HIGH PERFORMANCE COMPUTATIONAL MODELLING OF MICROSTRUCTURAL PHENOMENA IN POLYCRYSTALLINE METALS

K. Inal and K.W. Neale
Faculty of Engineering,
University of Sherbrooke,
Sherbrooke, Quebec, Canada J1K 2R1,
E-mail: Kenneth.Neale@USherbrooke.ca

Abstract

In this paper, applications of crystal plasticity theory to the numerical modelling of large strain plasticity phenomena are considered. In particular, instabilities and localized deformation phenomena for face-centred cubic (FCC) and body-centred cubic (BCC) polycrystals subjected to various deformation modes are investigated. In-house finite element analyses based on a rate-dependent crystal plasticity model have been developed to simulate the large strain behaviour for sheet specimens subjected to plane strain and plane stress deformation modes. In the formulation, the plastic deformation of an individual crystal is assumed to be due to crystallographic slip and simulations are performed using two approaches. In the first approach, each material point in the finite element analysis is considered to be a polycrystalline aggregate having a large number of FCC or BCC grains, and the Taylor theory of crystal plasticity is adopted to model the behaviour of the polycrystal. In the second approach, each grain is represented individually using one or more finite elements, and the constitutive response within each element is given by the single crystal constitutive model. Both approaches account for initial textures, as well as texture evolution during large plastic deformations. The numerical analyses incorporate parallel computing features. The results of simulations for the above-mentioned deformation modes are discussed, and in certain cases comparisons are made with experimental results for rolled aluminum sheet alloys and for draw quality steels.

Introduction

The mechanical properties of a polycrystalline metal depend on many attributes of its microstructure; consequently, considerable efforts have been devoted to the study of micromechanics. These studies indicate that, among the factors which result in the plastic deformation of single crystals and polycrystals, crystallographic slip occurring by the migration across the slip planes of atomic defects, termed dislocations, is the dominant one.

Crystallographic slip induces lattice rotations, which result in a non-random distribution of the crystal orientations in polycrystals. The textures developed during forming processes are macroscopic averages of such non-random orientations. Research indicates that texture occurs in many metal forming processes such as drawing, extrusion, rolling and sheet metal forming. These textures not only have profound effects on the mechanical and thermal properties of metals, but also have great influence on subsequent fabrication processes as well as on the quality of the products. Thus, it is obvious that accurate simulations of large strain phenomena should consider initial texture and its evolution, as well as the anisotropy induced by the evolution of microstructure and microscopic properties.

To model processes such as texture evolution and its influence on deformation-induced anisotropy, micromechanically based models of plastic behaviour are required. In particular, constitutive relations formulated on the concepts of crystal plasticity must be adopted. Since Taylor's pioneering work in 1938, the prediction of the deformation behaviour of polycrystalline solids from the response of their single crystal constituents has been the focus of many investigations. Thus, many crystal plasticity

M. Pandey et al. (eds), Advances in Engineering Structures, Mechanics & Construction, 583–593.

models have been proposed or modified to simulate the behaviour of polycrystalline metals during plastic deformation from the response of their single crystal constituents.

The mathematical modelling of material behaviour is a very effective way of reducing time and costs involved in optimizing manufacturing processes. Indeed, numerous complex forming operations have been simulated using numerical methods in order to predict critical parameters. Up to the 1980's, most applications involving numerical techniques such as the finite element method have been based on phenomenological constitutive models since microscopic models are significantly more demanding in terms of computational resources. However, the introduction of parallel computers has rendered metal forming modelling based on crystal plasticity feasible since they offer more computational power and storage than serial computer architectures. With proper parallelization techniques, realistic applications based on crystal plasticity can be performed on parallel supercomputers.

In this paper, applications of crystal plasticity theory to the numerical modelling of large strain plasticity phenomena are considered. Crystal plasticity theory is employed to model both FCC and BCC polycrystals where modelling of the polycrystalline aggregates is carried out at various scales. We first recapitulate the constitutive model. Then the parallel computing algorithms are briefly presented. In the last section we present two different applications where crystal plasticity theory is employed to simulate instabilities and localized deformation phenomena for FCC and BCC polycrystals subjected to plane strain tension and plane stress tension.

Constitutive Model

The polycrystal plasticity model formulated by Asaro and Needleman (1985) is employed in the analyses. Accordingly, the total deformation of a crystallite is taken to be the result of two distinct physical mechanisms: crystallographic slip due to dislocation motion on the active slip systems, and elastic lattice distortion. Within an FCC crystal, plastic deformation occurs by crystallographic slip on the 12{111}<110> slip systems. For a BCC crystal, crystallographic slip is assumed to occur on 24 slip systems, the 12{110}<111> + 12{112}<111> systems.

In the rate-sensitive crystal plasticity model employed, the elastic constitutive equation for each crystal is specified by:

$$\overset{\nabla}{\boldsymbol{\sigma}} = \boldsymbol{L}\boldsymbol{D} - \dot{\boldsymbol{\sigma}}^{0} - \boldsymbol{\sigma}\mathrm{tr}\boldsymbol{D} \tag{1}$$

where $\overset{\nabla}{\boldsymbol{\sigma}}$ is the Jaumann rate of Cauchy stress, $\boldsymbol{D}$ represents the strain-rate tensor and $\boldsymbol{L}$ is the tensor of elastic moduli. The term $\dot{\boldsymbol{\sigma}}^{0}$ is a viscoplastic type stress-rate that is determined by the slip rates on the slip systems of a FCC and BCC crystal. A detailed presentation of the crystal plasticity constitutive model can be found in Wu et al. (1997) and will not be repeated here.

The slip rates are governed by the power-law expression

$$\dot{\gamma}_{(\alpha)} = \dot{\gamma}_{(0)}\, sgn\,\tau_{(\alpha)} \left| \frac{\tau_{(\alpha)}}{g_{(\alpha)}} \right|^{1/m} \tag{2}$$

where $\dot{\gamma}_{(0)}$ is a reference shear rate taken to be the same for all the slip systems, $\tau_{(\alpha)}$ is the resolved shear stress on slip system α, $g_{(\alpha)}$ is its hardness and m is the strain-rate sensitivity index. The $g_{(\alpha)}$

characterize the current strain-hardened state of all the slip systems. The rate of increase of the function $g_{(\alpha)}$ is defined by the hardening law:

$$g_{(\alpha)} = \sum_{\beta} h_{(\alpha\beta)} \left| \dot{\gamma}_{(\beta)} \right| \tag{3}$$

where $g_{(\alpha)}(0)$ is the initial hardness, taken to be a constant τ_0 for each slip system, and where the $h_{(\alpha\beta)}$ values are the hardening moduli. The form of the moduli is given by

$$h_{(\alpha\beta)} = q_{(\alpha\beta)} h_{(\beta)} \text{ (no sum on } \beta) \tag{4}$$

where $h_{(\beta)}$ is a single slip hardening rate and $q_{(\alpha\beta)}$ is the matrix describing the latent hardening behaviour of the crystallite.

The single slip hardening law employed in this investigation takes the following power-law form of the function $h_{(\beta)}$

$$h_{(\beta)} = h_0 \left(\frac{h_0 \gamma_a}{\tau_0 n} + 1 \right)^{n-1} \tag{5}$$

where h_0 is the system's initial hardening rate, n is the hardening exponent and γ_a is the accumulated slip.

Two different models are employed to obtain the response of a polycrystal comprised of many grains. In the Taylor model, the material response is obtained by invoking the Taylor assumption. Accordingly, at a material point representing a polycrystal of N grains, the deformation in each grain is taken to be identical to the macroscopic deformation of the continuum. Furthermore, the macroscopic values of all quantities, such as stresses, stress-rates and elastic moduli, are obtained by averaging their respective values over the total number of grains at the particular material point. In the FE/grain model an element of the finite element mesh represents a single crystal, and the constitutive response at a material point is given by the single crystal constitutive model. This approach enforces equilibrium and compatibility between grains throughout the polycrystalline aggregate in the weak finite element sense.

Parallel Computing

In general, Taylor-type polycrystal models are ideally suited for the parallelization of the computational procedures. Especially, when CPU time is considered, the simulations fall in the category of "embarrassingly parallel" (e.g., Sorensen et al. (1995)) applications, and they provide significant computational improvements. However, such "embarrassingly parallel" applications are strictly feasible only if the total program size fits within a single processor of the parallel computer. This is not the case for the simulations presented in this paper, and it was necessary to implement the polycrystal FE model in a data parallel form as described by Beaudoin et al. (1993) and Inal et al. (2002a, 2003).

The parallel computing algorithms employed in the simulations are designed to distribute data on the microscopic level (crystal data) over the processors of a distributed memory supercomputer. By this method, the global size of the simulation is distributed between the processors of the parallel

computer. To illustrate this, consider a simulation with a total number N of crystals (Fig.1). The basic idea in the finite element formulation is that each material point is representing a polycrystal comprised of N crystals and the constitutive response is given through the Taylor polycrystal model (Fig. 1a). The global crystal data is distributed between the processors (Fig. 1b) such that each processor runs a part of the global program for $B = N/A$ crystals where A is the total number of processors used in the simulation. (Note that the processors read only the crystal data to which they are assigned and all arrays containing microscopic quantities have the maximum size of B instead of N.) Thus all processors compute microscopic arrays (for the set of crystals that they have assigned) independently. However, to compute the global stiffness matrix, the macroscopic values of stresses, stress rates and the moduli are required. These values are obtained by collective communication between the processors using the Message Passing Interface.

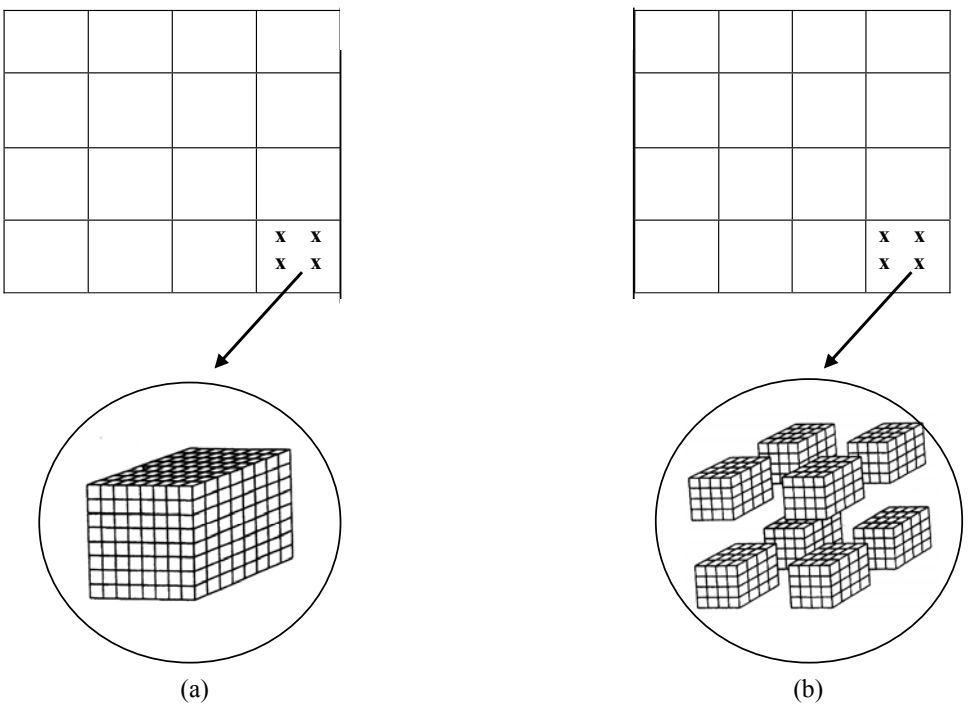


Figure 1. (a) Polycrystal aggregate comprised of N crystals, (b) the distribution of this polycrystal aggregate between processors

The parallel computing algorithms which we have developed are essential for the simulations presented in this paper. These parallel sub-routines enable simulations with sufficiently fine meshes necessary to capture the key features of localized deformation for the aluminum alloy analysed.

Numerical Simulations

In this paper, crystal plasticity theory has been employed to simulate the effects of through-thickness texture gradients in the aluminum alloy AA5754 and the effects of strain paths in localized deformation in drawing quality (DQ) steel. It should be mentioned that the finite element meshes employed in both applications consist of four-node quadrilateral elements, made up of four 'crossed' constant strain triangular sub-elements. In presenting results, the quadrilateral is regarded as the basic element, and when reporting values of the field quantities the average value of the triangles is associated with the centroid of the quadrilateral.

The Effects of Through-Thickness Texture Gradients

It has already been mentioned that, to model processes such as texture evolution and its influence on deformation-induced anisotropy, models based on crystal plasticity have been employed in numerous studies. In these studies it has been assumed that the textures employed are representative of the entire volume. However, most forming processes do not produce materials with uniform spatial distributions of texture. Indeed, without sufficient care in the forming process, significant texture gradients develop (e.g., surface-to-midplane texture gradients in rolled materials, surface-to-core gradients in wires). Thus from a theoretical or practical point of view, it is important to investigate these texture gradient effects on plastic deformation properties.

In this section, a thin, orthotropic sheet specimen submitted to uniaxial tension is modelled (Fig. 2 where 40 x 56 elements are employed) under the assumption of plane strain conditions. The analyses assume no initial geometric imperfection. Localized deformation occurs as a result of the so-called "clamped" boundary conditions applied at the ends ($x_1 = \pm L_0$). With the tensile axis aligned in the x_1 direction, and x_3 being the direction normal to the sheet, the boundary conditions are

$$\begin{aligned} u_3 &= 0 \text{ along } x_1 = \pm L_0 \\ \dot{u}_1 &= \text{V (applied velocity) along } x_1 = L_0 \\ \dot{u}_1 &= \text{-V (applied velocity) along } x_1 = -L_0 \end{aligned} \tag{6}$$

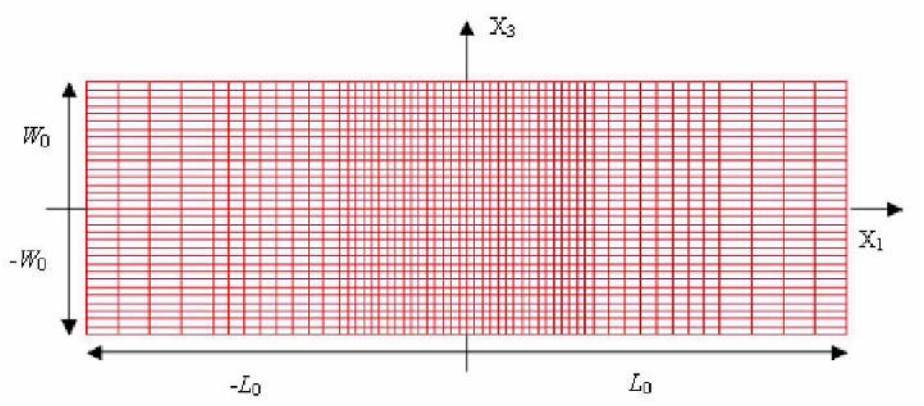
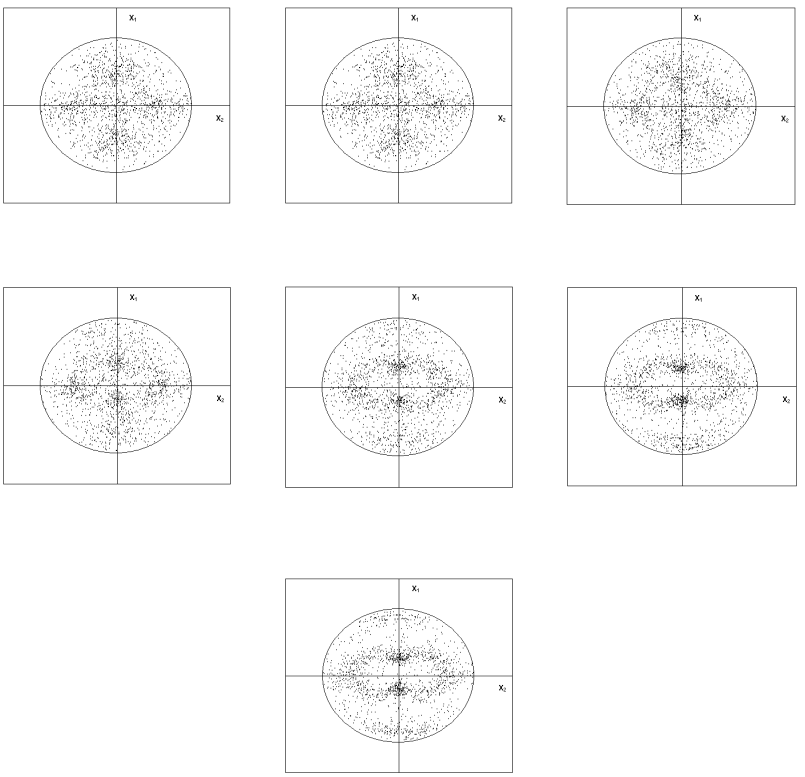


Figure 2. Finite element mesh used in the simulations

A set of discretized orientations of approximately 400 grains, measured at 7 different locations through the thickness of the aluminium alloy AA5754 is employed in the simulations (Figs. 3a-g). It can be seen that the initial textures become sharper towards the centre of the sheet. Thus, the degree of anisotropy increases towards the centre of the sheet. The values of the material properties used in the simulations are

$$\tau_0 = 95 \text{ MPa},\ h_0/\tau_0 = 1.2,\ \tau_s/\tau_0 = 1.16,\ h_s/\tau_0 = 0,\ q = 1.0 \tag{7}$$

The slip system reference plastic shearing rate $\dot{\gamma}_0$ and the slip rate sensitivity parameter m are taken as $\dot{\gamma}_0 = 0.001 \text{s}^{-1}$, and m=0.002, respectively with the crystal elastic constants taken as C_{11} =206 GPa, C_{12} =118 GPa and C_{44} =54 GPa.

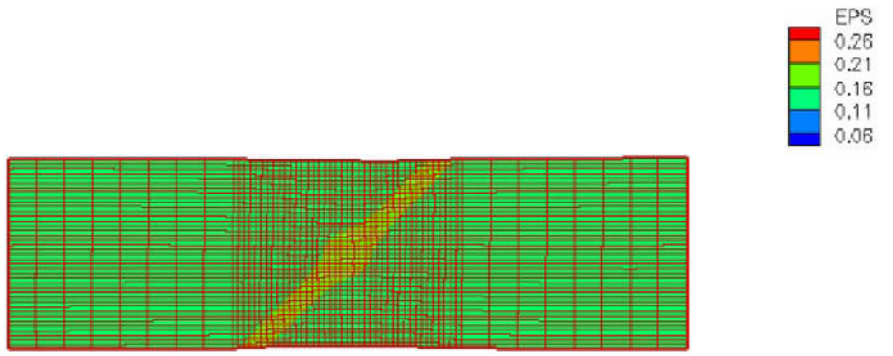


Figures 3a-g. Initial textures of the aluminum alloy AA5754 represented by {111} stereographic pole figures from the surface towards the centre of the sheet

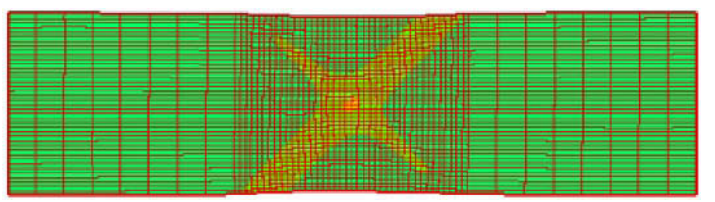
A quantitative representation of shear band development is presented in Fig. 4 where contours of true strain (in the rolling direction) are plotted versus normalized elongation. It can be seen that at an elongation of $U/L_0 = 0.065$, a shear band passing through the centre of the specimen has already developed (Fig. 4a). With further stretching ($U/L_0 = 0.07$), even though strain has began to concentrate in this well defined shear band, a second shear band has developed perpendicular to the first one (Fig. 4b). The fully developed shear bands at $U/L_0 = 0.15$ are presented in Fig. 4c. Note that, although there are two fully developed shear bands intersecting at the centre of the specimen, the primary (first formed) shear band is sharper and wider than the secondary shear band. This pattern is due to the existing through-thickness texture gradients. Previous studies (Inal et al. (2002b, 2002c)) have indicated that when a single layer of texture was employed in the simulations (no texture gradients), multiple shear bands occurred simultaneously with the same intensities. It should also be mentioned that simulations of plane strain tension, where only a single layer of the initial textures (Figs. 3 a-g) was employed (no texture gradients), always predicted a single shear band.

A recent study by Inal et al. (2002b) has shown that when texture evolution is excluded from the analyses, localized deformation in the form of shear bands was not predicted during plane strain tension. To investigate the effect of through-thickness texture gradients on the predicted localisation modes (necking and/or shear banding), the simulation described above was performed once more, but with texture evolution excluded from the polycrystal model. Thus the stretching and rotation of the lattice vectors were excluded in the numerical analysis. Simulations have shown that, when through-

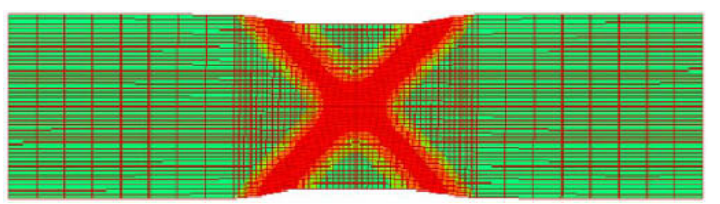
thickness texture gradients are considered, even without texture evolution, localised deformation in the form of shear bands were predicted during plane strain tension (Fig. 5).



(a) $U/L_0 = 0.065$



(b) $U/L_0 = 0.07$



(c) $U/L_0 = 0.15$

Figures 4a-c. True strain at various elongation levels

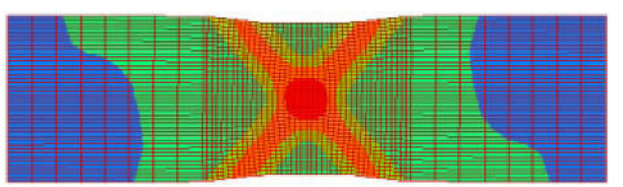


Figure 5. Deformed mesh at $U/L_0 = 0.12$ for the simulation without texture evolution

The Effects of Strain Paths on Localized Deformation in Drawing Quality (DQ) Sheet Steel

Many industrial processes require sheet metal to be subjected to several complex strain paths before the final product is manufactured. One such process is tube hydroforming, where tubed material is

typically bent into a desired shape, placed within a die, then hyrdoformed to alter the tube cross-section. The strain path is complex in that the sheet material is first subjected to a near-plane strain path in the axial direction (i.e., bending), followed by a near-plane strain path in the circumferential direction (i.e., hydroforming). To simulate this process, sheet specimens were first pre-strained in the rolling direction (RD), then were rotated 90° clockwise and pulled along a second (orthogonal) path, such that the transverse direction (TD) was then aligned along the tensile axis (Fig. 6).

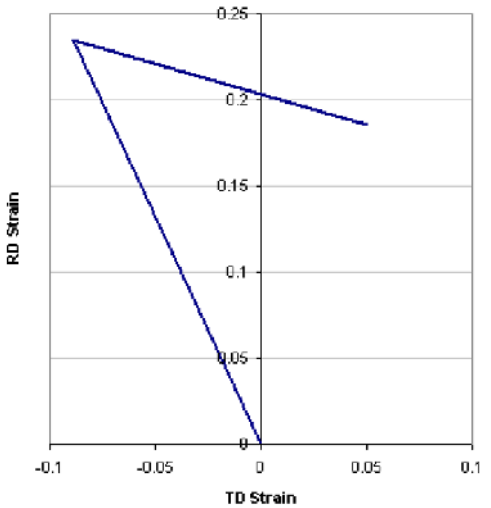


Figure 6. Experimentally observed strain paths for DQ sample

A so-called finite element (FE)/grain model together with a unit cell approach was employed to simulate the strain paths described above. In this model, each element of the finite element mesh represents a single crystal, and the constitutive response at a material point is that given by the single crystal constitutive model. A unit cell is defined as a globally small region of the sheet that contains all the essential micro-structural and textural features that characterize the sheet (e.g., Inal et al. (2005)). The sheet itself is subject to plane stress conditions (i.e., $\dot{\sigma}_{33} = 0$). Orientations within the measured texture data are randomly assigned in the mesh/unit cell. In other words, each element of the mesh represents an orientation from the measured texture. The loading imposed on the edges of the unit cell is assumed to be constant (Fig. 7), such that

$$\frac{\dot{\varepsilon}_{22}}{\dot{\varepsilon}_{11}} = \rho \tag{8}$$

where $\dot{\varepsilon}_{22}$ and $\dot{\varepsilon}_{11}$ are the (principal) logarithmic strain rates. The initial texture for the DQ steel represented by 400 grains/orientations is shown in Fig. 8. In this figure X_1 and X_2 correspond to the rolling and transverse direction of the sheet respectively. The values for the material parameters in the crystal plasticity analysis are $\dot{\gamma}_0 = 0.001\text{s}^{-1}$, m=0.05, $h_0 / \tau_0 = 28$, $\tau_0 = 54.5$ MPa, n= 0.18 and q=1.

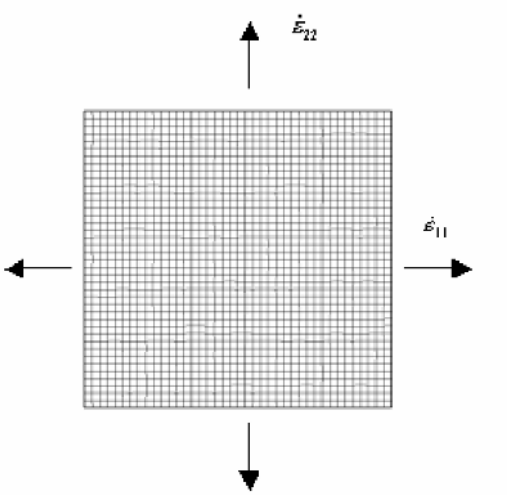


Figure 7. Schematic representation of a unit cell

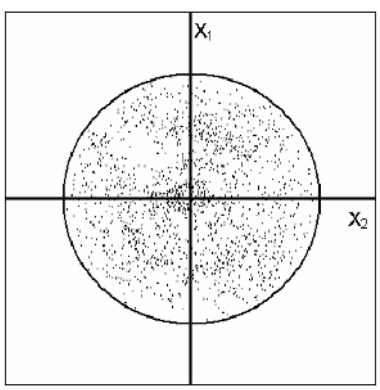


Figure 8. Initial texture represented in terms of {111} pole figure.

The strain paths observed in the experiments (Fig. 6) were imposed at the edges of the unit cell (Equation 8) and numerical simulations were performed with 1600 elements. Thus each grain in the initial texture is represented four times in our simulations. Figs. 9-10 present the measured and predicted textures after the strain paths defined in Fig. 6. It can be seen that the simulated texture is in good agreement with the measured texture. However, the simulated texture is slightly sharper than the measured one. This is probably due to the major drawback of the FE/grain model; i.e., the inevitable inhomogeneous spatial orientation distribution introduced numerically (since the initial texture is assigned randomly to the finite elements). To reduce the effect of spatial distribution of texture components in numerical simulations, the measured crystal orientations are randomly assigned N times to elements in the mesh. In our simulations N, was taken as 4. Usually the higher the N, the lower the effect of the inhomogeneous spatial orientation distribution introduced numerically. Thus, employing higher values on N will improve the overall predicted macroscopic and microscopic responses; predictions were slightly improved when N was taken as 8. However, employing electron

backscattering diffraction (EBSD) data as input is the most efficient technique to minimize the effects of the spatial orientation distribution dependency.

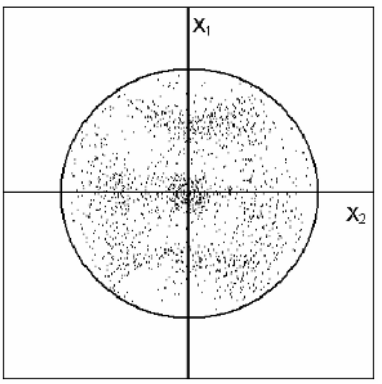


Figure 9. Experimentally measured texture

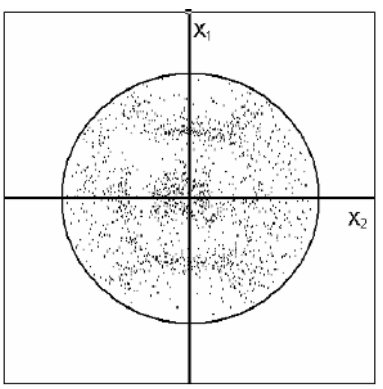


Figure 10. Simulated texture by FE/grain model

Conclusions

In this paper, the implementation of crystal plasticity constitutive relations in the numerical modelling of large strain phenomena was discussed. In particular, the effects of through-thickness texture gradient.

The common metals of industrial practice are polycrystalline aggregates which consist of single crystals or individual grains with lattice structures. As has already been discussed, the mechanical properties of a polycrystalline metal depend on many attributes of its microstructure. Thus, accurate modelling of large strain phenomena should include the effect of the initial microstructure and its evolution. Although phenomenological models are acceptable for many applications, they cannot explicitly include the basic physics of plastic deformation. However, large strain phenomena can be modelled more accurately based on crystal plasticity theories where the initial texture and its evolution, as well as the anisotropy induced by the evolution of microstructure and microscopic

properties, are accounted for. Furthermore, with proper parallelization techniques and supercomputers, realistic applications with crystal plasticity theory are now feasible.

Numerical simulations have shown that both the Taylor model and the FE/grain model can be employed to simulate large strain plasticity phenomena in polycrystalline metals. It should be mentioned that the FE/grain model accounts for the grain morphologies (e.g., grain shapes and sizes), which cannot be modelled with the Taylor approach. However, the major drawback of the FE/grain model is the inevitable inhomogeneous spatial orientation distribution introduced numerically (since the initial texture is assigned randomly to the finite elements). By contrast, the spatial orientation distribution does not present this type of problem in simulations with the Taylor model since this model employs average values obtained from individual grains that do not depend on their relative locations.

Acknowledgements

This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC). K.W. Neale holds the Canada Research Chair in Advanced Engineered Material Systems, and the support of this program is gratefully acknowledged.

References

Asaro, R.J., and Needleman, A. (1985): Texture development and strain hardening in rate dependent polycrystals. Acta Metallurgica, 33, 923-953.

Beaudoin, A.J., Mathur, K.K., Dawson, P.R., and Johnson, G.C. (1993): Three-dimensional deformation process simulation with explicit use of polycrystal plasticity models. International Journal of Plasticity, 9, 833-860.

Inal, K., Neale, K.W., Hamelin, C.J., Diak, B.J., and Pilkey, A.K. (2005): Numerical and experimental investigation of strain path effects on localized deformation in steel alloys. SAE Transactions, (in print).

Inal, K., Wu, P.D., and Neale, K.W. (2003): Parallel computing techniques for metal plasticity applications. High Performance Computing Systems and Applications, D. Sénéchal, Ed., NRC Research Press, Ottawa, Ontario, 133–137.

Inal, K., Neale, K.W., and Wu, P.D. (2002a): Parallel finite element algorithms for the analysis of multiscale plasticity problems. Applications of High-Performance Computing in Engineering VII, C.A. Brebbia, P. Meli and A. Zanasi, Eds., WIT Press, 75–84.

Inal, K., Wu, P.D., and Neale, K.W. (2002b): Instability and localized deformation in polycrystalline solids under plane-strain tension. International Journal of Solids and Structures, 39, 983-1002.

Inal, K., Wu, P.D., and Neale, K.W. (2002c): Finite element analysis of localization in FCC polycrystalline sheets under plane stress tension. International Journal of Solids and Structures, 39, 3469–3486.

Sorensen, N.J., and Andersen, B.S. (1995): A parallel finite element method for the analysis of crystalline solids. DCAMM Report, The Technical University of Denmark, 1-15.

Wu, P.D., Neale, K.W., and Van der Giessen, E. (1997): On crystal plasticity FLD analysis. Proceedings of the Royal Society of London, 453, 1831-1848.