# A new cluster-type statistical model for the prediction of deformation textures

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**Abstract.** An attempt was done to improve the quality of deformation texture predictions by statistical models through the introduction of "clusters" of *N* grains thus defining a third, intermediate length scale. The interaction between each cluster and the macroscopic length scale is of the Taylor type, whereas inside each cluster a VPSC scheme is used. Predictions of cold rolling deformation textures were quantitatively compared with experimental results for a steel alloy. The results are encouraging.

## 1. Introduction

During the plastic deformation of polycrystalline materials, the boundary conditions (forces, displacements) applied at the outer borders of the work piece are somehow transmitted to the individual grains (stresses, strains). This process is quite complex, and can be captured by CPFE [1] or CP-FFT [2] models, which could be used for deformation texture predictions. However, these models are so far too computation-intensive for certain applications, such as FE simulations of industrial deep drawing processes in which the evolution of texture and plastic anisotropy in every integration point is tracked and accounted for *during* the FE simulation. Statistical models may still be preferred in that case [3]. Note that only single-phase materials are considered in what follows.

## 2. Boundary conditions as used in statistical models for deformation textures

These models operate on discrete sets of crystals, each modelled by at least their crystal orientation and weight factor. Such set must be statistically representative for the initial condition of the material of which a metal forming operation is to be simulated. Statistical models use simple assumptions about the transmission of external forces and displacements throughout the polycrystal. They are usually formulated in terms of 'interactions': the long range interaction is the relationship between the stresses and velocity gradients of the RVE (Representative Volume Element) at the macroscopic length scale (see Fig. 1) and those of the RVEs at smaller length scales, usually grains (at what is called here 'mesoscale', Fig. 1). Short-range interactions are those between directly neighbouring grains. The well-known Taylor model adopts for example the following assumption about a long range interaction: the plastic velocity gradient at macroscale must be equal to the one at the mesoscale (grain scale). This is a very strong interaction. As a result of this, all grains are supposed to have the same plastic strain; this assumption constitutes strong short-range interaction applied by the model. In contrast to this, no assumptions about short-range stress interactions (between directly neighbouring grains) are adopted. Concerning the long range stress interaction, it is merely assumed that the macroscopic stress is the volume average of the stresses in the mesocopic RVEs (grains). The model also assumes homogeneous distributions of stresses and plastic strains inside the grains. The equally well-known VPSC model [4-5] also assumes homogeneity of stress and plastic strain rate inside the grains (called 'inclusions'). As for the long-range interaction, it (i) requires that the stresses and plastic strain rates of the macroscopic RVE are the volume averages of those of the inclusions and (ii) treats each grain as an inclusion embedded in the macroscopic RVE

(assumed to be homogenous) and solves for the local stresses and (plastic) strains as would be done in an Eshelby-type inclusion model. In this, the constitutive model used for the inclusions is visco-plasticity, which can be seen as an approximation of the Generalized Schmid Law. The classical Eshelby solution, which uses linear elasticity, had of course to be adapted to this [4]. Note that this procedure leads to a much more subtle long-range interaction between the mesoscopic RVEs (grains) and the macroscopic RVE. On the other hand, short range interactions (which take place at grain boundaries) are not directly modelled. Compared to this, the Taylor model strictly models both the long-range and the short range strain-rate interaction, but no short range stress interaction at all. In this, it must be pointed out that in truth, all grains interact to different extents with all other ones; short range and long range interactions are just extreme cases. The CPFE (see for example [1]) and CP-FFT (see for example [2]) models can in principle capture the entire range of interactions, however at a rather high computational cost. "Cluster models" try to make a compromise between statistical models and CPFE / CP-FFT models by introducing a third length scale which is intermediate between the macroscopic and the mesoscopic length scales. This is done by subdividing the polycrystal into *M* "clusters" of *N* grains. Such cluster can then be seen as the RVE of a third intermediate length scale, here called "mesoscopic-2". The interaction between each cluster and the macroscopic length scale is of the Taylor type, whereas inside each cluster a VPSC [4-5] scheme is used.

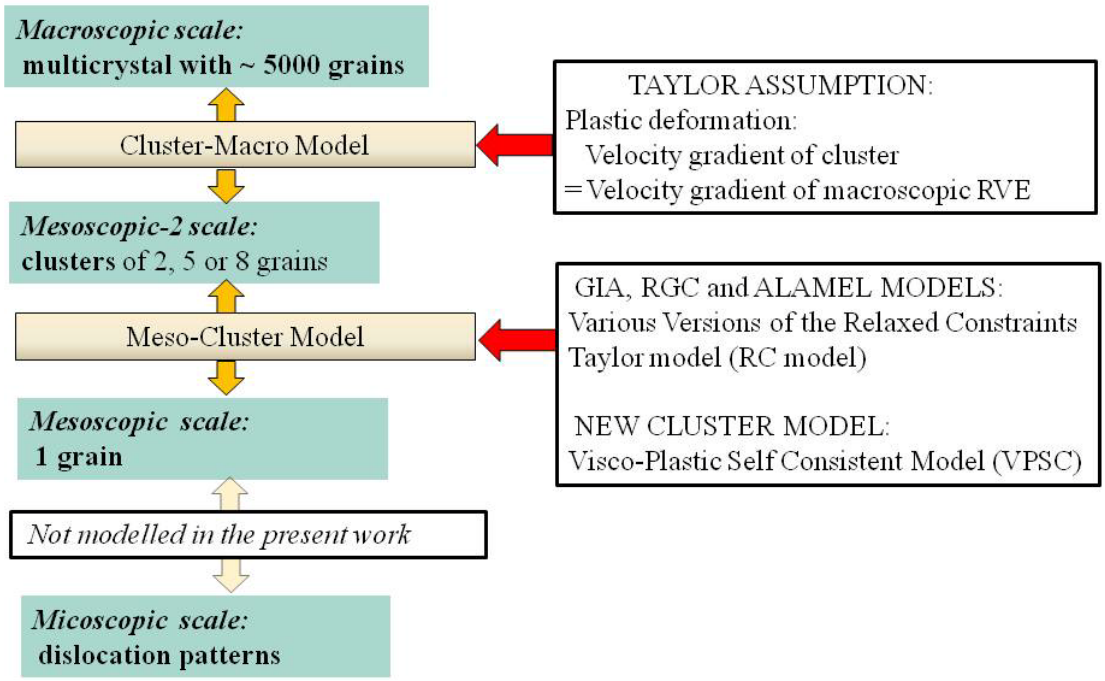


Fig. 1 Length scales as used in the present work.

## 3. Cluster Models

### *3.1. Existing Models*

The LAMEL model [6] adopts the Taylor-interaction between a cluster ($N$=2) of two grains and the macroscopic RVE. It focuses on short-range interaction. It is of limited use, as has been designed to simulate plane strain deformation only (the strain mode at mid-plane in rolling). The internal grain boundary of the cluster needs to be parallel with the rolling plane. The velocity gradient of the two grains must be equal to each other, except for the two simple shears for which the shear plane is parallel to the internal grain boundary. The average plastic velocity gradient of the two grains needs to be equal to the macroscopic velocity gradient (Taylor assumption for the cluster). The solution for the slip rates in the

two grains is sought by minimizing the total rate of plastic work dissipated in the cluster taken as a whole, using the Generalized Schmid Law for each grain but respecting the conditions described above. This results in (i) geometrical compatibility at the internal grain boundary and (ii) equilibrium of shear stresses at the grain boundary [6].
The GIA model [7] (which is in fact older than the LAMEL model) and the closely related RGC model [8] can be seen as a sort of generalization of the LAMEL model. These models look at a brick-shaped cluster subdivided into 8 grains by 3 planes, which are normal to ND, RD and TD, respectively. This creates 12 internal grain boundaries, as opposed to a single one in the case of LAMEL. Each internal grain boundary is treated in a similar way as the one of LAMEL. This leads to 24 possible shear-type relaxations. An extra complication is that these may cause voids or overlaps inside the cluster, which are kept under control by the adoption of a penalty term in the overall minimization procedure. The ALAMEL model is another generalisation of the LAMEL model [9]. It is very similar to it as it also works with a cluster of two grains ($N$=2). It no longer assumes that the internal grain boundary is parallel to a rolling plane. Its initial orientation is chosen at random (for each cluster separately) from a 'grain boundary orientation distribution function'. The cluster is supposed to represent two thin layers of material draped at both sides of a grain boundary segment. The orientation changes of these internal grain boundaries are tracked during the simulation of a large strain. The application of this model is not restricted to plane strain.

*3.2. New Model*
Fig. 1 describes how the new cluster model [10] works. The interaction between the cluster and the macroscopic RVE is of the Taylor type, as in LAMEL, ALAMEL, GIA and RGC. The interaction between each grain and the cluster as a whole is modelled by the "Neffect-VPSC"-software [10] from the Los Alamos National Lab, with $n^{eff}$=10. In this, the cluster, i.e. the mesoscopic-2 RVE, was used as the "macroscopic" RVE of the VPSC software. So far, tests have been done with $N$=2 and $N$=5.

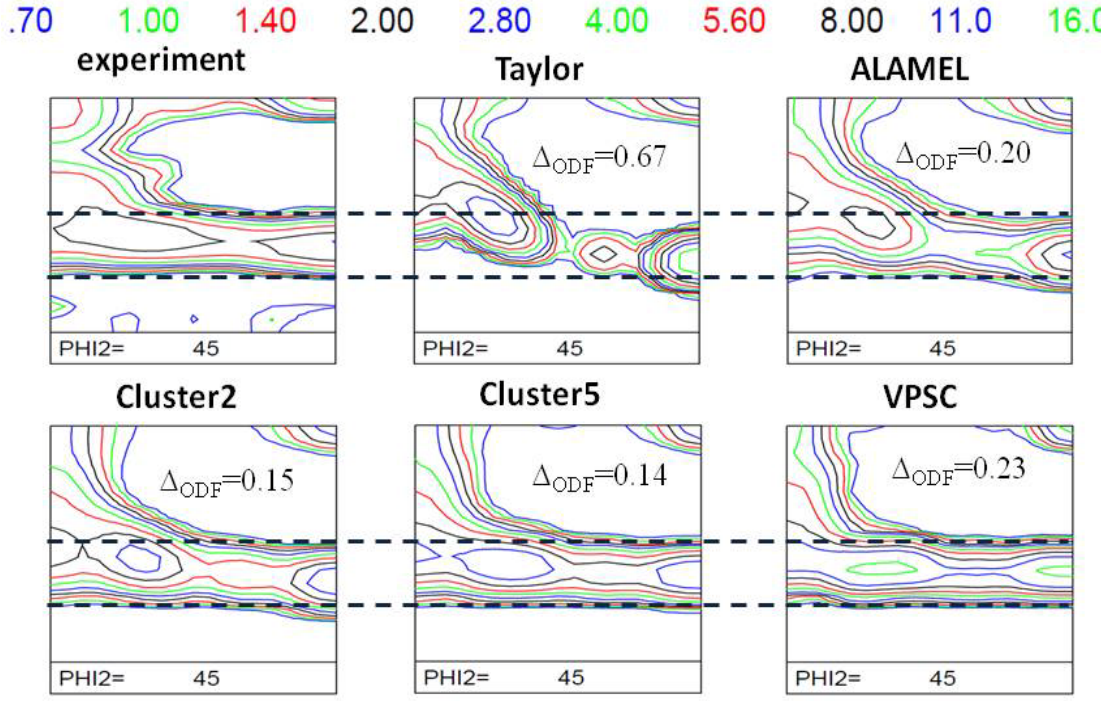


Fig.2 $\varphi_2$=45° sections of the ODFs of the experimental cold rolling texture and model predictions for the T61 cup drawing steel. $\Delta_{ODF}$ is the normalized error integral.

## 4. Results

Experimental validations for cold rolling applied to two steel qualities (DC06 and T61) and one aluminium alloy (AA6016) have been described in [10], as well as results for simple shear tests on DC06. Fig. 2 reproduces some of the results for T61, which is a low carbon steel with 0.04 wt% C for beverage cans. Sheets of it have been cold rolled to 0.2 mm thickness followed by continuous annealing, after which the material was further cold rolled (60 % reduction) in the laboratory. The figure also gives the normalized error integral $\Delta_{ODF}$, i.e. the square of the difference between the values of the ODF of the cold rolling texture as predicted by the models and the experimentally measured one, integrated over entire Euler space, and then divided by the texture index of the experimental ODF.

## 5. Conclusions

The results reported in Fig. 2 and in [10] all indicate, that (i) the quantitative agreement between the measured and predicted ODFs after rolling and shearing are much better for the ALAMEL, VPSC and the new cluster models with $N$=2 or 5, than for the Taylor model; (ii) the two New Cluster models perform better than ALAMEL and VPSC and (iii), the New Cluster model with $N$=5 performs slightly better than the one with $N$=2. Further research should indicate whether even better results might be obtained with $N$>5. Note also that in case $N$=5 would indeed be the best choice, it could be concluded that the simple Taylor assumption of homogeneous plastic strain would very well model the interaction between the mesoscopic-2 RVE corresponding to $N$=5 and the macroscopic RVE.

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