Simulation of Crystallographic Texture and Anisotropie of Polycrystals during Metal Forming with Respect to Scaling Aspects

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Abstract

We present a method to map and track textures in crystal plasticity finite element simulations using texture components. The use of such functions allows us to conduct forming simulations with full anisotropy update on all size scales ranging from the microscopic to the large-scale regime. The article presents the concept and some applications to the investigation of scaling aspects associated with texture and anisotropy during metal forming.

1 Introduction

Our main aim in polycrystal research lies in developing methods for mapping crystallographic anisotropy into mathematical methods for predicting large strain plastic deformation. A second even more demanding goal is the prediction of the *change* in crystalline anisotropy during deformation. This is necessary since the crystals rotate during deformation owing to their elastic-plastic spins. The microstructural processes involved during these reorientation processes of the grains in polycrystalline matter cannot be captured in terms of simple empirical constitutive laws but require the use of physically-based concepts. In this context the crystal plasticity finite element constitutive methods have gained momentum [1-6].

This article addresses the question how textures can be merged with crystal plasticity finite element constitutive descriptions in a rigorous, scalable, and efficient way. A particular challenge in this context lies in the reduction of redundant texture information to a level where sufficient details can be recovered without loosing physical significance.

This problem of representing large texture sets in plasticity simulations can be split into two separate tasks. The first one is the formulation of a basic solution method which uses crystallographic orientation as a state variable. This is achieved by formulating an orientation dependent constitutive law which maps the requested physical anisotropy at the single crystal scale and by embedding this formulation into a finite element code. For this we use the approach of Raabe et al. [2-8] and Kalidindi [1]. The numerical implementation then tackles the interaction of the differently oriented volume portions and thereby predicts the integral response of the sample under loads. Any such formulation requires a discrete representation of the orientation distribution function or a portion of it at each integration point. Therefore, the second task consists in feeding one single rotation matrix (crystal orientation) directly on each Gauss point of the finite element mesh. This amounts to mapping or respectively decomposing orientation distributions in such a way that they can be subsequently mapped on a mesh in a discrete manner thereby matching the initial overall distribution. For this task we use the texture component method [9,10] which approximates the orientation distribution function by a superposition of sets of simple standard functions with individual spherical coordinates, orientation density, and scatter in orientation space.

2 Theoretical background

We use the texture component method for reproducing orientation distributions. This mean that the texture is approximated by a superposition of model functions with individual height and individual full width, i.e.

$$f(g) = F + \sum_{c=1}^{C} I^{c} f^{c}(g) = \sum_{c=0}^{C} I^{c} f^{c}(g) \text{ where } I^{0} = F, f^{0}(g) = 1$$
(1)

where g is the orientation, f(g) is the orientation distribution function (ODF) and F is the random texture component. The intensity I^c describes the volume fraction of all crystallites belonging to the component c. The ODF is defined by

$$f(g) dg = 8 \mathbf{p}^2 \frac{dV_g}{V}$$
 which implies $f(g) \ge 0$ (2)

where V is the volume and dV_g the volume of all crystals with an orientation g within $dg=sin(\phi) d\phi d\phi_1 d\phi_2$. Normalization requires

$$\oint f^{c}(g) \, \mathrm{d}g = 1 \qquad \text{which implies} \qquad \sum_{c=0}^{C} I^{c} = 1 \tag{3}$$

As a rule texture components require positivity, i.e.

 $f^{c}(g) \ge 0$ for all $g \in G$ and $I^{c} > 0$ (4)

where G is the orientation space. For the components we use spherical Gauss-functions which are described by

$$f^{c}(g) = N^{c} \exp\left(S^{c} \cos \widetilde{w}\right) \tag{5}$$

where N^{c} is a normalization factor and \tilde{w} the orientation distance. Further details on texture components are given in [9,10]. The constitutive crystal plasticity model was also described in previous works [1-8].

3 Mapping texture components in the crystal plasticity finite element constitutive model

One important challenge of polycrystal plasticity simulations lies in identifying an efficient way of mapping *statistical* orientation distributions on the integration points of a grid of a crystal plasticity finite element model. This applies in particular when aiming at the simulation of larger parts typically containing more than 10^{10} crystals. The new concept we suggest for this task is based on mapping small sets of spherical Gaussian texture components on the integration points of a crystal plasticity finite element model.

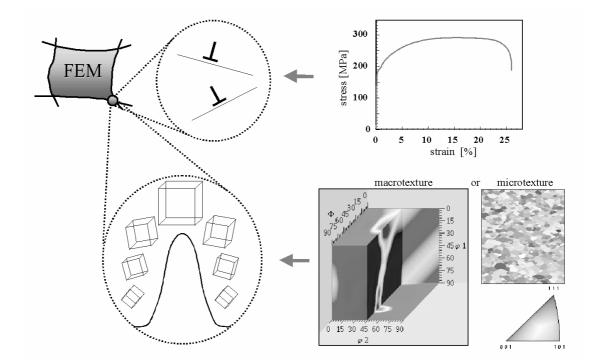


Fig. 1: Principle of the texture component crystal plasticity finite element method.

Fig. 1 shows the principle of the new approach. After recovering texture components from experimental or theoretical data they are mapped onto the integration points of a finite element mesh. This is conducted in two steps. First, the discrete preferred orientation g^c (center orientation) is extracted from each of the texture components and assigned in terms of its respective Euler triple (ϕ_1 , ϕ , ϕ_2), i.e. in the form of a

single rotation matrix, onto *each* integration point (**Fig. 2a**). In the second step, the mapped single center orientations of the texture components are rotated in such a fashion that the resulting overall distribution of *all* rotated orientations reproduces exactly the texture function which was originally prescribed in the form of a compact texture component (**Fig. 2b**).

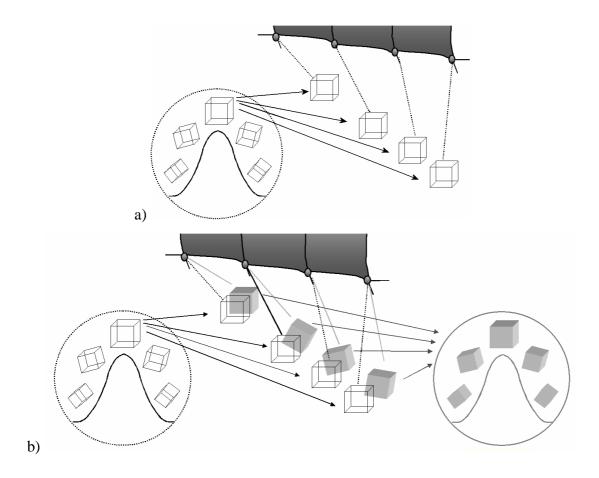


Fig. 2: Main steps of the spherical decomposition of a texture component.

In other words the orientation scatter individually described by each texture component function is mapped onto the finite element by systematically modifying the orientations at each point in a way which exactly imitates the scatter prescribed by the texture component. This means that the scatter which was originally only given in orientation space is now represented by a distribution both, in real space and in orientation space, i.e. the initial spherical distribution is transformed into a spherical *and* lateral distribution. It is important in this context, that the use of the Taylor assumption locally allows one to map more than one preferred crystallographic orientation on each integration point and to assign to them different volume fraction (**Fig. 3**).

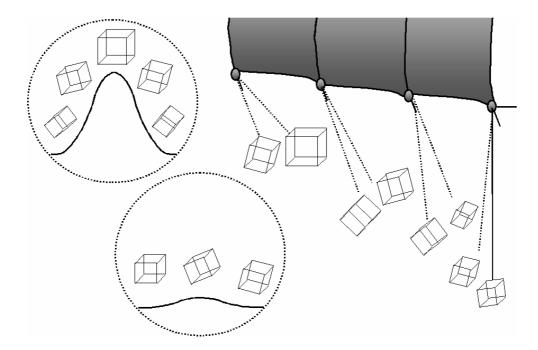


Fig. 3: Mapping of a *set* of texture components on a mesh.

This means that the procedure of mapping and rotating single orientations in accord with the initial texture component scatter width is individually conducted for all prescribed components as well as for the random background extracted from initial experimental or theoretical data by use of the component method. After having mapped the texture components by decomposing them into a group of single orientations which are arranged in the form of a lateral and spherical distribution on the mesh, the texture component concept is no longer required in the further procedure. During the subsequent crystal plasticity finite element simulation each individual orientation originally pertaining to one of the texture components can undergo individual orientation change as in the conventional crystal plasticity methods. This means that the texture component method loses its significance during the simulation. In order to avoid confusion one should, therefore, underline that the texture component method is used to *feed* textures into finite element simulations on a strict physical and quantitative basis. The components as such, however, are in their original form as compact functions not tracked during the simulation. On the other hand the mapped orientation points which were extracted from the components must not be confused with individual grains, but they mark points of an exact distribution function.

4 Simulation Results and Experimental Results

In the following we present some cup drawing applications of the new texture component crystal plasticity finite element simulation method, **Fig. 4**. Simulations of cup drawing tests depend on details of the contact between tool and specimen. The present cup drawing simulations were conducted under the assumption that the circular blank being drawn had an initial radius of 100 mm and an initial thickness of 0.82 mm. The interaction between the blank and the blank holder was assumed as a soft contact to impose the appropriate clamping pressure in the thickness direction of the element between blank, die, and blank holder. The simulations used an exponential soft contact function.

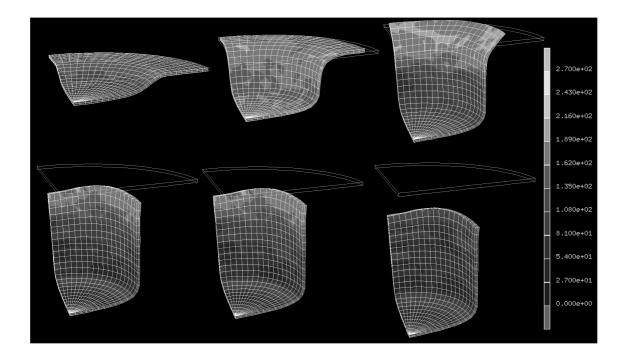


Fig. 4: Shape change during drawing of an aluminum sample containing about 10^{10} crystals. The gray scale scheme represents the von Mises equivalent stress.

Different friction properties (μ =0 to 0.2) were checked and the results showed that friction properties had under these contact conditions only little influence on the *relative* ear height. This is an important aspect compared to conventional J2-based continuum plasticity simulations which generally reveal stronger dependence on friction. Consequently the μ =0 case was selected to save computing time.

Fig. 5 shows simulation results for a specimen the texture of which was approximated using a volume fraction of 70.97 % of an orientation close to the cube component (Euler angles at Gauss maximum: ϕ_1 =197.87°, ϕ =6.47°, ϕ_2 =245.00°) and the rest as random texture background component. The texture recalculated by the component method given in terms of {111} and {200} pole figure projections shows good agreement with the original experimental data. The pole figures are shown in stereographic projections using 1.0, 2.0, 3.0, 4.0, 7.0 contour levels. The predicted distribution of the relative earing height reveals a very good correspondence with the simulation result.

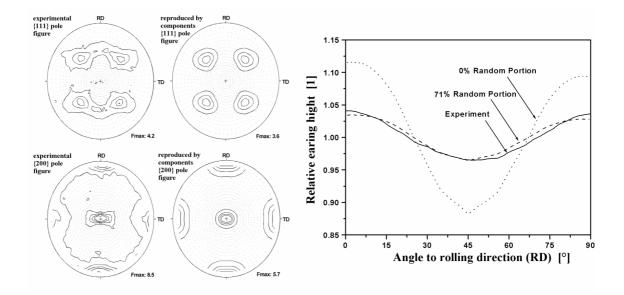


Fig. 5: Simulation and experiments for earing in an aluminum sample the texture of which was approximated by a volume fraction of 70.97 % of a component close to cube (Euler angles at Gauss maximum: $\phi_1 = 197.87^\circ$, $\phi = 6.47^\circ$, $\phi_2 = 245.00^\circ$) and the rest as random texture background component. The recalculated texture shows good agreement with the original experimental pole figure. The predicted distribution of the relative earing height reveals a very good correspondence with the simulation result.

5 Conclusions

The study presented a new finite element method which includes and updates crystallographic texture during forming simulations. The method is based on feeding discrete localized spherical texture components onto the Gauss points of the mesh of a finite element simulation which uses a crystal plasticity constitutive law. The method was tested and the results were compared to experimental data.

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6 References

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