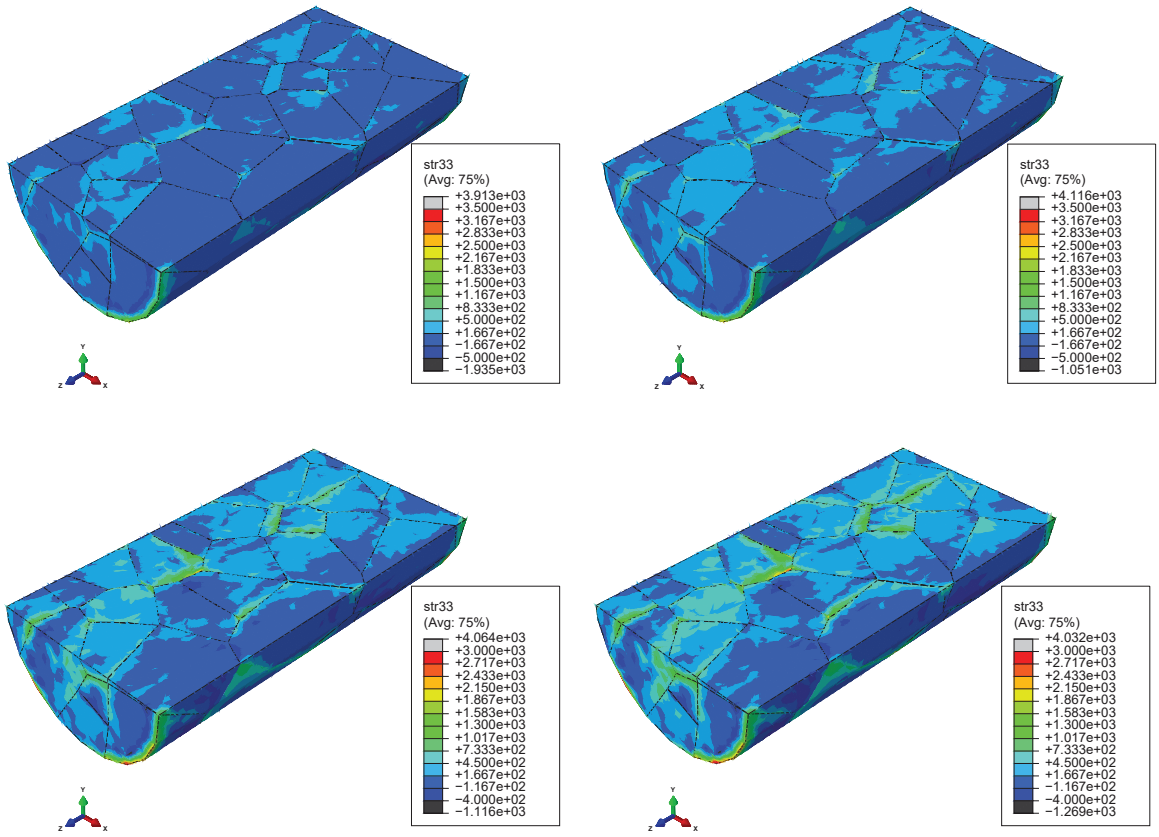

FIGURE 1: Stress distribution for $\kappa = 0$ (upper-left), $\kappa = 1$ (upper-right), $\kappa = 3$ (lower-left) and $\kappa = 5$ (lower-right) values of the grain boundary strength.

elements do not possess any kind of mechanical cohesive behavior and does not cause discontinuity in displacement field. In the solution phase, the displacement continuity across the grain boundary is fulfilled by means of equality constraints (rigid ties) enforcing the same displacement field for the corresponding nodes of on the two sides of an interface element.

To illustrate the effect of the grain boundaries on the microstructure deformation heterogeneity and the macroscopic constitutive response a cylindrical uniaxial specimen with $50\mu m$ length and $12.5\mu m$ radius with 50 grains having random orientations is considered, where 5 slip systems are considered to be active in each grain. The grain structure is obtained through Voronoi tessellation, [6]. The effect of the orientation mismatch has been studied in the recent studies by the authors (see e.g. [3],[4]) in both 2D and 3D bi-crystal specimens. However, these studies concentrated rather on single slip systems to explicitly analyze the effect of mismatch and the orientation of the grain boundary on the spatial distribution of stress and strain. A realistic microstructure study has not been conducted yet. Therefore in this study, the microscopic and macroscopic effects of the grain boundary strength parameter in a realistic specimen is addressed shortly. The material parameters are presented in Table 1.

In the advanced strain gradient crystal plasticity models, without a grain boundary model, the users can only prescribe soft (transmission of dislocations from one grain to other without any resistance) and hard (zero slip or complete accumulation of dislocations) conditions at the boundaries. However in a polycrystalline material the behavior of the grain boundary is quite complicated and it is not physical to treat them by using two limiting conditions. On the other hand, the current model could simulate the situations in between based on the orientation mismatch, the grain boundary orientation and the strength of the grain boundary. It is discussed previously that increasing the mismatch

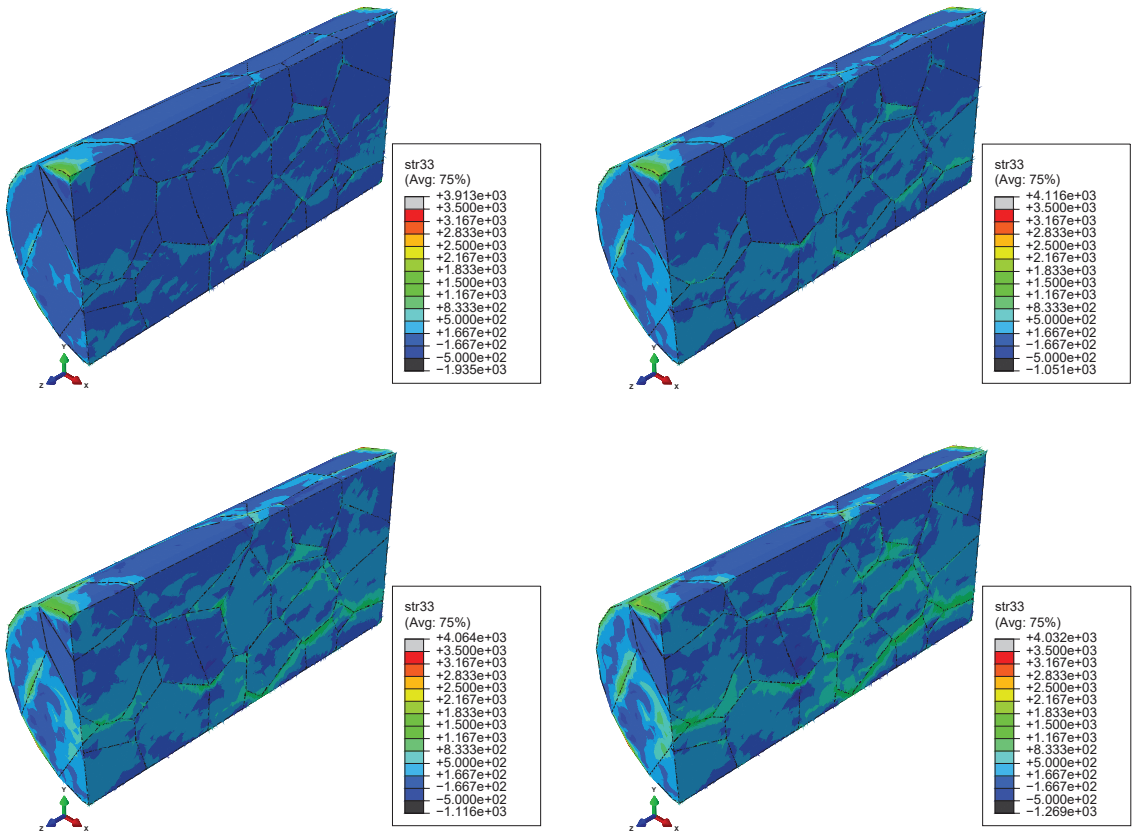

FIGURE 2: Stress distribution for $\kappa = 0$ (upper-left), $\kappa = 1$ (upper-right), $\kappa = 3$ (lower-left) and $\kappa = 5$ (lower-right) values of the grain boundary strength.

results in a harder grain boundary with a non-zero κ value. When there is no mismatch the grain boundary behaves soft for any value of κ. In the numerical example here, there is certain mismatch between the grains due to the random orientation distribution. It is expected that for different values of κ grain boundary behavior should change between soft and hard cases. It is important to note that κ is a size dependent parameter, and the effect of the magnitude should be evaluated accordingly.

In Fig. 1 and 2 the spatial stress distribution in the loading direction is presented for $\kappa = 0, 1, 3,$ and 5 values for both horizontal and vertical cuts. Without a grain boundary value or for $\kappa = 0$ case, even though there is orientation difference between grains the intensity of stress concentration is relatively low at grain boundaries, while experimental observations, e.g. for aluminum alloys under uniaxial deformation, illustrates pronounced localization and stress concentration at GBs (see e.g. [7]). This behavior is obtained by increasing the value of κ which amplifies the effect the orientation mismatch at grain boundaries. Similar observation is presented for the strain distribution in Fig. 3. Soft-like grain boundaries with $\kappa = 0$, approaches to zero slip condition at higher values, e.g. for $\kappa = 5$. The model and the κ parameter give the users the freedom to validate their models for such microstructures with limited number of grains, which would be still quite large to handle for detailed MD and DD calculations. This is not possible neither with standard crystal plasticity models resulting in jump between grains nor with the strain gradient crystal plasticity models, which could only define two limiting cases. Note that for the current specimen size $\kappa = 5$ is a rather big value making GB almost hard, it would be quite small value for a mm size specimen where the behavior would be much closer to the soft boundary.

The macroscopic response of the different microstructures due to different κ values is presented in Fig. 4. The

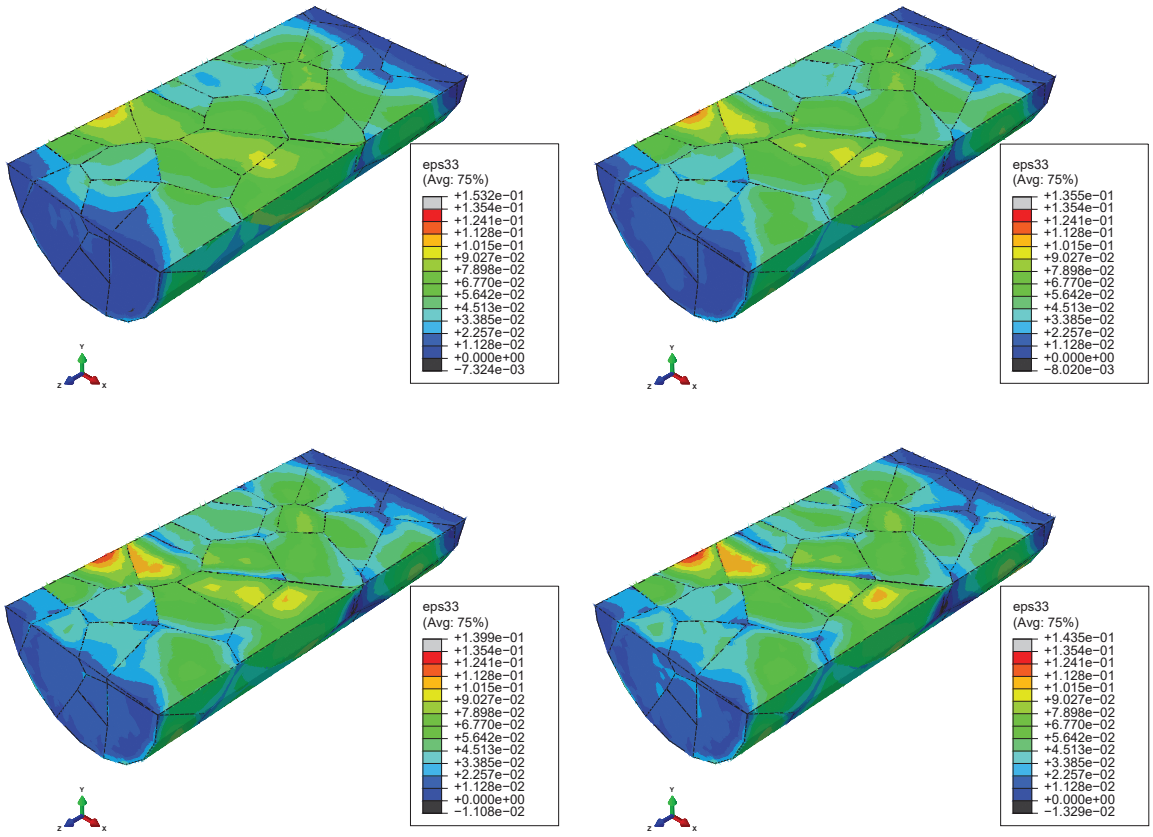

FIGURE 3: Strain distribution for $\kappa = 0$ (upper-left), $\kappa = 1$ (upper-right), $\kappa = 3$ (lower-left) and $\kappa = 5$ (lower-right) values of the grain boundary strength.

change in the grain boundary strength does not only result in an altered evolution of microstruture it also affects substantially the macroscopic stress-strain behavior. High κ values leads to considerable increase in the hardening of the material.

CONCLUSION AND OUTLOOK

In this paper the grain boundary model from Gurtin [1], is incorporated into a strain gradient crystal plasticity framework to analyze its performance in polycrystalline micron size 3D samples. The formulation of the grain boundary model is based on the grain boundary Burgers tensor which takes into account both the effect of the mismatch between the grains and the orientation of the grain boundary. The geometric structure of a grain boundary is described by the grain misorientation and the grain boundary normal vector, Wolf and Yip [8]. Therefore the current formulation fully captures the geometric structure of a grain boundary. The framework illustrate the coarse grained representation of complex grain boundary-dislocation slip interaction mechanisms such as dislocation transmission and accumulation at the grain boundary. In classical crystal plasticity models microstructure evolution at the grain boundaries evolves solely due to orientation mismatch and it is not possible to account for any type of dislocation–grain boundary interaction. However in the current model the parameter κ gives the possibility to adjust the amount of localization and stress concentration around the grain boundaries, which makes the experimental comparison and validation tasks easier. Even though there is no mechanical behavior included in the grain boundaries in the current version of the

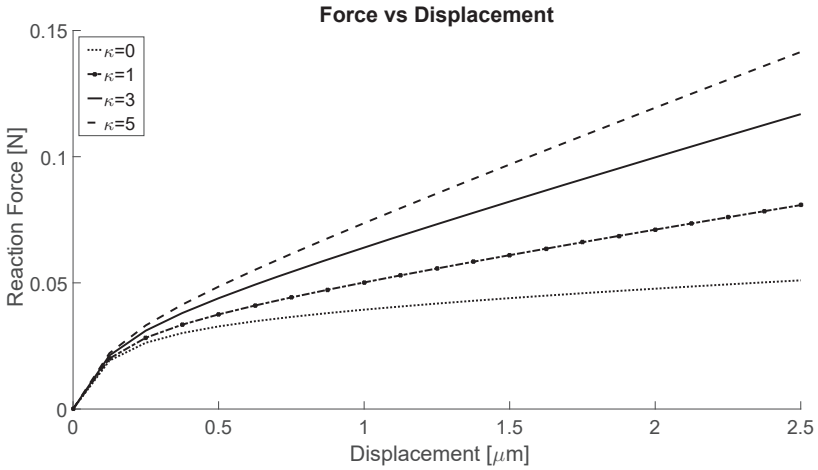

FIGURE 4: Force vs displacement response for different κ values.

model, the intrinsic evolution of stresses at the boundaries would give the possibility of a smooth incorporation of cohesive behavior. Then the model could be used for the simulation of small scale inter-granular crack initiation and propagation as well. The study includes a virtual polycrystalline material and the results are not compared with any experimental data yet. However, it shows a great potential to be used in different crystalline structures upon tuning the material parameters and using the real crystallographic data. It is one of the rare studies combining a gradient crystal plasticity model with physical grain boundary model to simulate the evolution of 3D polycrystalline microstructure in metallic alloys.

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