Int J Mater Form (2009) Vol. 2 Suppl 1:523–526
DOI 10.1007/s12289-009-0561-2

TEXTURE PREDICTION FROM A NOVEL GRAIN CLUSTER-BASED HOMOGENIZATION SCHEME

P. Eisenlohr[1]*, D.D. Tjahjanto[1], T. Hochrainer[2], F. Roters[1], D. Raabe[1]

[1] Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
[2] Fraunhofer Institut für Werkstoffmechanik IWM, Freiburg, Germany

ABSTRACT: We propose a method, termed relaxed grain cluster (RGC), which homogenizes the response of polycrystals, subjected to mechanical loads, from the monocrystal constitutive law in order to predict the evolution of deformation resistance and microstructure properties, e.g. texture. Generalizing existing grain interaction models, we consider a cluster of $2 \times 2 \times 2$ homogenous grains at each continuum material point. Allowing for additional displacements of the grain interfaces introduces relaxations with respect to the classical full-constraints (FC) Taylor model. This decouples the local grain deformation gradients, but may induce interfacial mismatch between grains. The relaxations are determined as minimizers of the cluster's total mechanical work density being biased by a (penalty) energy density associated with the interfacial mismatch. In this work the bias is neglected, thus the minimum energy criterium is equivalent to stress equilibrium at each interface. As an example, the evolution of texture for plane-strain compression (simplification for cold rolling) of a commercial aluminum alloy is compared for different configurations of interfacial relaxations. We discuss the resulting variation in texture intensity in light of the different relaxation modes allowed and point out the fully-relaxed RGC scheme to be closest to and in decent agreement with experimental reference.

KEYWORDS: Grain interaction, Homogenization method, Texture evolution

1 INTRODUCTION

Several advancements of the full-constraints (FC) Taylor model lead to improved texture predictions. Relaxed-constraints models (e.g., [1–3]) diminish the strict Taylor assumption of an equal strain (rate) tensor for each grain by allowing for deviations in one or several components of each strain tensor. This may be justified for special anisotropic grain shapes (e.g. flat or elongated). Beyond such global relaxations, particular grain interactions are not considered in these models.

By contrast, grain cluster models compose a meso-scale aggregate of interacting grains (typically two or eight) for which the boundary conditions are jointly imposed. The deformation can be relaxed among the grains within a cluster as long as the external boundary conditions are fulfilled for the entire cluster. The most simple grain cluster model is the so-called LAMEL model [4]. It considers a stack of two grains that are free to move their shared interface in its plane. The inherent anisotropy due to a single stacking direction is addressed by the so-called advanced LAMEL model (ALAMEL [5]), which considers grain interactions in a statistical way and divides each grain into a number of grain boundary regions treated in the spirit of LAMEL. Another route is followed by the grain interaction (GIA) model [6] (see also [7] and references therein for further developments), which considers aggregates of $2 \times 2 \times 2$ grains. A characteristic feature of the GIA model is the penalizing of incompatibilities, which develop among grains, by assigning energy contributions to them. Those are associated with the build-up of geometrically necessary dislocations at the grain boundaries.

The objective of the present research is to develop an efficient homogenization scheme, termed relaxed grain cluster (RGC) model, which is based on the generalization of the grain cluster concept. As an example, the scheme will be used to simulate texture evolution in cold rolling. Furthermore, we investigate the effects of various relaxation modes on the development of particular texture components.

2 RELAXED GRAIN CLUSTER MODEL

We consider the macro-scale material point to be a cluster of $2 \times 2 \times 2$ hexahedral grains of (initially) equal shape and size, which is to be periodically repeated in all three dimensions (see Fig. 1). In the present model, the finite deformation framework is adopted. The effective deformation gradient $\bar{\boldsymbol{F}}$ and the work-conjugated first Piola–Kirchhoff stress $\bar{\boldsymbol{P}}$ of the grain cluster are taken as the volumetric average of the respective local quantities, $\boldsymbol{F}^g$ and $\boldsymbol{P}^g$ (assumed homogeneous), and read

$$\bar{\boldsymbol{F}} = \sum_{g=1}^{8} v_0^g \boldsymbol{F}^g \quad \text{and} \quad \bar{\boldsymbol{P}} = \sum_{g=1}^{8} v_0^g \boldsymbol{P}^g \,, \tag{1}$$

*Corresponding author: Max-Planck-Str. 1, 40237 Düsseldorf, Germany. Phone: +49 211 6792983. Email: p.eisenlohr@mpie.de

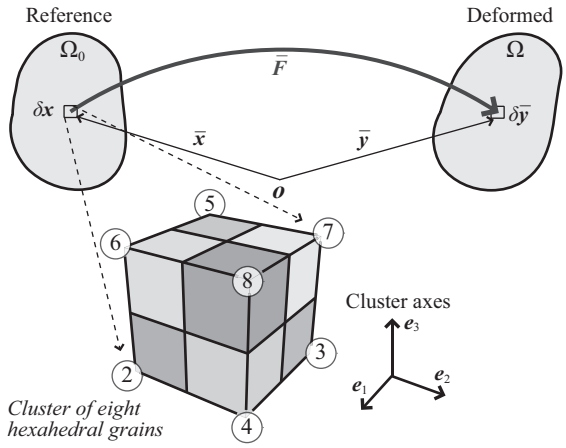

Figure 1: *Macro-scale body in the reference and deformed configurations, where a material point is represented by a cluster of eight hexahedral grains.*

with v_0^g the volume fraction of grain g in the reference configuration. The stress of individual grains results from the local constitutive model $\boldsymbol{P}^g = \hat{\boldsymbol{P}}^g(\boldsymbol{F}^g)$. The relaxation of the local deformation gradient can be conveniently described in terms of *relaxation vectors* $\boldsymbol{a}_\alpha^g$, each attached to one face α of grain g, yielding

$$\boldsymbol{F}^g = \bar{\boldsymbol{F}} + \frac{1}{v_0^g} \sum_{\alpha=1}^{3} \left(\boldsymbol{a}_\alpha^g \otimes \boldsymbol{n}_\alpha^g + \boldsymbol{a}_{-\alpha}^g \otimes \boldsymbol{n}_{-\alpha}^g \right) \qquad (2)$$

with $\boldsymbol{n}_\alpha^g$ the unit vector normal to face α of grain g. There are, in total, $6 \times 8 = 48$ vectors in the whole cluster.

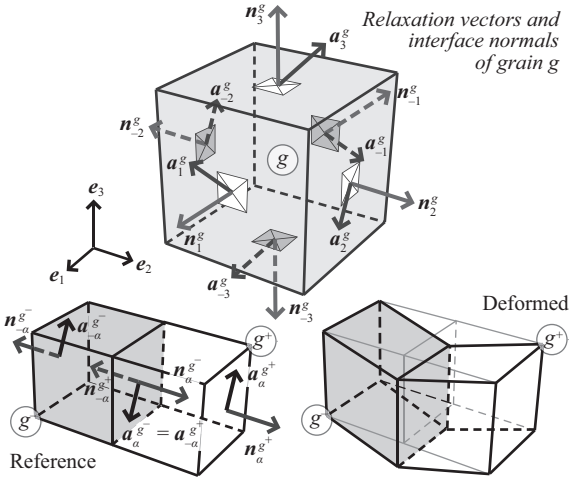

Figure 2: *Relaxation vectors applied at six faces of grain g (top). The effect of relaxation vector $\boldsymbol{a}_\alpha^{g^-} = \boldsymbol{a}_{-\alpha}^{g^+}$ at the shared interface between grains g^- and g^+ (bottom).*

Let g^- and g^+ be two neighboring grains (see Fig. 2 bottom), where face α of grain g^- is identical to face $-\alpha$ of grain g^+. To exclude rigid-body translation of grains, we necessarily impose the kinematical constraints:

$$\boldsymbol{a}_{-\alpha}^{g^+} = \boldsymbol{a}_\alpha^{g^-} \;,\; \boldsymbol{a}_{-\alpha}^{g^-} = -\boldsymbol{a}_\alpha^{g^-} \text{ and } \boldsymbol{a}_\alpha^{g^+} = \boldsymbol{a}_{-\alpha}^{g^-} . \qquad (3)$$

In the case of $2 \times 2 \times 2$-grain cluster, the constraints given by Eq. (3) reduce the number of independent relaxation vectors to 12—corresponding to the interior interfaces in the grain cluster. In the present RGC scheme, these 12 relaxation vectors characterize the local deformation gradients $\boldsymbol{F}^g$ for all grains $g = 1, \ldots, 8$ for any given macroscale deformation gradient $\bar{\boldsymbol{F}}$ (see Eq. (2)).

The independent relaxation vectors are determined by minimizing the total deformation energy density of the cluster, which is taken as the volumetric average of the energy density of individual grains. The solution of this minimization is equivalent to stress equilibrium at each interface, i.e.,

$$\boldsymbol{P}^{g^+} \boldsymbol{n}_{-\alpha}^{g^+} + \boldsymbol{P}^{g^-} \boldsymbol{n}_\alpha^{g^-} = \boldsymbol{0} \,, \qquad (4)$$

for all pairs of connecting grains g^- and g^+, where the normals of the interface $\boldsymbol{n}_{-\alpha}^{g^+} = -\boldsymbol{n}_\alpha^{g^-}$.

Note that for clusters extending in more than one dimension, the relaxation of an interface may cause incompatible deformations or mismatch at other (perpendicular) interfaces. For simplicity, the effect of interfacial mismatch on the cluster response is intentionally neglected in the present formulation. A more detailed description of the RGC model can be found elsewhere [8].

3 ROLLING TEXTURE SIMULATION

We use cold rolling of a face-centered cubic (fcc) commercial AA3104 aluminum alloy as an approximate plane-strain test case and analyze the texture evolution of RGC and variants of it. The first variant, S-RGC, differs from RGC by restricting the interface relaxation vectors according to $\boldsymbol{a}_\alpha^g \cdot \boldsymbol{n}_\alpha^g = 0$, which correspond to shear-only relaxations. The second variant, AFGIA, follows similar concepts as the RGC scheme, but is formulated in the (symmetric) infinitesimal strain framework yet does not enforce symmetry of corresponding interface relaxations.

3.1 TEXTURE AND BOUNDARY CONDITIONS

In this study textures are represented by sets of 8000 grains, thus all of the grain cluster homogenization schemes are evaluated for 1000 clusters consisting of eight grains each. Identical boundary conditions are applied to all 1000 clusters; each cluster acts independently from all others, hence no account is taken for any interaction among material points.

The right-handed coordinate system attached to the rolling direction (RD), transverse direction (TD), and normal direction (ND) of the rolled sheet material is $\boldsymbol{e}_1 \parallel$ RD, $\boldsymbol{e}_2 \parallel$ TD, and $\boldsymbol{e}_3 \parallel$ ND. Then, the rolling process as a function of time t can be idealized as isochoric plane-strain compression, which is expressed as a deformation gradient in the finite deformation framework by

$$\left[\bar{F}\right] = \begin{bmatrix} 1+\dot{\varepsilon}t & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1/(1+\dot{\varepsilon}t) \end{bmatrix} , \qquad (5)$$

where $\dot{\varepsilon} = 0.007\ \mathrm{s}^{-}1$ is the engineering strain rate in tension. In this case, t runs up to 1280 s, which corresponds to about 90 % thickness reduction.

3.2 RESULTS AND DISCUSSION

Figures 3 and 4 present the texture evolution in terms of, respectively, the fcc α-fiber (Euler angles $\phi = 45°, \varphi_2 = 0°$) and β-skeleton intensity plus location of maximum intensity predicted by the FC Taylor, AFGIA, S-RGC, and RGC homogenization schemes in comparison to data measured by Hydro Aluminium Deutschland, Bonn.

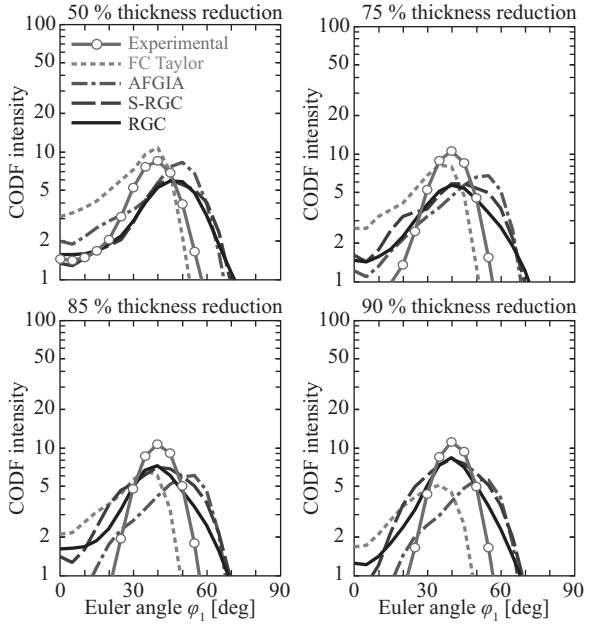

Figure 3: *Evolution of α-fiber intensity during cold rolling predicted by various grain cluster-based schemes compared to experimental data.*

The RGC and S-RGC schemes most closely match the experimental intensity distribution. The β-skeleton intensity in Fig. 4 exhibits a systematic reduction between the $\{1\,1\,2\}\langle 1\,1\,\bar{1}\rangle$ orientation at $\varphi_2 = 45°$ (Cu component) and the $\{1\,2\,3\}\langle 6\,3\,\bar{4}\rangle$ orientation at $\varphi_2 \approx 63°$ (S component) in the order of FC Taylor, AFGIA, S-RGC and RGC. The intensity close to the $\{1\,1\,2\}\langle 1\,1\,\bar{1}\rangle$ orientation at $\varphi_2 = 90°$ (Brass component) is, however, not influenced to a large extent by the choice of homogenization.

The development and in-grain orientation scatter of the Cu, S, and Brass components were studied in detail in some earlier works [9, 10] and crucially depend on the details of the boundary conditions imposed in a model calculation. These studies showed that the development of those components is promoted by the relaxation of certain grain-to-grain shear constraints within a grain cluster or for the overall aggregate (in the case of a simpler model). Specifically, the exact position and intensity of the Brass component seemed to depend on the micro-mechanical relaxation of the shear between rolling and transverse direction (RD and TD). The current results clearly show that

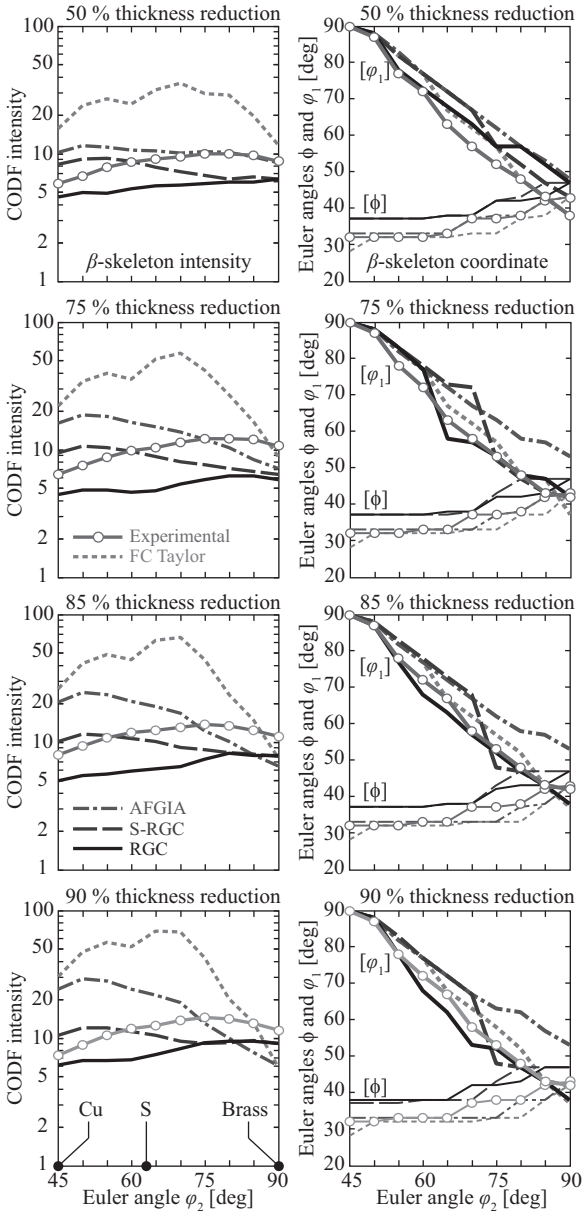

Figure 4: *Comparison of β-skeleton intensity and coordinate resulting from different grain cluster schemes to experimental reference.*

this orientation is much less sensitive to the details of relaxation and strain constraints than are the S and Cu orientations. This is not surprising since the Brass orientation is also the stable Sachs orientation, which is formed when using a Tucker stress state in conjunction with single crystal mechanics and no strain constraints. This means that from an fcc single crystal Schmid estimate the crystallographic $\{1\,1\,0\}$-direction is gradually oriented parallel to the compression axis and the $\langle 1\,\bar{1}\,2\rangle$-axis parallel to the rolling direction. Since the slip systems with the highest Schmid factors are also dominant systems in polycrystal models which impose strain constraints one can conclude that the Brass orientation might be less sensitive to changes in the boundary conditions than the other two components.

The systematic decrease of intensity occurring between the Cu and S component coincides with an increase in the degree of relaxation allowed by the different schemes. For a cubical cluster of eight grains the maximum number of constraints possible in the framework of infinitesimal strain is 8 grains $\times$ 6 components of (symmetric) strain $= 48$, while in the finite deformation framework it is 8 grains $\times$ 9 components of deformation gradient $= 72$. In either framework, the FC Taylor model allows for zero relaxations. Analyzing the remaining relaxation schemes reveals the sequence of increasing number of possible relaxations to be 20 for AFGIA, 24 for S-RGC, and 36 for RGC.

This finding is in-line with the observation that the S component is in fcc crystals generally much less stable than the Brass component. Beaudoin *et al*. [11] showed by detailed crystal plasticity finite element simulations for a grain cluster aggregate consisting of eight different variants of the S orientation that this component tends to undergo strong in-grain orientation fragmentation. The orientation spread that was observed after plane-strain deformation of this grain ensemble extended through the entire α-fiber. This earlier observation underlines that the S component is very sensitive to the internal boundary conditions as is also evident from the large deviations among the different models observed here.

The results for the Cu component after 90 $\%$ thickness reduction show two groups with different tendency. The first class of rather stiff models (FC Taylor and AFGIA) predicts a quite strong orientation density. The second class of more compliant models (S-RGC and RGC) predicts a more modest orientation density for this component. This result is interesting and reflects the different model approximations and their effect on the different texture components. The Cu orientation is relatively close (7°) to the Taylor orientation $\{4\,4\,11\}\langle 11\,11\,\bar{8}\rangle$, which is the most stable orientation in FC Taylor simulations for fcc crystals. Hence, the Cu orientation is promoted by stiff boundary conditions. However, if these stiff constraints are relaxed, the orientation density in the Cu component drops. This characteristic behavior of the Cu component is in contrast to the high stability of the Brass component, which does not change much under different relaxation modes. The Brass component is stress-stabilized as pointed out above, i.e., the main slip systems which are activated under plane-strain will under most relaxation states dominate the deformation of this component.

The Cu orientation, in contrast, is strain-stabilized. Its stability does not result, as for the Brass orientation, from a characteristic set of highly stressed slip systems. The active slip systems (under plane-strain) of the Cu orientation are not so highly stressed as in case of the Brass orientation and, therefore, depend more sensitively on the boundary conditions. This means that the closer the constraints of a model are to the FC Taylor assumption, the stronger the orientation density of the Cu component should be. This is reflected by the current results.

4 CLOSING REMARKS

The relaxed grain cluster (RGC) scheme illustrated in this work shows a very encouraging concurrence with experimental texture evolution in cold rolling of fcc aluminum. Likely, the most crucial novelty in this scheme is the adoption of the finite deformation framework in contrast to earlier grain cluster models. Its dissociation from any particular grain constitutive law recommends the scheme for application in multi-mechanism and/or multi-phase settings.

REFERENCES

[1] H. Honneff and H. Mecking. Analysis of the deformation texture at different rolling conditions. In *Proc. 6th Int. Conf. on Texture of Materials (ICOTOM-6)*, volume 1, pages 347–355, Tokyo, 1981. The Iron and Steel Institute of Japan.

[2] U.F. Kocks and H. Chandra. Slip geometry in partially constrained deformation. *Acta Metall.*, 30 (3):695–709, 1982.

[3] P. Van Houtte. On the equivalence of the relaxed Taylor theory and the Bishop–Hill theory for partially constrained plastic deformation of crystals. *Mater. Sci. Eng.*, 55(1):69–77, 1982.

[4] P. Van Houtte, L. Delannay, and I. Samajdar. Quantitative prediction of cold rolling textures in low-carbon steel by means of the LAMEL model. *Textures Microstruct.*, 8-9:109–149, 1999.

[5] P. Van Houtte, S. Li, M. Seefeldt, and L. Delannay. Deformation texture prediction: from the Taylor model to the advanced Lamel model. *Int. J. Plasticity*, 21(3):589–624, 2005.

[6] P. Wagner. *Zusammenhänge zwischen mikro- und makroskopischen Verformungsinhomogenitäten und der Textur*. PhD thesis, RWTH Aachen, 1994.

[7] M. Crumbach, M. Goerdeler, and G. Gottstein. Modelling of recrystallisation textures in aluminium alloys: I. Model set-up and integration. *Acta Mater.*, 54:3275–3289, 2006.

[8] D.D. Tjahjanto, P. Eisenlohr, and F. Roters. A novel grain cluster-based homogenization scheme. submitted.

[9] J. Hirsch and K. Lücke. Overview no. 76: Mechanism of deformation and development of rolling textures in polycrystalline f.c.c. metals–I. Description of rolling texture development in homogeneous CuZn alloys. *Acta Metall.*, 36(11): 2863–2882, 1988.

[10] J. Hirsch and K. Lücke. Overview no. 76: Mechanism of deformation and development of rolling textures in polycrystalline f.c.c. metals–II. Simulation and interpretation of experiments on the basis of Taylor-type theories. *Acta Metall.*, 36(11): 2883–2904, 1988.

[11] A.J. Beaudoin, H. Mecking, and U.F. Kocks. Development of localized orientation gradients in fcc polycrystals. *Philos. Mag. A*, 73(6):1503–1517, 1996.