Article I. Statistical models for deformation texture prediction using vortex-type accommodation of local strain misfits

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Abstract. Many advanced models for deformation texture prediction make use of crystal plasticity finite element or fast Fourier methods. They manage to deal with strain heterogeneities at very small length scales. However, they demand a lot of calculation power, too much for daily use as tools for computer aided design/manufacturing of forming operations of steel or aluminium sheet parts. So-called statistical models for deformation texture and plastic anisotropy are still of interest in such cases, as they are fast and can indeed be incorporated as constitutive models in finite element simulations of metal forming processes. The present work discusses the existing statistical models. Predicted ODFs of rolling textures of a few steel and aluminium alloys will be compared with those of older models as well as with experimental results. A currently undertaken attempt to further improve the quality of the predictions of one of the statistical models (ALAMEL) will be proposed. Not only the effect of local deviations from homogeneous strain ("relaxations") on the plastic work in the grains will be considered, but also the increase of plastic work due to the plastic accommodation of these misfits. This is done by assuming the existence of certain flow patterns in the matrix surrounding the grains, some of which resembling the "vortices" sometimes observed in liquids.

1. Introduction

Sheet metal (aluminum or steel, used in the metal forming industry for the production of car bodies) usually features a strong crystallographic texture which causes a strong plastic anisotropy in the material. For various applications (product design, quality monitoring) it is then desirable to model the deformation process including its effect on the change of the material properties. This sets the following problem: to properly model the forming process, one needs to know the texture in a given location in the workpiece, because it makes the constitutive law anisotropic. But this anisotropy itself is constantly changing due to the progress of the forming process. So one needs a modelling procedure that simulates the intricate coupling between the mechanical deformation, the texture evolution being caused by it, and the evolution of the plastic anisotropy (itself caused by the evolution of the texture). In principle this could be dealt with by a crystal-plasticity finite element code (CP-FEM), see e.g. Roters et al. [1], or by a Crystal-Plasticity Fast Fourier (CP-FFT) model, see e.g. Lebensohn et al. [2]. Using CP-FEM for the entire polycrystal would require an enormous computational power in case the objective would be to optimize an industrial production process; even the much more efficient CP-FFT method would (at the time being) require a calculation power beyond reach of SMEs or single research groups at universities. So we have recently proposed the "Hierarchical Multi-Scale method" (HMS) [3]. It would not treat the entire workpiece as a single polycrystalline material in which each grain has a different velocity gradient, but rather try to capture its over-all behavior by introducing "integration points" at three different length scales:

- largest: "engineering length scale", looking at the entire work piece, modelling its elastic-plastic or visco-plastic behavior by an standard engineering FE model such as Abaqus. The smallest "items" considered at this length scale are the integration points used by this software.
- these integration points are then considered as polycrystals with typically 5000 grains. They are the representative volume elements (RVEs) of the 'macroscopic' length sale. A 'polycrystal deformation model' will be used to obtain the anisotropic stress-strain relationship at the macroscopic length scale, to be used by the constitutive model at the engineering length scale.

Now, consider that all this is done for a single time increment. Abacus will then provide a new velocity gradient for each of its own integration points (at the 'engineering length scale'). This means that the effect of the deformation step can now be implemented at the smaller length scales. Indeed, a strain increment tensor is obtained from the velocity gradient (and for a given time increment) at each
Abacus-integration point, leading to a typical polycrystal problem: given the average strain increment of the polycrystal, what is the strain increment of each of its grains? The problem can in principle be solved by means of a **polycrystal deformation model**, leading to new textures at the integration points of the 'engineering length scale', i.e. the textures of the RVEs of the macro-scale (macro-RVEs). However, it should be noted that other updates must also be done, namely of the constitutive laws at each integration point (the anisotropic stress-strain relationship at the macroscopic length scale). Once this has been done, all is ready for the simulation of a next deformation step by Abacus (at the 'engineering length scale').

2. **Polycrystal deformation models**

So it is clear that a good polycrystal deformation model is needed. Just how good it needs to be is an other matter. The present authors are dedicated to texture research, so they have decided to work with macro-RVEs consisting of 2000 or 5000 grains, as in earlier work it had been found that a texture represented by a discrete set of 2000 grains was about good enough to make acceptable calculations of $r$-values of fcc metals, the standard deviation of the error on the $r$-values being of the order of 0.002 (Tóth and Van Houtte [4]). Another issue is the choice of the polycrystal model. Excellent quality is expected from CPFEM (see e.g. [1]) and CP-FFT methods (see e.g. [2]), but also from VPSC methods see e.g. Lebensohn and Tomé [5]. Of these methods, CPFEM requires most computer power followed by CP-FFT, in any case too much for the purpose set in the present work. Note that these two models try to explicitly model the heterogeneity of stresses and strain rates inside the individual grains as well as the mechanical interactions between them. In contrast to this the so called 'statistical methods' only adopt certain assumed relationships between for example the plastic velocity gradient tensors of individual grains and certain statistical quantities of the entire polycrystal (such as its average velocity gradient tensor). This is even true for the currently most complex statistical method: the visco-plastic self-consistent method (VPSC). Predictions (deformation textures, flow stresses etc.) made by statistical models are less precise as those made by CPFEM and CP-FFT models but nevertheless deserve a discussion (see e.g. Van Houtte et al. [6]) as some of these achieve good quality of predictions combined with high calculation speeds, which makes their application in the context of the HMS method [3] possible. Some well known statistical models have been described in detail by Van Houtte et al. [6]. The simplest is the Taylor-Bishop-Hill model which requires that the macroscopic displacement gradient applies to each of the individual grains.

![Diagram](image)

**Fig. 1** (a) Schematic representation of a rolling process applied on a stack of 2 grains, both of which originally had a square cross section. (b) After rolling (compression + elongation), their cross section has become rectangular, at least according to the Taylor model. (c) according to one of the relaxed constraints models (Pancake), each grain may have undergone an additional simple shear called 'relaxation'. These relaxations are chosen as to minimize the plastic work in the grain. There is no relationship between the relaxation shears of the two grains.

Another class of models are the conventional relaxed constraints models, which differ from the Taylor-Bishop-Hill model by the fact that some of the 'simple shear' components of the macroscopic displacement gradient tensor are NOT enforced on the individual grains, but instead chosen in such
way that that the plastic work required to deform the grain is minimized (Fig. 1c). This deviation from the prescribed macroscopic velocity gradient is described by a tensor called 'relaxation tensor' which is the product of a user-defined velocity gradient tensor describing a unit shear rate with a scalar \( \dot{\gamma}_r \). This scalar is a sort of 'additional slip rate' to be estimated by the model in order to minimize the plastic work required to deform the grain.

3. Cluster models

Such models subdivide the grains of a polycrystal in 'clusters' of \( n \) grains, neighboring each other or not (Fig. 2d-e). It is requested that the average velocity displacement gradient tensor of each cluster is equal to the average at the macroscopic length scale (i.e. overall average of the polycrystal). This consistency requirement is easily achieved in case of the ALAMEL model [6] (Fig. 2e).

![Fig. 2](image-url)

**Fig. 2** As fig. 1, except: (d) is a cluster of 2 grains. The relaxations come in pairs of opposite shears so that the average relaxation is zero. Usually a second pair of relaxations is also applied, which has the same shear plane but a shear direction perpendicular to the plane of the drawing. (e) ALAMEL model: similar to (d), but in addition it is assumed that the two grains have a common grain boundary, which is parallel to the shear plane of the relaxation.

More general cluster models have been proposed by other authors: the GIA model by Crumbach et al. [7] and the RGC model by Eisenlohr et al. [8] operate on 8 grains organized in a 2x2x2 cluster. The grains touch each other (Fig. 3a). Initially the 8 grains have the same brick shape. The cluster has 3 mutually orthogonal symmetry planes. Their intersections form an orthogonal reference frame. Each relaxation consists of a set of 2 shears with opposite signs at both sides of one of the symmetry planes. Note that this preserves the consistency, the average relaxation of the cluster being kept equal to zero. Fig. 3 illustrates a configuration that would be obtained in case of rolling. The plane of the figure is one of the symmetry planes of the process (the plane formed by ND and RD). The effects of 2 out of the 6 relaxations can be seen in this figure. Please note that each of the 8 grains will feel the overlapping effects of 3 of the 6 relaxations, themselves organized in 3 pairs of 2 relaxations with opposite sign. So three independent values (called \( \dot{\gamma}_I, \dot{\gamma}_{II}, \text{ and } \dot{\gamma}_{III} \)) characterize the 6 relaxations. Their effect on the strain rate in each of the 8 grains can easily be mathematically described, and so can their effect on the strain rate tensor of each of the 8 grains. The authors of this model have used the latter in a mathematical model based on crystal plasticity to calculate the rate of plastic work in each of the grains, as a function of the three relaxations. Note however that the authors of the GIA model [7] have realized that such shear relaxations would create additional misfits between the 8 grains of the cluster and the matrix surrounding the cluster. This would require additional plastic accommodation strains in the matrix and/or the grains. In some variants of their model this is taken into account by estimating the density of geometrically necessary dislocations (GNDs) which would
Fig. 3. Cluster model: sideview on a cluster of 8 brick-shaped grains in the microstructure of a rolled polycrystal. The deformation of the grains is supposed to be 'relaxed' by 6 pairs of opposite shear relaxation systems. Pair I (with \( \gamma_I \)) operates along the rolling plane in RD. Pair II (with \( \gamma_{II} \), not visible in the figure) also operates along the rolling plane, but in TD. In a similar way, pairs III and IV operate along the plane normal to RD (in ND with \( \gamma_{III} \) as well as in TD with \( \gamma_{IV} \), not visible). Finally, pairs V and VI operate along the plane normal to TD (in RD and ND, \( \gamma_v \) and \( \gamma_{VI} \) both invisible in the figure).

Some remarks can be given about the stress equilibrium issue. Van Houtte [9] published a short summary of work done mainly by other authors demonstrating that the introduction of a shear-type relaxation in a Taylor-Bishop-Hill type model is equivalent to requesting that the corresponding shear stress is zero. Doing this for all grains would means that the model sets the corresponding shear stress component to zero in all grains. Introducing a relaxation in the form of opposite shears in adjacent grains (as is done by cluster models) creates equilibrium of the corresponding shear stress components at the grain boundary [6]. However, it remains true that the requirement for stress equilibrium at all grain boundaries is far from being satisfied by these statistical models; this remains the privilege of CPFEM and CP-FFT models. Benchmarks can be done by comparing the results of cluster models with those of CPFEM models. This was done for ALAMEL [10], giving insight in the degree of approximation of CPFEM: not perfect, but acceptable given the difference in calculation time.
4. VPSC model and associated cluster model

The visco-plastic model for metallic crystals uses a linear relationship between the deviatoric stress and the plastic strain rate. The effect is rather weak: multiplying the strain rate by 100 might only slightly increase the stress. The effect can nevertheless be used to establish a formula giving a linear relationship between stress deviators and plastic strain rates. That has allowed several authors to develop the 'Visco-Plastic Self Consistent (SC) model' [5, 11-12], inspired by the self-consistent method from elasticity theory. It uses the Eshelby relations which derive the relationship between stress concentrations acting on an 'inclusion' which for some reason undergoes a different strain as the nominal average strain of the material. In the VPSC method, the linear relationship between stresses and elastic strains is replaced by one between stress and plastic strain rate deviators. The model assures consistency between the macroscopic and the mesoscopic levels: the macroscopic stress and plastic strain rate deviators are made equal to the volume averages of the corresponding values in each grain. Note that:

- as to the main strain mode: in contrast to the Taylor-Bishop-Hill theory and its 'relaxed' versions, the model sees it that 'hard' grains are less deformed than 'soft' grains;
- note however that the VPSC model has not been designed to assure stress equilibrium at grain boundaries, as CPFEM does.

Xie et al. [13] have proposed a cluster model called 'cluster 2' (2-grain clusters) or 'cluster 5' (5-grain clusters). It makes use of the VPSC method. Note that:

- the average strain rate of each of these clusters needs to be equal to the macroscopic strain rate.
- the grains in the clusters need not be direct neighbors. Each cluster is treated independently as a small polycrystal by the Neffect-VPSC model (Tomé [12]) which delivers the strain rates and deviatoric stresses of each of the grains. Some results will be given in Table 2.

Comment: as far as the interaction between grains is concerned, an intermediate length scale is introduced between the macroscopic and the mesoscopic (=grain) length scales.

5. Some results of the existing models for cold rolling

| Reduction | 40%    | 63%    | 86%    | 95%    | 98%    |
|-----------|--------|--------|--------|--------|--------|
| FC        | 0.208  | 0.584  | 0.636  | 0.272  | 0.388  |
| VPSC      | 0.429  | 0.824  | 0.501  | 0.409  | 0.465  |
| GIA       | 0.208  | 0.355  | 0.257  | 0.190  | 0.253  |
| LAMEL     | 0.344  | 0.653  | 0.346  | 0.183  | 0.196  |
| ALAMEL    | 0.189  | 0.433  | 0.306  | 0.156  | 0.171  |
| I_{exp}   | 2.59   | 2.45   | 4.51   | 6.87   | 9.23   |

Table 1 Normalised texture index (ID_N) of difference ODFs for AA1200.

FC= FC Taylor theory; VPSC: Visco-Plastic Self-Consistent Model (Lebensohn et al.[5]); GIA (Crumbach et al. [7]); LAMEL: as ALAMEL starting with elongated grains [14]; ALAMEL: standard version [6], starting with equiaxed grains.

Table 1 (from [6]) gives an idea about ID_N after cold rolling of an AA1200 aluminum alloy. The ODF of the initial texture had been measured and used as initial texture in the simulations. The quality of agreement between predicted deformation and observed textures was then assessed by means of the following parameters:

\[ ID = \int \left[ f_1(g) - f_2(g) \right]^2 dg \quad \text{and} \quad ID_N = \frac{ID}{I_{exp}} \]

in which \( f_1(g) \) is the experimental ODF and \( f_2(g) \) the predicted one. The integral \( ID \) is taken over entire Euler space. \( ID_N \) is the value of \( ID \) normalized by the texture index \( I_{exp} \) (integral of the square of the ODF) of the experimental texture. \( ID_N \) can only be 0 when both ODFs (experimental and predicted)
are exactly equal to each other in all 6859 (=19³) points of the discrete representation of both ODFs. Table 2 compares IDₙ results obtained by the new cluster model described above with those of other models.

|                     | Taylor | ALAMEL | Cluster2 | Cluster5 | VPSC |
|---------------------|--------|--------|----------|----------|------|
| DC06 compression ND 40% | 0.04   | 0.05   | 0.04     | 0.04     | 0.09 |
| DC06 simple shear RD 40% | 0.18   | 0.14   | 0.09     | 0.07     | 0.07 |
| DC06 simple shear RD 100% | 0.45   | 0.25   | 0.12     | 0.13     | 0.21 |
| AA6016_cold rolling _86% reduction | 0.51   | 0.24   | 0.25     | 0.22     | 0.37 |
| T61 30% cold reduction  | 0.20   | 0.10   | 0.05     | 0.06     | 0.10 |
| T61 60% cold reduction  | 0.67   | 0.20   | 0.15     | 0.14     | 0.23 |

Table 2 Normalized texture index of the difference ODFs (IDₙ) for Taylor FC, ALAMEL, VPSC, Cluster2 with 2500 clusters and Cluster5 with 1000 clusters[13].

6. Current work

6.1. Concept

CPFEM models applied on polycrystalline materials (e.g. 1000 grains or more) are expected to be able to capture effects due to the heterogeneity of plastic deformation in a real polycrystal. The average plastic deformation differs from one grain to another, which in fact can only be achieved when the internal deformation of each crystal is heterogeneous, otherwise the integrity of the material is lost. Only in this way material integrity can be achieved everywhere in the material while simultaneously guaranteeing stress equilibrium everywhere. Now, suppose that one needs at least 30 elements to capture the heterogeneity of stress and strain rate inside a grain, while at least 1000 grains at least are needed to predict the overall anisotropy of a polycrystal in a satisfactory way. That means that CPFEM models with 30000 elements or more would be needed to make satisfactory texture and anisotropy predictions. The present authors then consider it a challenge to try to develop new statistical models which would offer a good compromise: still sufficiently accurate for industrial applications however less of course as CPFEM or CP-FFT models. When looking at their own models (especially ALAMEL), the present authors feel that what is mainly lacking is a way to deal with the misfits that are created between the grains of the polycrystal. CPFEM does offer solutions without such misfits - but at a price. So a 2-grain cluster model (Fig. 2 d) is currently being developed, which

- tries to describe the reduction of plastic work in the grains due to shear relaxations as an analytical function f₁ of these shear relaxations;
- assumes that each grain is surrounded by a "matrix" which has the average plastic properties as the polycrystal in the current condition;
- uses a kinematically admissible velocity field in the matrix that would indeed accommodate the misfit created in the matrix;
- calculates the increase of plastic work that this would cause in the matrix, also in the form of an analytical function: f₂⁺;
- minimizes the sum f₁ + f₂⁺ by choosing the best values for the shear relaxations.

The authors believe that this can be done, although they do not yet know whether the resulting model would deserve the effort.

6.2. Constitutive model of the matrix

The direct surroundings of each grain of such ‘cluster’ model will be treated as if they have the average plastic properties of the entire polycrystal. In the first version of the model a von Mises model will be used for these. At the beginning of each deformation step, the Taylor model will be used to estimate the flow stress of the polycrystal for the nominal strain mode, however taking the current texture into
account. This particular flow stress/strain rate combination must then be reproduced by the 'matrix' model, i.e. the von Mises model mentioned above.

**Fig. 4** Kinematical model for a grain with a shear relaxation. The grain is in this example is already elongated. It is supposed to undergo plane strain deformation as in cold rolling. The shear relaxation in the grain is indicated by velocity vectors. The matrix regions RA1 and RA2 right and left of the grains are supposed to locally accommodate the grain relaxation by a rigid body rotation overlapping the deformation of the matrix itself. This rotation does not require additional plastic work in RA1 and RA2. The regions in the matrix above and below the grain (SA3 and SA4) accommodate the grain relaxation by an opposite shear (overlapped on the nominal strain rate in the matrix). Note that the velocity caused by the relaxation at the top of SA3 and the bottom of SA4 is zero. This is not the case at the half circular outer boundaries of RA1 and RA2. The tangential velocities there are continued in SA1 and SA2 where they decrease linearly when moving in outward direction, to become zero when arriving at the outward boundary with the matrix; this resembles a vortex-type pattern.

6.3. **Kinematic model for a shear-type relaxation and its accommodation by the matrix**

Fig. 4 shows a 2-D kinematically admissible model (i.e. no density changes anywhere in the material) for a grain undergoing shear relaxation, including the accommodation of this shear relaxation by the matrix around the grain. That means that at the outer boundary of the accommodation zone the change of the material velocity due to the relaxation is exactly zero in all points. As a result this hypothetical accommodation field does not violate the integrity of the material. It has been inspired by one which has been proposed many years ago by Brown [16] in a paper called 'Transition from laminar to rotational motion in plasticity' in which he proposes a model for the hardening of an aluminium alloy by hard particles. It is possible to generalize the velocity field of fig. 4 in order to also achieve such compatibility at the interfaces not shown in the figure (those which are parallel to the plane of the drawing). Note also that before the era of powerful computers, scientists and engineers already used kinematically admissible velocity fields to estimate the metal flow and the forces required for it, using the 'upper bound theorem' [17] from plasticity theory to get an upper limit of the plastic work required to achieve the forming operation. The application of this theorem would in the present case mean that the relaxations must be chosen in such way that the total dissipated plastic work in the grain and in the matrix must be minimized (relaxations decreasing the plastic work in the grain, but increasing it in the matrix). In the present work, it will be tried to use only analytical equations for the estimation of the dissipated plastic work in order to get a good compromise between
accuracy and calculation time. All equations had been already developed at the time that the present paper was written. The software tests have however not yet been completed.

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