Grain Interactions in Crystal Plasticity

K.P. Boyle and W.A. Curtin

Division of Engineering, Brown University, Providence, RI, 02912

Abstract. The plastic response of a sheet metal is governed by the collective response of the underlying grains. Intragranular plasticity depends on intrinsic variables such as crystallographic orientation and on extrinsic variables such as grain interactions; however, the role of the latter is not well understood. A finite element crystal plasticity formulation is used to investigate the importance of grain interactions on intragranular plastic deformation in initially untextured polycrystalline aggregates. A statistical analysis reveals that grain interactions are of equal (or more) importance for determining the average intragranular deviations from the applied strain as compared to the orientation of the grain itself. Furthermore, the influence of the surrounding grains is found to extend past nearest neighbor interactions. It is concluded that the stochastic nature of the mesoscale environment must be considered for a proper understanding of the plastic response of sheet metals at the grain-scale.

INTRODUCTION

Sheet metal deformation is ultimately governed by the collective response of the underlying grains. Polycrystalline plasticity seeks to understand this aggregate behaviour from the vantage point of the single crystal. Macroscopic plastic properties can be derived from attributes of the single crystal by using appropriate homogenization theories or by finite element computations. Although homogenization schemes, such as the Taylor isostrain assumption or the isodeformation gradient [1] assumption, are often invoked, a large body of experimental evidence indicates that intragranular deformation is not homogeneous. The study of intragranular heterogeneity, within the context of crystal plasticity, is important for understanding and predicting a variety of phenomena including damage evolution and ductile fracture, strain localization, and crystallographic texture evolution. Aernoudt et al. [2] give a concise overview of the nature of the experimental observations with regards to heterogeneous flow at the grain-scale.

The plastic response of a polycrystalline aggregate is always constrained by the global boundary conditions. However, the intragranular plastic response is mediated by the relative constraints provided by interactions among grains in the precise local grain topology. The extent to which grain interactions influence intragranular plasticity is not well understood. This lack of understanding stems partly from the difficulty in monitoring in-situ intragranular deformation. Experiments are usually limited to intermittent surface measurements and to avoid the complications of sub-surface structure the measurements are often performed on large grains with quasi-columnar grain structures [3,4,5]. Nevertheless the importance of grain interactions has been demonstrated; Korbel et. al. [6] have shown that grain interactions influence the initiation and growth of unstable plastic flow patterns, Kalidindi et al. [7] have shown that the evolution of grain-scale orientation heterogeneities depend on grain interactions, and strain mapping techniques have been used to demonstrate the prevalence of inhomogeneous intragranular deformation [8,9]. New experimental methods, such as 3-dimensional X-ray diffraction microscopy [10,11], hold promise for a more comprehensive in-situ study of intragranular plasticity and grain interactions.

Finite element crystal plasticity computations, which use a minimum of one element per grain, are ideally suited for studying grain interactions because model aggregate grain configurations can be simulated, no homogenization schemes need to be invoked, both compatibility and equilibrium are satisfied, and the evolution of the field quantities inside the grains can be followed. Results obtained...
from finite element crystal plasticity simulations focused on the study of grain interactions indicate that the local grain neighborhood strongly influences the deviations from isostrain behaviour [12,13,14,15,16]. Our goal is to quantify the influence of grain interactions and to understand the relative importance of grain interaction as compared to crystallographic orientation on the inhomogeneity of deformation at the scale of the grain. We do so by statistically analyzing the evolution of heterogeneity with deformation for a central grain embedded in different specific grain neighborhood configurations all corresponding to realizations of a random average texture. The question addressed is important not only for assessing homogenization theories but also for understanding the origins of intragranular inhomogeneity. The results indicate that grain interactions play a dominant role in determining the intragranular deviations from the applied strain in any one grain, and that the influence of the surrounding grains extend past near-neighbor interactions.

**COMPUTATIONAL PROCEDURE**

**Finite Element Crystal Plasticity Simulations**

A rate-dependent finite element crystal plasticity constitutive law, as described in [17], is followed. The rate of shear strain on slip system \( \gamma^{(a)} \), is given by a power law representation given by,

\[
\dot{\gamma}^{(a)} = \gamma_0^{(a)} \left( \frac{\tau^{(a)}}{\tau_c^{(a)}} \right)^m \text{sgn} (\tau^{(a)})
\]

where \( \gamma_0^{(a)} \) is a reference shear strain rate, \( \tau^{(a)} \) the resolved applied shear stress, \( \tau_c^{(a)} \) the critical shear strength, and \( m \) characterizes the material strain rate sensitivity. The critical slip system shear strength is taken to evolve according to the relationship,

\[
\tau_c^{(a)} = H^{(a\kappa)} |\dot{\gamma}^{(a)}|
\]

where the hardening modulus \( H^{(a\kappa)} \) is expressed as a latent hardening coefficient \( q^{(a\kappa)} \) multiplied by a self-hardening modulus \( h^{(a)} \), where no summation over \( \kappa \) is taken. Isotropic latent hardening is assumed, i.e. \( q^{(a\kappa)} = 1 \). The self-hardening modulus is given by,

\[
h^{(a)} = (h_i - h_f) \text{sech}^2 [h' \gamma'] + h_i,
\]

where \( h' = (h_i - h_f) / (\tau_j - \tau_o), \gamma' = \int_0^t \dot{\gamma}^{(a)} dt \) and \( h_i, h_f \) are initial and saturation hardening rates. The material parameters are given in Table I; \( c_{11}, c_{12} \) and \( c_{44} \) are the standard anisotropic elastic moduli for cubic materials. An f.c.c. material is modeled and therefore the \( \{111\} <110> \) slip system is operative. The crystal plasticity constitutive law was implemented into the commercial finite element code ABAQUS [18] as a material user subroutine [19].

**Aggregate Configurations**

This study is focused on the influence of the topology of the crystallographic orientation of the surrounding grains on the plastic response of a central grain in a computational cell of crystallites. The computational cell used here consists of a cube containing 342 cubic grains in a 7x7x7 array.

Three regions are defined in the computational cell: region R1 corresponds to the central grain; region R2 corresponds to the layer of 26 near-neighbor grains surrounding region R1; and region R3 contains 315 grains and corresponds to the remaining two layers of grains surrounding region R2 (see Fig. 1a). Five ideal texture components prominent to f.c.c. sheet metals are chosen for the central grain: the copper (\( \{111\}\langle110\rangle \)), Goss (\( \{110\}\langle001\rangle \)), S (\( \{123\}\langle634\rangle \)), rotated cube (\( \{001\}\langle110\rangle \)) and brass (\( \{110\}\langle112\rangle \)) orientations. Five different configurations of crystallographic orientations, distributed randomly in orientation space, are assigned to each of the sets of grains in regions R2 and R3. A total of 125 specific configurations are thus tested. The simulations are organized into a three-dimensional matrix of test configurations (Fig. 1b). The independent variable for each axis (dimension) of the matrix is the crystallographic orientations of the grains in one of the corresponding three regions described. The notation \( \Omega_{pqr} \) denotes this matrix of test configurations, where the indices \( p, q, r = 1-5 \) correspond to the five grain orientations for region R1 and the five particular realizations of random texture in regions R2 and R3 respectively.

The computational cell is discretized with 1, 8 and 27 elements per grain so that three simulations are

| \( \tau_j \) | 1.8 \( \tau_o \) | \( h_o \) | 8.9 \( \tau_o \) | \( h_o \) | 0.1 \( \tau_o \) | \( \dot{\gamma}_0 \) | 0.001 s\(^{-1}\) | \( m \) | 0.005 | \( c_{11} \) | 850 \( \tau_o \) | \( c_{12} \) | 620 \( \tau_o \) | \( c_{44} \) | 375 \( \tau_o \) |
performed for each specific configuration $\Omega_{pqr}$. The use of 8-integration-point linear hexahedral brick elements leads to a total of 2744, 21952, and 74088 integration points in the cell. Plane strain compression is the chosen deformation path. The laboratory frame of reference is chosen such that direction 3 is the direction of applied compression, 2 is the direction of plane strain and 1 is the direction of free extension. All faces of the computational cell are constrained to remain planar. The cell was deformed in plane strain compression up to $\varepsilon_{y1}=0.80$ and with an initial true strain rate of 0.00014 s$^{-1}$.

**Statistical Analysis**

A strain deviation parameter is developed to quantify the influence of grain interactions on the inhomogeneity of intragranular deformation. A residual strain at each integration point $k$ is defined with respect to the applied strain $\varepsilon_{ij}^a$ and is divided by the norm of the applied strain to obtain a normalized strain deviation parameter $\Delta \varepsilon_{ij}^k$ given by,

$$\Delta \varepsilon_{ij}^k = \sqrt{\left(\varepsilon_{ij}^k - \varepsilon_{ij}^a\right)^2 / \varepsilon_{nn}^a \varepsilon_{nn}^a} \quad (4)$$

The average strain deviation parameter within a grain for a fixed configuration $\Omega_{pqr}$ is obtained by averaging over the $N$ integration points within the central grain, i.e.,

$$\langle \Delta \varepsilon_{ij} \rangle_{\Omega_{pqr}} = \frac{1}{N} \sum_{k=1}^{N} \Delta \varepsilon_{ij}^k \quad (5)$$

Equation (5) represents the average mean square deviation of the strain in the grain relative to the applied strain. The Taylor isostrain assumption corresponds to $\Delta \varepsilon_{ij}^k = 0$ and $\langle \Delta \varepsilon_{ij} \rangle_{\Omega_{pqr}} = 0$. As the grain surroundings (regions R2 and/or R3) are changed for a fixed region R1 orientation, e.g., $\Omega_{pqr}$ for varying $q$ and/or $r$ at fixed $p$, or as the region R1 orientation is changed for fixed grain surroundings (regions R2 and/or R3), e.g., $\Omega_{pqr}$ for varying $p$ at fixed $q$ and/or $r$, we are interested in the dependence of the strain deviation parameter on the specific orientations of each configuration. A comparison of the influence of different grain neighborhoods on the average intragranular inhomogeneity is achieved by calculating the standard deviation of the average strain deviation parameter with respect to the various orientations tested. For example, for the case when the configurations for regions R2 and R3 are fixed, the standard deviation over the variation of the average strain deviation parameters for region R1 is,

$$s_{\Delta \varepsilon_{ij}}^{\Omega_{pqr}} = \sqrt{\frac{1}{5} \sum_{p=1}^{5} \left(\langle \Delta \varepsilon_{ij} \rangle_{\Omega_{pqr}} - \langle \Delta \varepsilon_{ij} \rangle_{\Omega_{ave}} \right)^2} \quad (6)$$

where the average value of $\langle \Delta \varepsilon_{ij} \rangle_{\Omega_{ave}}$ is given by,

$$\langle \Delta \varepsilon_{ij} \rangle_{\Omega_{ave}} = \frac{1}{5} \sum_{p=1}^{5} \langle \Delta \varepsilon_{ij} \rangle_{\Omega_{pqr}} \quad (7)$$

Therefore, in equations (6) and (7) one of the indices for $\Omega_{pqr}$ is free, which is indicated by $\langle \rangle$. The standard deviation parameter describes the variability of the average strain in region R1 as a function of the specific orientation configurations in the aggregate averaged over either region R1, region R2, or region R3. If the standard deviation parameter is small, then the influence of the orientations being averaged over is small, i.e. the specific grain region being averaged
over is not important in determining the deformation of the central grain. If the standard deviation parameter is large, then the orientations being averaged over have a significant effect on the deformation of the central grain.

RESULTS AND DISCUSSION

The macroscopic flow curves derived from the computational cell are insensitive to the mesh discretization or to the orientation configurations used, suggesting that 342 grains discretized with one element per grain are sufficient to reproduce the macroscopic flow behaviour. Barbe et al. [20] obtained similar results. Furthermore, the simulated flow curves are consistent with the expected flow behaviour obtained by integrating Eqn. 2 and by using the appropriate Taylor factor for a non-textured material in plane strain compression (Fig. 2).

![Figure 2](image)

**FIGURE 2.** Macroscopic stress-strain response comparing simulations with 1, 8 and 27 elements per grain.

Figure 3 shows the evolution of the strain deviation parameter \(\Delta e_{ij}^{\text{iso}}\) for the 1-3 strain component versus the applied compressive strain \(\varepsilon_{33}\) for the computational cell discretized with 8 elements per grain. The results are grouped according to either central grain orientation (R1) or grain surroundings (R2 and/or R3) held fixed. In Fig. 3a, the central grain is held fixed in the brass orientation (\(p = 1\)), the near-neighbor grains in region R2 are held fixed at \(q = 1\), while the grain topologies for region R3 are varied (\(\Omega_{r1}\) where \(r = 1, 5\)) whereas in Fig. 3b, the grain topologies for regions R2 and R3 are held fixed at \(q\) and \(r = 1\) while the central grain R1 orientation is varied (\(\Omega_{p11}\) where \(p = 1, 5\)). Comparing Figs. 3a and b, it is clear that the variation among samples with varying central region R1 is smaller than that when the central grain is held fixed and region R3 is varied. This result shows that the specific grain texture in region R3 is more important to the deformation of the central grain (region R1), with regards to the 1-3 component of strain, than the central grain orientation. The trend is quantified by the standard deviation \(sd_{ij}^{p,q,r}\) and \(sd_{ij}^{r,q,p}\) parameters for these configurations, as shown in Fig. 4a, where the standard deviation for the configurations grouped according to \(\Omega_{p11}\) is higher than that grouped according to \(\Omega_{q1r}\).

Standard deviation parameters are calculated for each of the region R1 orientations for a fixed region R2 (\(q = 1\)) and by averaging over region R3 for \(r = 1, 5\) (i.e. for the configurations grouped according to \(\Omega_{r1}, \Omega_{r2}, \Omega_{r3}, \Omega_{r4}\) and \(\Omega_{r5}\) where \(r = 1, 5\)) and for each of the region R3 configurations for a fixed region R2 (\(q = 1\)) and by averaging over region R1 for \(p = 1, 5\) (i.e. for each of the configurations grouped according to \(\Omega_{p11}, \Omega_{p12}, \Omega_{p13}, \Omega_{p14}\) and \(\Omega_{p15}\) where \(p = 1, 5\)). The five standard deviation parameters calculated for each of the region R1 orientations is averaged (i.e. for \(sd_{ij}^{q,p,r}\) where \(p = 1, 5\)) and similarly, the five standard deviation parameters calculated for each of the region R3 configurations is averaged (i.e. for \(sd_{ij}^{r,q,p}\) where \(r = 1, 5\)); the average standard deviation parameters for the 1-3 strain component are shown in Fig. 4b. The results indicate that on average the standard deviation parameters for the central grain orientations with varying region R3 configurations are higher than the standard deviation parameters for fixed region R3 configurations with varying central region R1 orientations.

The results analyzed for all configurations and all computational discretizations, as described above, can be summarized as follows. The deviation from the applied strain for the 1-2 strain component in the central grain R1 is more sensitive to self-orientation than to the surrounding grain environment (R2, R3) for all configurations tested. However, the intragranular strain deviations for the 1-3 and 2-3 strain components are more sensitive to the mesoscale surrounding grain environment (R2, R3) as compared to grain self-orientation. The 2-2 strain component shows very little deviation from the isostrain condition and neither self-
For most configurations tested, deviations from the applied strain for the 1-1 and 3-3 strain components are more sensitive to the mesoscale surrounding grain environment (R2, R3) than to grain self-orientation (R1).

The results indicate that the deviations from the applied strain are primarily influenced by interactions with the surrounding grain environment, not by grain self-orientation. The consistent exception is the 1-2 strain component. As well, significant grain interactions clearly extend past the first layer of grains; the grain orientation topology in the outermost layers (region R3) often controls the evolution of intragranular inhomogeneity in the central grain, irrespective of self-orientation. Furthermore, the crystallographic texture of these grains was initially random, and so our results are not a consequence of any special assumed starting textures. This leads us to conclude that the stochastic nature of the mesoscale environment out to at least the third neighbors must be considered for a proper understanding of local grain deformations in any given polycrystalline aggregate.

The need to account for the mesoscale grain topology in order to rationalize experimental observations implies that less correlation is expected between deformation processes at the grain-scale and crystallographic orientation for any given grain (or likewise parameters based on crystallographic orientation, such as the Taylor factor or Schmid factor, which characterize the plastic response of the grain with respect to the applied stress). One example
pertinent to sheet metal deformation includes the characterization of a grain's resistance to strain localization; the Taylor factor for a single grain or the average Taylor factor for an aggregate of grains may be inappropriate for characterizing the resistance to strain localization of the local mesoscale environment, for which strain percolation patterns emerge which likely influence the stability of local grain environment to mesoscale shear localization.

The importance of considering grain interactions with respect to the evolution of intragranular plastic inhomogeneity raises a number of questions regarding the accuracy of various homogenization theories as used in crystal plasticity. Basic homogenization schemes assume that all grains with the same initial orientation evolve in an equivalent manner; i.e. the state of each grain after deformation can be linked to the initial orientation and therefore grain topology is ignored. However, grain interactions influence the evolution of the average orientation and spread in orientations within the grain. Average grain orientations, for the same initial orientation, can evolve differently for different mesoscale environments and therefore averaging based on equivalent initial orientation becomes inaccurate and evidently the applicability of these basic homogenization schemes for details beyond the average stress-strain response and average texture evolution becomes questionable.

Beaudoin et al. [21] have concluded, based on a finite element crystal plasticity study, that the spread in orientation in a grain is dictated increasingly by the mesoscale environment, so that as deformation proceeds the grain loses identity of the initial orientation and they infer that the evolution of the microstructure becomes rather insensitive to the details of the initial microstructure and is basically controlled by the overall texture as a characteristic of the average environment. However, our findings show that the initial stochastic influence of the mesoscale environment is not lost as deformation proceeds even though all configurations tested develop a strong "copper-type" texture typical for plane strain deformed f.c.c. materials. Therefore, the discrete nature of the interactions between a grain and its mesoscale surroundings are maintained for highly textured mesoscale environments and the collective response of grain aggregate and the strain percolation patterns that evolve are stable with respect to small perturbations in the orientation topology (i.e. for changes in the crystallographic orientation of grains in region R1).

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