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Micromechanical Modelling of Size Effects in Microforming

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Abstract

This paper deals with the micromechanical modelling of the size dependent mechanical response of polycrystalline metallic materials at micron scale through a strain gradient crystal plasticity framework. The model is implemented into a Finite Element software as a coupled implicit user element subroutine where the plastic slip and displacement fields are taken as global variables. Uniaxial tensile tests are conducted for microstructures having different number of grains with random orientations in plane strain setting. The influence of the grain size and number on both local and macroscopic behavior of the material is investigated. The model is capable of capturing both size effect due to statistical distribution of the grains and their size taking into account the grain boundary conditions.

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Keywords: Microforming, strain gradient plasticity, crystal plasticity, non-local modelling, grain boundary conditions

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1. Introduction

In many industrial clusters such as, electronics, communication, aerospace, biomedical devices, defense and automotive, miniaturization of the products have recently become a global trend, which requires advanced manufacturing technologies at micron level. Microforming is a plastic deformation procedure for the production of parts having at least two dimensions at micron scale. At this scale there are various factors affecting the deformation behavior, process performance, and the quality of micro-formed parts (see e.g. [1] for an overview).

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In addition to geometry, tooling design, process parameter configuration and deformation conditions the microstructure and the grain size play a crucial role in the plastic behavior of the material (see [2] for a detailed literature review). There have been various theories developed for the modelling of macro scale plastic deformation during conventional metal forming processes and many of these frameworks are implemented in commercial finite element simulation tools. In all these local plasticity and damage models, the specimen size and the grain size do not enter the frameworks. Therefore, these classical simulations are not able to capture the effect of the size on the mechanical response of the material, which is crucial at micron scale. Recent studies have shown that on the scale of several micrometers and below, crystalline materials behave differently from their bulk equivalent due to micro-structural effects (e.g. grain size, lattice defects and impurities), gradient effects and surface constraints (see [3] for an extensive review). These effects could lead to stronger or weaker material response depending on the size and unique micro-structural features of the material. Moreover, as the size goes down statistical size effect comes into play as well due to the decisive behavior of individual grains, which are quite limited in number. It has been a challenge to establish models taking into account the size effect due to the microstructural and the statistical phenomena.

Current paper studies both the intrinsic and the statistical size effects through a strain gradient polycrystalline plasticity framework developed for microstructural patterning in single crystals in [4] and [5] and used for different microstructure evolution phenomena in [6] and [7]. Different specimen and grain sizes are considered using Voronoi tessellation, where the polycrystalline aggregate is generated using probability theory. Applying the constitutive model to 2D (plane strain) polycrystalline structure, the micro tensile tests for various microstructures are numerically simulated by finite element method (FEM) in Abaqus software through the developed implicit user element subroutine. The attention is focused on the effect of different boundary conditions for the spatial deformation evolution and the macroscopic size-dependent behavior of the material. Some recent studies address the influence of the boundary conditions in micro scale specimens through strain gradient models (see e.g. [8], [9]), however conclusions are mostly drawn for bi-crystals or specimens with very restricted number of grains or grain shapes (see [10]). A thorough study considering different microstructural parameters and grain boundary conditions has not yet been conducted. The current study illustrates the intrinsic size-effect for various microstructures with different grain size and grain number as well as the statistical effect, which fades away with the increasing number of grains.

2. Constitutive Model

The constitutive model in this paper is a strain gradient crystal plasticity framework, which is originally developed to model the deformation patterning in single crystals (see [4]). Like all the other crystal plasticity models the evolution of the plastic strain is obtained through a plastic slip evolution equation based on a power law relation,

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha}\left(|\tau^{\alpha} + \nabla \cdot \boldsymbol{\xi}^{\alpha}|/s^{\alpha}\right)^{\frac{1}{m}} \mathrm{sign}(\tau^{\alpha} + \nabla \cdot \boldsymbol{\xi}^{\alpha}). \tag{1}$$

The gradient effect is included in the model through the micro-stress vector $\xi^{\alpha} = \partial\psi_{\nabla\gamma}/\partial\nabla\gamma^{\alpha}$ bringing the plastic slip gradients via a quadratic plastic slip potential $\psi_{\nabla\gamma}$ into the formulation. The other stress contribution affecting the evolution of plastic slip is the classical Schmid stress, which is the stress projected on the slip systems, $\tau^{\alpha} = \boldsymbol{\sigma} : \mathbf{P}^{\alpha}$ 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. Internal length scale parameter enters the formulation through the scalar quantity$A$, and in this work it is defined as $A = ER^2/\left(16(1 - \nu^2)\right)$ where R is a typical length scale for dislocation interactions. In the following examples we relate R to a certain percentage of the grain size to study its influence. The slip evolution equation together with the linear momentum balance are taken as the governing equations for the finite element solution procedure. They are weighted, integrated, linearized, discretized and the obtained coupled linear set of equations are solved implicitly in an incremental manner through a user element subroutine in ABAQUS software. For the post-processing of the results a Python script is developed to convert the data into a file that could be read by the finite element software.

3. Numerical Examples

Numerical examples address the plastic behavior of polycrystalline specimens at micron scale with microstructures having 5, 50 and 110 grains obtained through Voronoi tessellation. The initial average grain size in these simulations are set to D_{av} = 150 μm. Then the effect of the grain size is analyzed through a scaling operation using the internal length scale parameter, which would give values from 100 μm to 375 μm. Horizontal tensile specimens are considered. Displacement is applied to the right edge in the global +x direction, resulting in macroscopic $\langle \varepsilon_{11} \rangle = 2.5\%$. The symbol $\langle \ \rangle$ represents the Macaulay bracket, indicating a macroscopically averaged value. The left edge is constrained in the x direction and rigid body movement is prevented by fixing the bottom left corner of the model in global y direction. The material parameters, presented in Table 1, are not directly related to any engineering materials, rather used to demonstrate the strain gradient effects in the polycrstalline aggregates. Crystallographic orientations of grains are randomly distributed (0-360°). Two slip systems (120, 60) are considered in the following examples.

Table 1. Material properties of the strain gradient crystal plasticity model.

Young modulus E [MPa]	Poisson raito $\nu [\,/\,]$	Reference slip rate $\dot{\gamma}_0 [\mathrm{s}^{-1}]$	Slip resistance s [MPa]	System orientations [°]	Material length scale R [μm]
210000.0	0.33	0.05	20.0	120, 60	1, 1.5, 2.5, 3.75

The intrinsic size effect could be analysed through a change in the grain size or a change in the internal length scale parameter, where both would influence the macroscopic constitutive behaviour and the spatial evolution of the plastic strain in the same manner. Therefore, this effect is studied through different D_{av}/R ratio values. A small D_{av}/R value represents a microstructure with small grain size or large internal length scale parameter, which induces large internal stresses penalizing high plastic slip gradients. This behaviour results in a more spread geometrically necessary dislocation distribution and therefore the boundary layer thickness is increased.

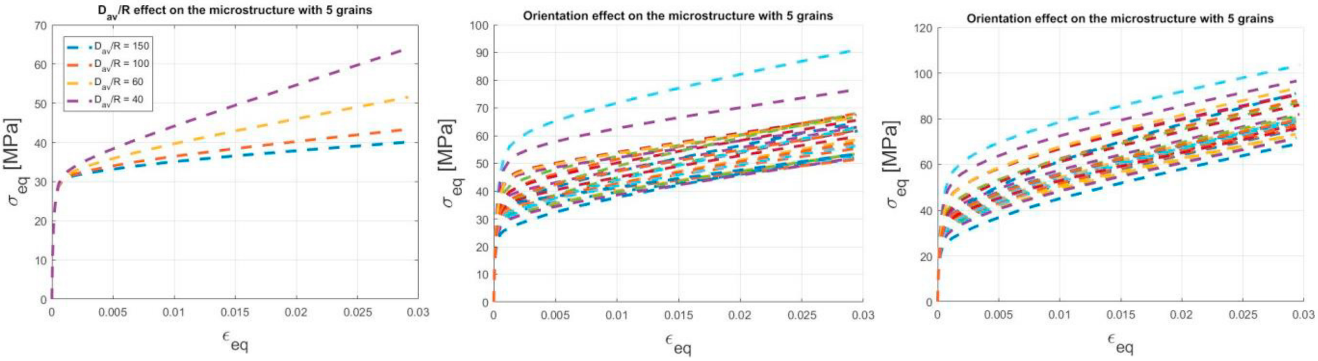

Fig. 1. Intrinsic size effect on the macroscopic stress strain response (left), Orientation effect on the macroscopic response (for 30 different randomly oriented microstructure) for soft grain boundary conditions (center), and for hard grain boundary conditions (right).

Fig 1(left) illustrates the intrinsic size effect on the constitutive behaviour of a specimen having a microstructure with 5 grains and different D_{av}/R ratios. The case with the smaller grain size shows stiffer response. In Fig. 1(centre) and Fig. 1(right) the effect of the random orientation on the global constitutive behaviour is presented for soft and hard boundary conditions respectively for 30 randomly oriented grain systems. The bandwidth of the scatter for the soft boundary condition is quite large while it gets smaller for the hard boundary condition. In the soft case the plastic slips are not restricted at the grain boundaries and the mismatch of orientation is reflected severely at the macroscopic constitutive response. In the case for hard boundary conditions, the plastic slip is enforced to be zero at the grain boundaries, which is a strong condition reducing the effect of orientation mismatch. The randomness of the orientation introduces a statistical effect, which is prominent at the microstructures with low number of grains.

In Fig. 2 and 3 the local equivalent stress and equivalent plastic strain distributions are plotted for different D_{av}/R

ratios to illustrate the effect of the grain size. For the hard boundary case (figure 2) the plastic strain field is constrained at the grain boundaries, reaching to zero level at the boundary which induces a boundary layer. For small D_{av}/R

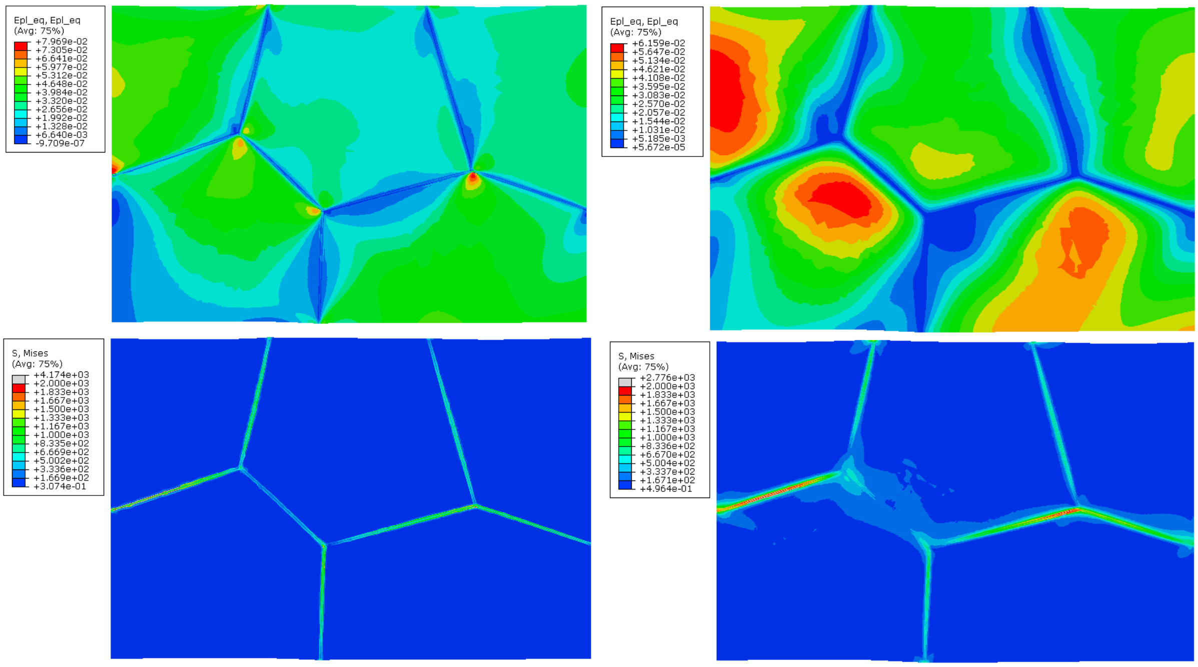

Fig. 2. Local equivalent plastic strain (top) and equivalent stress distribution (bottom) with hard grain boundary conditions for large (left) $D_{av}/R = 400$ and small (right) $D_{av}/R = 40$ values representing large and small grain sized specimens.

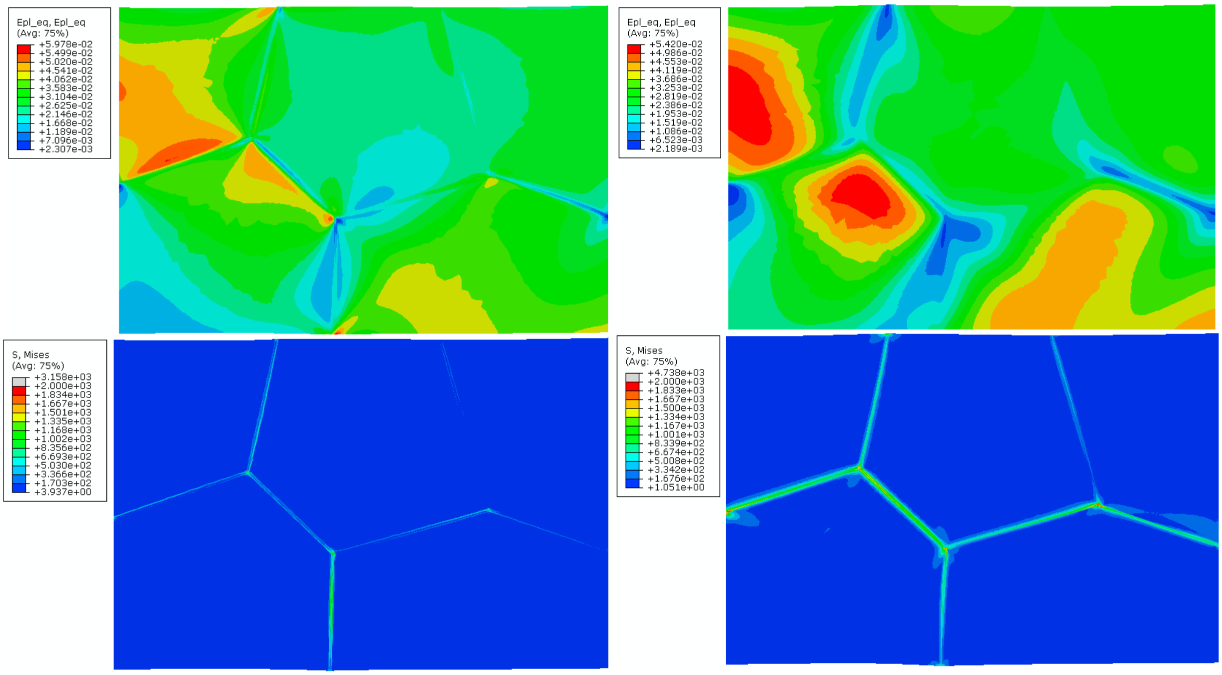

Fig. 3. Local equivalent plastic strain (top) and equivalent stress distribution (bottom) with soft grain boundary conditions for large (left) $D_{av}/R = 400$ and small (right) $D_{av}/R = 40$ values representing large and small grain sized specimens.

values, representing the case with small grain boundaries, wider grain boundary layer corresponding to more distributed geometrically necessary dislocation density are observed. Same influence is observed for the stress evolution at the grain boundaries and more pronounced stress concentration is obtained for the small grain case. Same example with soft grain boundary conditions are addressed in Fig 3. The grain size effect on the equivalent plastic strain and equivalent stress distribution is same with the hard boundary case. In this case the stress concentrations at the grain boundary occurs solely due to orientation mismatch since there is no constraint on the plastic slip evolution at the grain boundaries. Note that in all of the simulations in this work only two slip systems (60^{o} and 120^{o}) are considered and increasing the number of slip systems does not cause a major change in the results for the current plane strain problem.

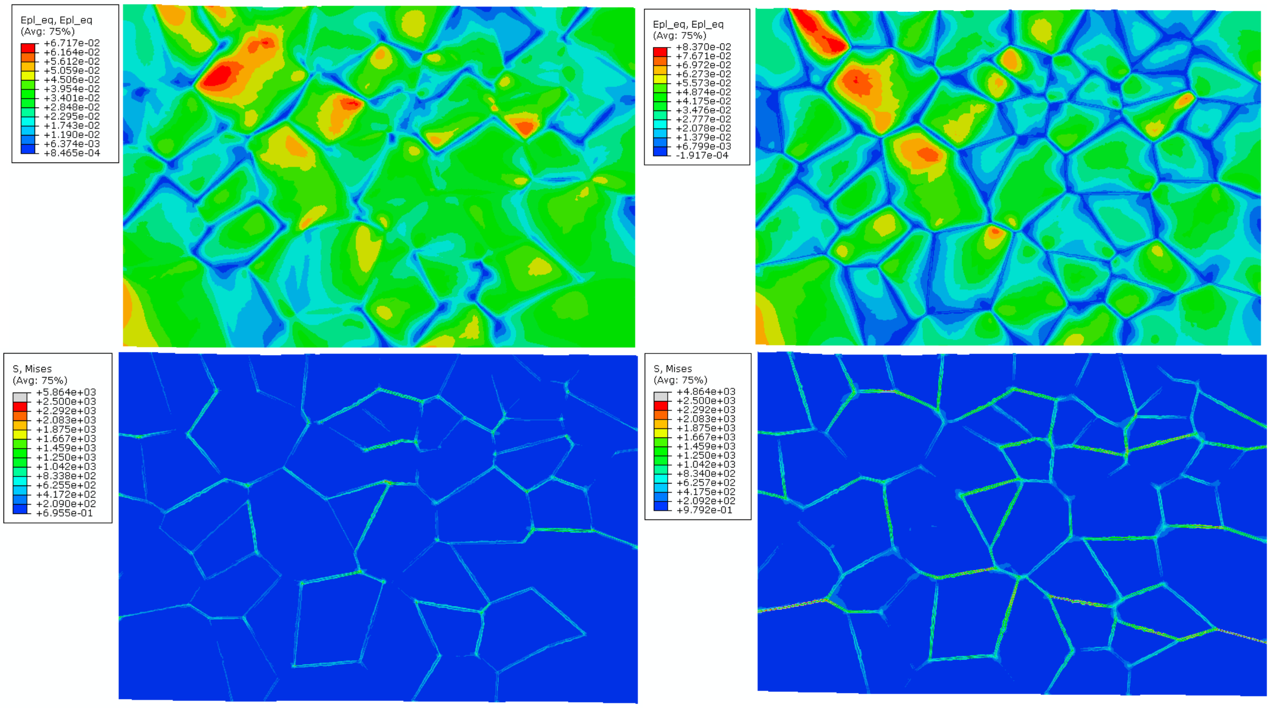

Fig. 4. Local equivalent plastic strain (top) and equivalent stress distribution (bottom) with soft grain boundary conditions (left) and hard boundary conditions (right) for a 50 grain microstructure with $D_{av}/R = 60$.

Fig. 4 represents the differences in local response between soft and hard grain boundary conditions for the microstructure with 50 grains having the grain size ratio $D_{av}/R = 60$. For the hard case, due to the imposed conditions, the grain boundaries are strongly present in the local response figures, where the zero slip constraint and stress concentration are observed clearly. The soft case is a good example to illustrate the orientation mismatch effect in both local stress and plastic strain distribution.

In Fig. 5, the orientation effect for the case with high number of grains is represented in a microstructure with 110 randomly oriented grains, for 20 different set of orientations, having both hard and soft grain boundary conditions. The results presented in Fig. 1 depend highly on the orientation set and therefore the statistical effect is dominating. Increasing the number of grains reduces this effect as presented in Fig. 5 where the band of variation almost disappears. The boundary conditions play a crucial role here as well and for the hard boundary case the results almost converge to the isotropic material behaviour and there is almost no statistical effect. However, even though it is not presented here, the intrinsic size effect exists for this microstructure as well and it solely depends on the size of the grain.

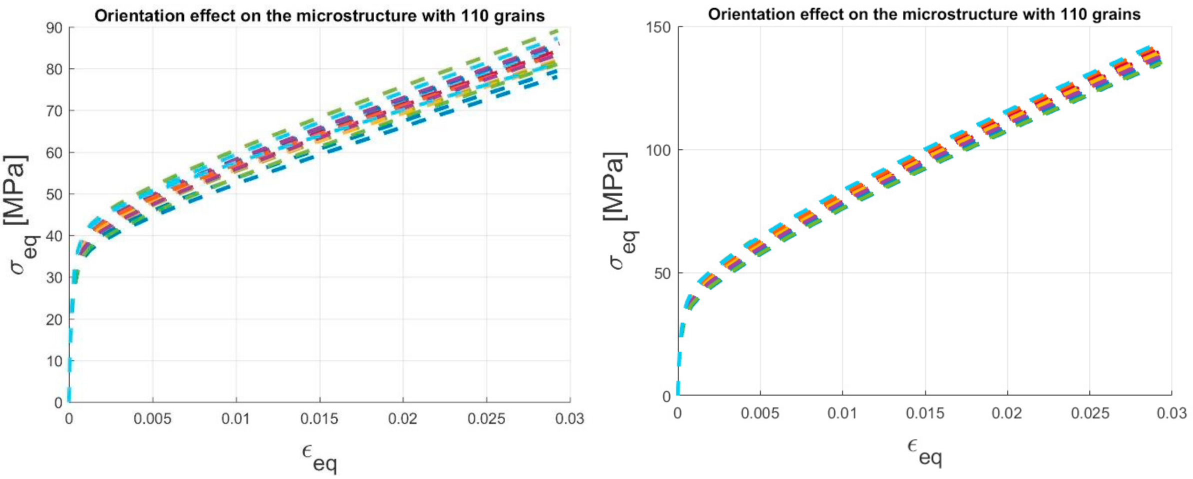

Fig. 5. Orientation effect (for 20 different randomly oriented microstructure) on the macroscopic response for soft grain boundary conditions (left), and for hard grain boundary conditions (right).

4. Conclusions

This study addresses the intrinsic and the statistical size effects in micron scale polycrystalline metallic specimens under plastic deformation through a non-local crystal plasticity framework. In samples including limited number of grains the statistical effect due to random grain orientation is quite dominating since the individual grain behaviour plays crucial role in material response and there is huge scatter in stress-strain curves. As the number of grains is increased the scatter band decreases. Moreover, a detailed study on the effect of the grain boundary conditions and grain size on the local response is presented as well. It is observed that hard conditions at the grain boundaries yield not only increase in the hardening behaviour but also decrease the scatter due to random orientation distribution.

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