

INTRODUCTION OF A LARGE-STRAIN TEXTURE-BASED FINITE ELEMENT METHOD

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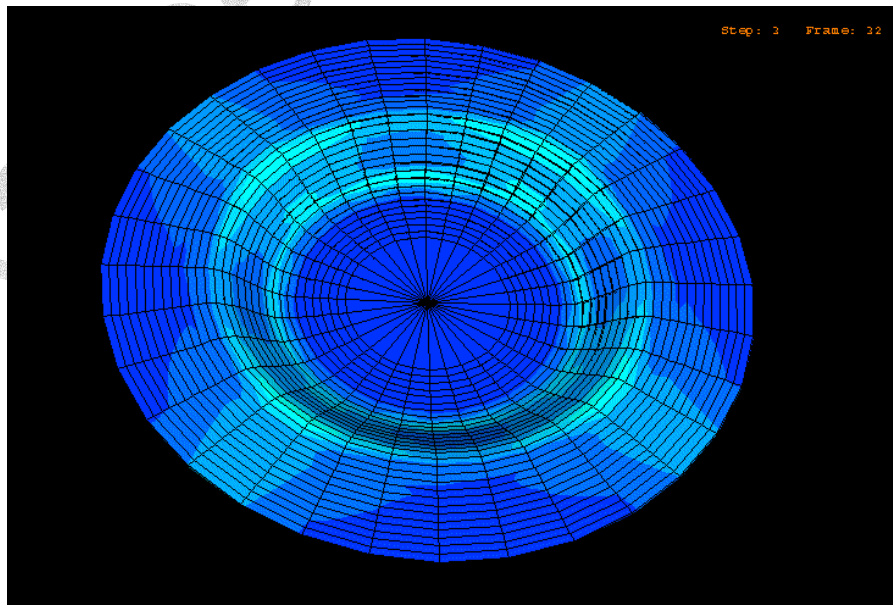
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Report abstract

This Max-Planck project report presents a time efficient and at the same time physically based approach for including and simulating elastic-plastic crystalline anisotropy during complex forming operations of metal polycrystals. The novel procedure is based on the direct integration of spherical crystallographic texture components into a commercial non-linear finite element program package. The method has been developed to perform very fast simulations of large strain industry-scale metal forming operations of textured polycrystalline materials including complete texture update during forming. Instead of using the yield surface concept or large sets of discrete crystalline orientations the method proceeds from a small though physically based set of discrete and mathematically compact Bessel-type Gaussian texture components which are used to map the orientation distribution function directly and in a discrete fashion onto the integration points of a viscoplastic crystal plasticity finite element model. The method merges approaches from crystallography, crystal plasticity, and variational mathematics. It increases the computational efficiency of microstructure-based anisotropy calculations dramatically and thus represents a feasible approach to incorporate and predict anisotropic behavior at the industrial scale. Applications of the new method are particularly in the field of predicting shape-sensitive anisotropic large strain - large scale forming operations such as encountered in the automotive and aerospace industry. This progress report gives an overview of existing anisotropy concepts which are commonly used in conjunction with finite element methods, provides an introduction to the new crystallographic texture component crystal plasticity finite element method, and gives examples of its application.



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1. Introduction

Metals are typically encountered in polycrystalline form where each grain can have a different orientation of its crystallographic axes with respect to the external reference system. The distribution of these orientations is referred to as texture. The discrete nature of crystallographic atomic-scale shear along densely packed lattice directions on preferred crystal planes entails a highly anisotropic, i.e. orientation dependent response of such aggregates during mechanical loading. This applies in particular for polycrystalline matter, where the grains interact with their neighbor crystals during forming and continuously change their crystal orientation (Fig. 1).

While the elastic-plastic deformation of a single crystal as a function of its orientation can nowadays be well predicted, plasticity of polycrystalline clusters is less well tractable. This is essentially due to two reasons. First, the intricate elastic-plastic interaction occurring during co-deformation among the highly anisotropic individual crystals and their respective neighbor grains as well as among different regions within the same crystal are not well understood. Second, crystals gradually change their orientation during forming and hence also alter the overall anisotropy of the entire polycrystalline specimen. The described processes entail strong heterogeneity in mechanically loaded crystalline matter in terms of strain, stress, and crystal orientation.

Besides fundamental questions from the field of polycrystal mechanics also engineering problems would considerably profit from novel theoretical approaches. Research on elastic-plastic anisotropy is a topic of high economic relevance since improved predictions of forming operations can help saving raw material, obtaining similar mechanical properties everywhere in a formed product, avoiding failure, and optimizing forming of light-weight constructional materials for instance in the automotive industry. Related issues of interest are the physically based prediction of internal stresses in microelectronic compounds or large scale power plant parts.



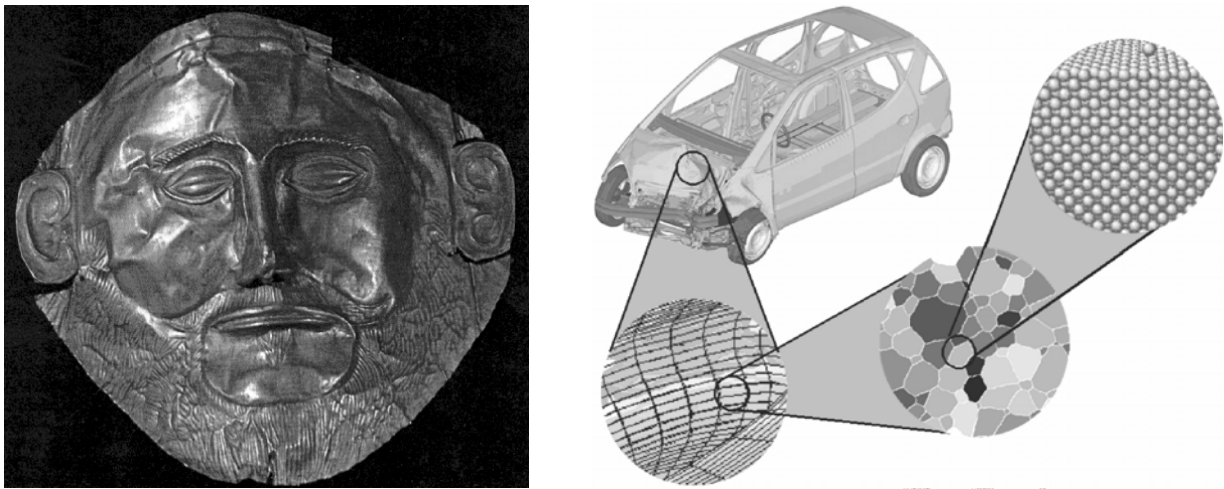


Fig. 1. Research on large strain plastic anisotropy of metals has been a topic for 4000 years. The reasons for that are obvious: Engineers want to save material, obtain similar mechanical properties everywhere in the material, and avoid failure. The computational treatment of crystal anisotropy requires close integration of approaches from metal physics, crystallography and mathematics of non-linear differential equations.

The computational treatment of crystal anisotropy requires close integration of approaches from metal physics, crystallography and mathematics of non-linear differential equations. The major challenge of the present initiative to directly integrate physically based crystal behavior into variational approaches lies in identifying an effective method of mapping a representative crystallographic orientation distribution onto the integration points of a finite element method using a compact mathematical form which permits texture update during mechanical loading. Based on these fundamental considerations we have developed a new physically based and highly time efficient prediction method for the simulation of polycrystal plasticity which accounts for all relevant crystallographic aspects. Its idea is to map a discrete representation of an orientation distribution onto each integration point of a non-linear crystal plasticity finite element formulation. When taking a practical perspective at the problem it is obvious that an appropriate representation of such a discrete texture requires the reduction of the information content to a level at which complex mechanical loading situations can be simulated without the help of a supercomputer. Hence, a texture reproduction method was chosen which is based on using discrete Bessel-type spherical Gauss texture functions. This approach provides a very small set of orientational components which are characterized by simple parameters of physical significance (Euler

angle triple, volume fraction, full width at half maximum). Using this method, only a few texture components are needed to describe the orientation distribution function. This data reduction increases computing efficiency dramatically. The required orientation components can be extracted from experimental data, such as pole figures stemming from x-ray, neutron-, or electron diffraction.

2. Methods for mapping plastic anisotropy in finite Element Models

Classical approaches for including anisotropy in finite element approximations can be grouped into 5 different strategies, namely, empirical anisotropic yield surface concepts (Fig. 2a), physically based anisotropic yield surface concepts (Fig. 2b), integration of continuum and crystal plasticity homogenization models (Fig. 2c), crystal plasticity finite element formulations (Fig. 2d), and texture component crystal plasticity finite element formulations (Fig. 2e).

The yield surface is the generalization of the yield point (e.g. $R_{p0.2}$), known from uniaxial tensile testing, to general states of stress. Extending the yield *point* into a yield *surface* is only required if the material under investigations reveals anisotropic plastic response, i.e. if it deforms differently in different directions. Classical empirical mathematical descriptions of an anisotropic yield surface were suggested in 1928 by von Mises [1] and in 1948 in a generalized form by Hill [2]. The shape coefficients of Hill's quadratic yield function can be fitted from experimentally obtained mechanical data taken along different directions of the sample, such as the Lankford coefficients R_0 , R_{45} , and R_{90} . The scaling is given by the yield stress obtained from uniaxial tensile testing. A number of optimized empirical anisotropic yield surface functions have been published in the last decades, such as those introduced by Barlat [3] which are particularly suited for aluminum and related face centered cubic alloys and those of Hill [4] which often match mechanical behavior of body centered cubic steels (Fig. 2a). The main advantages of empirical anisotropic yield surface functions are short calculation times and for cases with stable textures robust results. The main disadvantage lies in the fact that the anisotropy of metals changes during forming due to the evolution of texture. It must be noted in that context that the texture changes differently in different regions of the same specimen owing to the spatial differences in strain state and strain path.



Translating this into the yield surface concept means that each region of a plastically strained specimen has a different yield surface and also a different yield surface evolution. It is hence a main limitation of the yield surface concept that these changes in the physical origin of anisotropy are not mapped by a corresponding change of the shape of the yield surface individually at each integration point, i.e. the same yield surface shape is nowadays used throughout one finite element simulation.

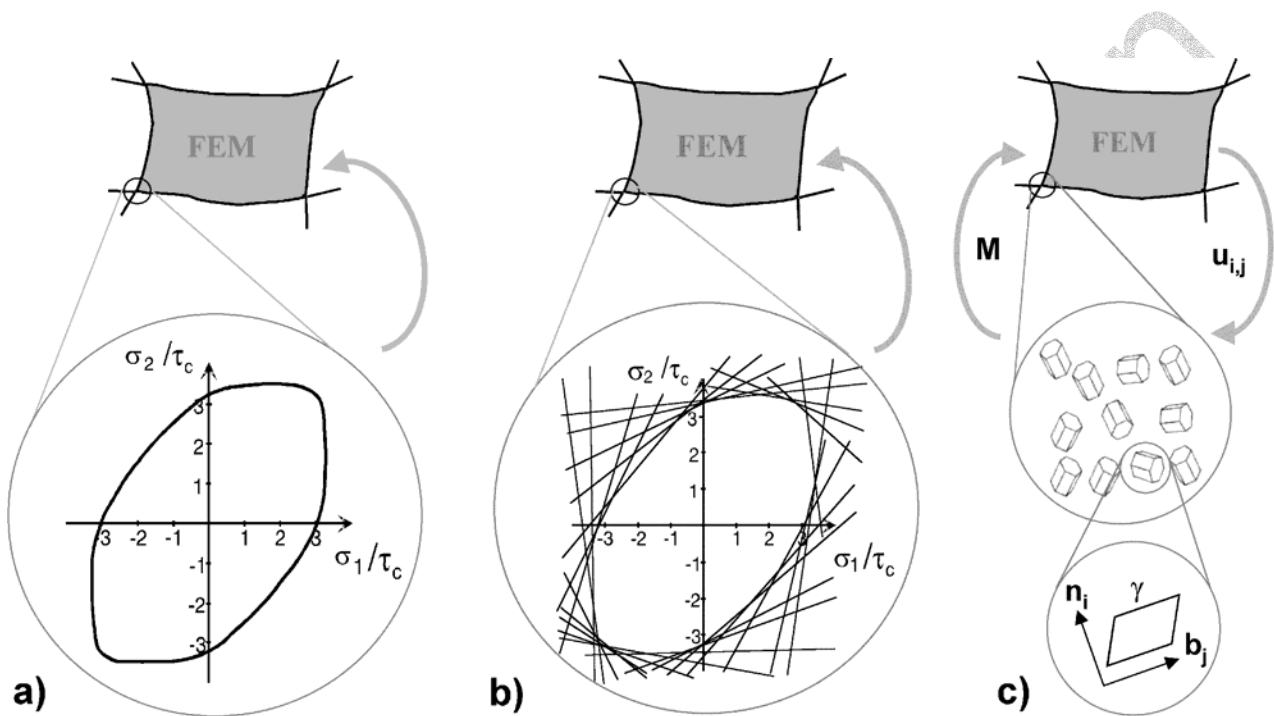


Fig. 2. Anisotropy in finite element models; a) empirical anisotropic yield surface, b) texture based anisotropic yield surface, c) integration of continuum and crystal plasticity homogenization models.

Polycrystalline alloys inherit and develop crystallographic textures during forming. These can directly serve as input data for the calculation of the crystallographically determined portion of the yield surface shape using Taylor-Bishop-Hill theory or rate-sensitive derivatives of these models. This applies for a single crystal yield surface as well as for the homogenization bounds of the polycrystal yield surface [5, 6]. The experimental input textures can be determined using x-ray, neutron, or electron diffraction. Since a texture-based yield surface uses the genuine crystallographic anisotropy information of a sample it is often superior to an empirical approach which relies on a small set of mechanical parameters. However, since the texture information is again not updated during the finite

element simulation, texture-based yield surface functions also have the shortcoming of neglecting possible texture changes during forming (Fig. 2b).

Another method of dealing with anisotropy lies in combining Taylor theory and finite element simulation [7]. In this approach the deformation tensor after each strain step prescribes the boundary conditions for a Taylor-type model. In this approach each finite element contains the representative crystallographic texture information in the form of a large set of discrete grain orientations. The Taylor factor calculated from homogenization is fed back into the finite element simulation as a correction factor for the flow stress in the ensuing simulation step (Fig. 2c). The strength of this method lies in the exact simulation of texture evolution. With respect to engineering applications a weakness of the approach lies in the fact that a large set of discrete grain orientations is required for a mathematically correct representation of the texture. This entails long computation times when simulating large strain metal forming operations with complete texture update.

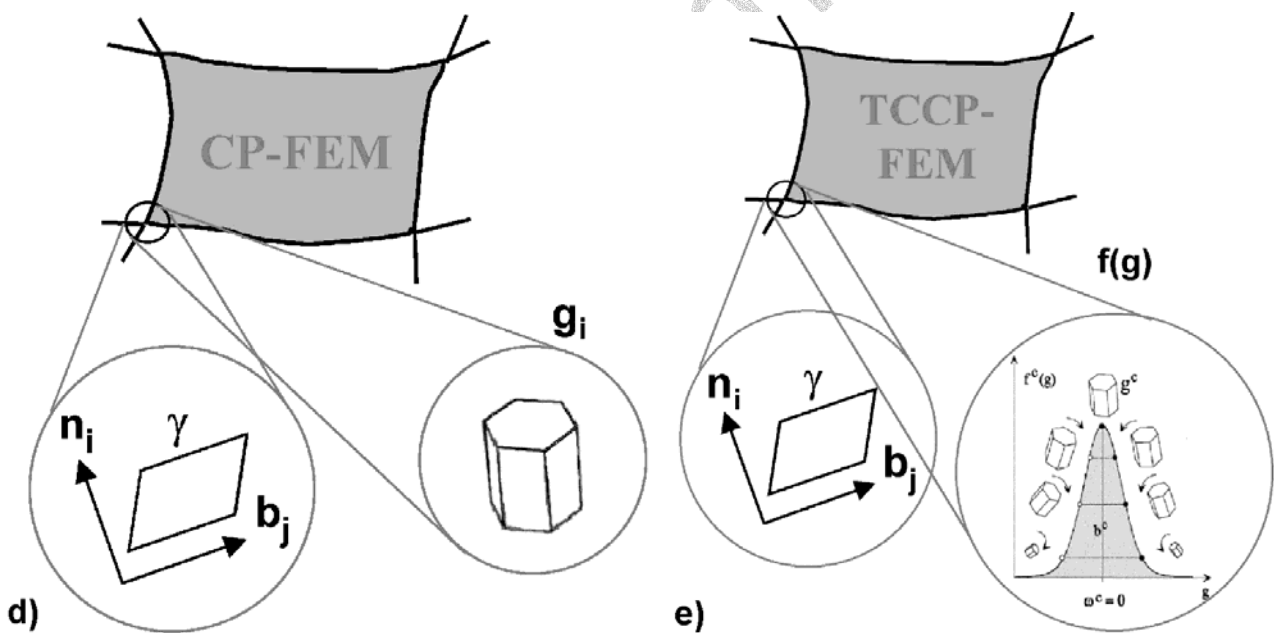


Fig. 2. Anisotropy in finite element models; d) crystal plasticity finite element formulations (CP-FEM), e) texture component crystal plasticity finite element formulations (TCCP-FEM).

The next step in sophistication lies in the direct implementation of crystal plasticity theory into finite element models [8-10]. Such models provide a direct means for updating the material state via integration of the evolution equations for the crystal lattice orientation and

the critical resolved shear stress. The deformation behavior of the grains is at each integration point determined by a crystal plasticity model which accounts for crystallographic slip and for the rotation of the crystal lattice during straining (Fig. 2d). Crystal plasticity finite element models represent elegant tools for detailed simulation studies of texture evolution under realistic boundary conditions. However, since each integration point represents one single orientation it entails long calculation times. The next chapter presents a new method to modify the crystal plasticity finite element approach with respect to applications in the field metal forming simulations. Its basic idea consists in using a more effective way of describing the texture of macroscopic samples at each integration point, turning the method into a *texture component* crystal plasticity finite element method (Fig. 3).

3. The texture component crystal plasticity finite element method

The major challenge of directly integrating constitutive polycrystal plasticity laws into finite element approaches lies in identifying an effective method of mapping a representative crystallographic texture on a finite element mesh using a compact mathematical form which permits individual texture update separately at each integration point during straining. This means that crystal plasticity finite element approaches which permit texture update require a *discrete* representation of the texture at each integration point. For this purpose we use a texture component method to fit the orientation distribution function. This method works with Bessel-based Gauss-type model functions with individual amplitude and individual full width at half maximum [11,12].

For demonstrating the method we use two experimental aluminium textures. Both samples were hot rolled and coiled at 315°C. Sample B was additionally cold rolled with a thickness reduction of 88% in order to obtain a texture different from sample A. Deep drawing tests were carried out and the ear profiles were measured on both samples. Sample A showed a recrystallization texture with strong cube orientation. Sample B revealed a typical plane strain deformation texture.



The experimental textures of sample A and B were analyzed using the component method of Helming [12] using discrete spherical Bessel-Gauss texture functions. The pole figures as reproduced by the component fit method are given together with the original experimental pole figures in Figs. 3 and 4. While only one texture component was sufficient to reproduce the texture of sample A, two components were necessary to fit the texture sample B. Both reproduced textures show good agreement with the experimental pole figures.

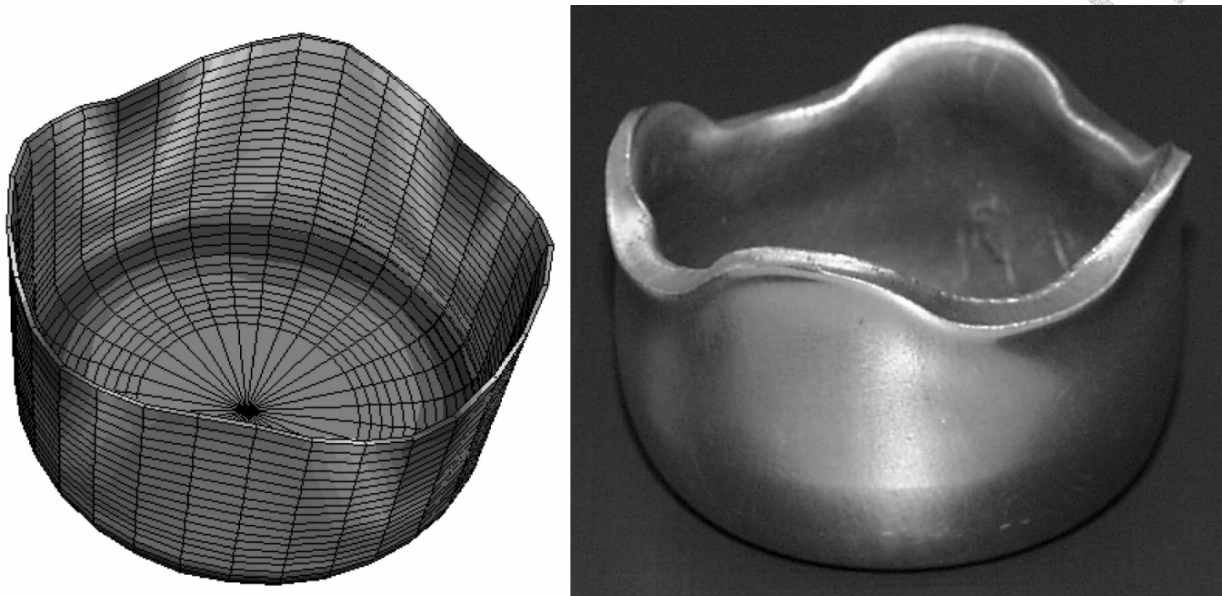


Fig. 3. Example of the application of the new texture component crystal plasticity finite element formulation. The calculation uses complete texture update individually at each integration point. The gray coding indicates the sheet thickness. The starting texture had a strong cube texture [14].

The finite element calculations were carried out using the commercial finite element program ABAQUS in conjunction with the user defined material subroutine UMAT [13,14]. The deformation behavior of the material was determined by a crystal plasticity model, which accounts for plastic deformation by crystallographic slip and for the rotation of the crystal lattice during deformation.

An implicit crystal plasticity procedure was implemented and used for the time integration of the constitutive equations. The constitutive approach permits homogenization at each integration point, i.e. locally the Taylor hypothesis may apply. This means that - if a set of orientations is considered at one integration point - the local deformation gradient in each of these grains, each represented by its rotational matrix, is homogeneous and identical to the

macroscopic deformation gradient at this particular material portion. The volume fraction of each individual texture component has to be taken into account separately. The random background part is used for rescaling.

Fig. 4 shows the relative ear height which we used for comparing the simulation results with the experimentally obtained data (solid line). The curve simulated directly from finite element modeling (0% random portion) qualitatively reproduces the experimental ear shape, though much sharper than the true profile. After normalization (71% random portion as obtained from texture component fit) the simulated curve is in very good agreement with the corresponding experimental data, both, in terms of shape and height.

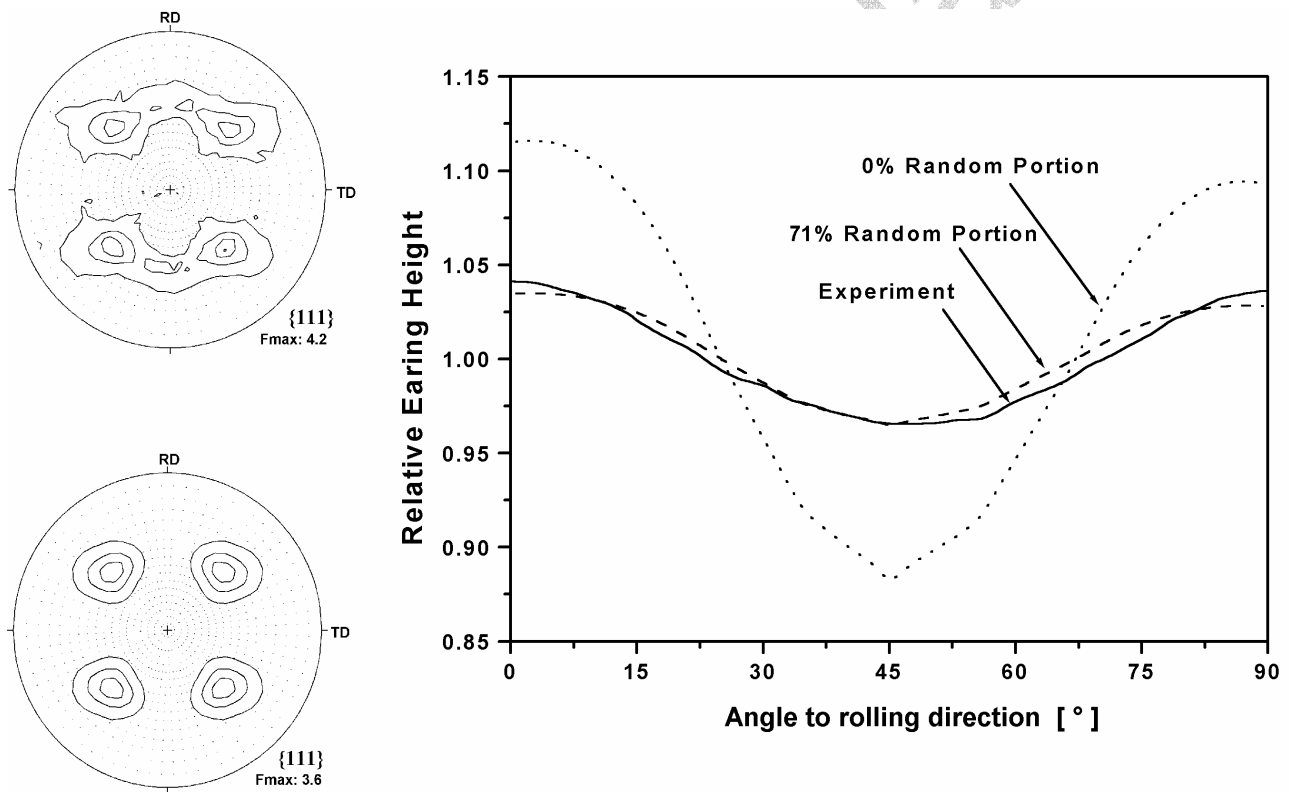


Fig. 4. Experimental and simulated earing profiles of sample A. The direct simulation result obtained from the crystal plasticity finite element method (dotted line) shows qualitative agreement with the experimental result (solid line). After renormalization the curve (dashed line) shows also good quantitative agreement with the experimental curve.

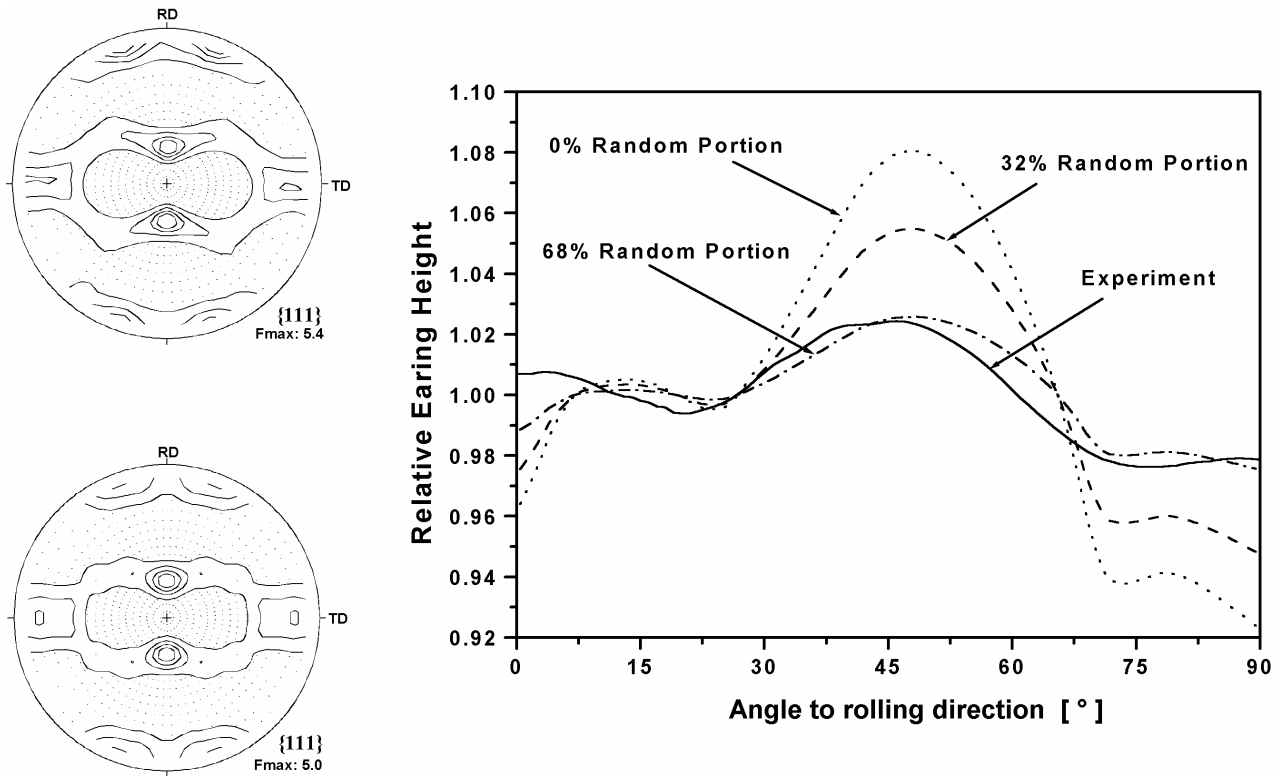


Fig. 5. Experimental and simulated earing profiles of sample B. The direct simulation result obtained from the crystal plasticity finite element method (dotted line) shows qualitative agreement with the experimental result (solid line) [14].

Fig. 5 shows the simulation results for sample B. Qualitative agreement between simulation and experiment is obtained even without normalization (0% random portion). After normalization (32% random portion as obtained from texture component fit) the simulated ear curve is still sharper than the experimental one. Best correspondence between simulation and experiment is found when using 68% random portion, which is larger than suggested by the texture component fit. The differences in agreement between simulation and experiment of samples A and B are interpreted in terms of differences in symmetry and scatter widths of the used texture components. While the texture of sample A essentially consists of a highly symmetric cube orientation, sample B with its deformation texture reveals lower symmetry. Further examples of the method are shown in Figs.6-8.

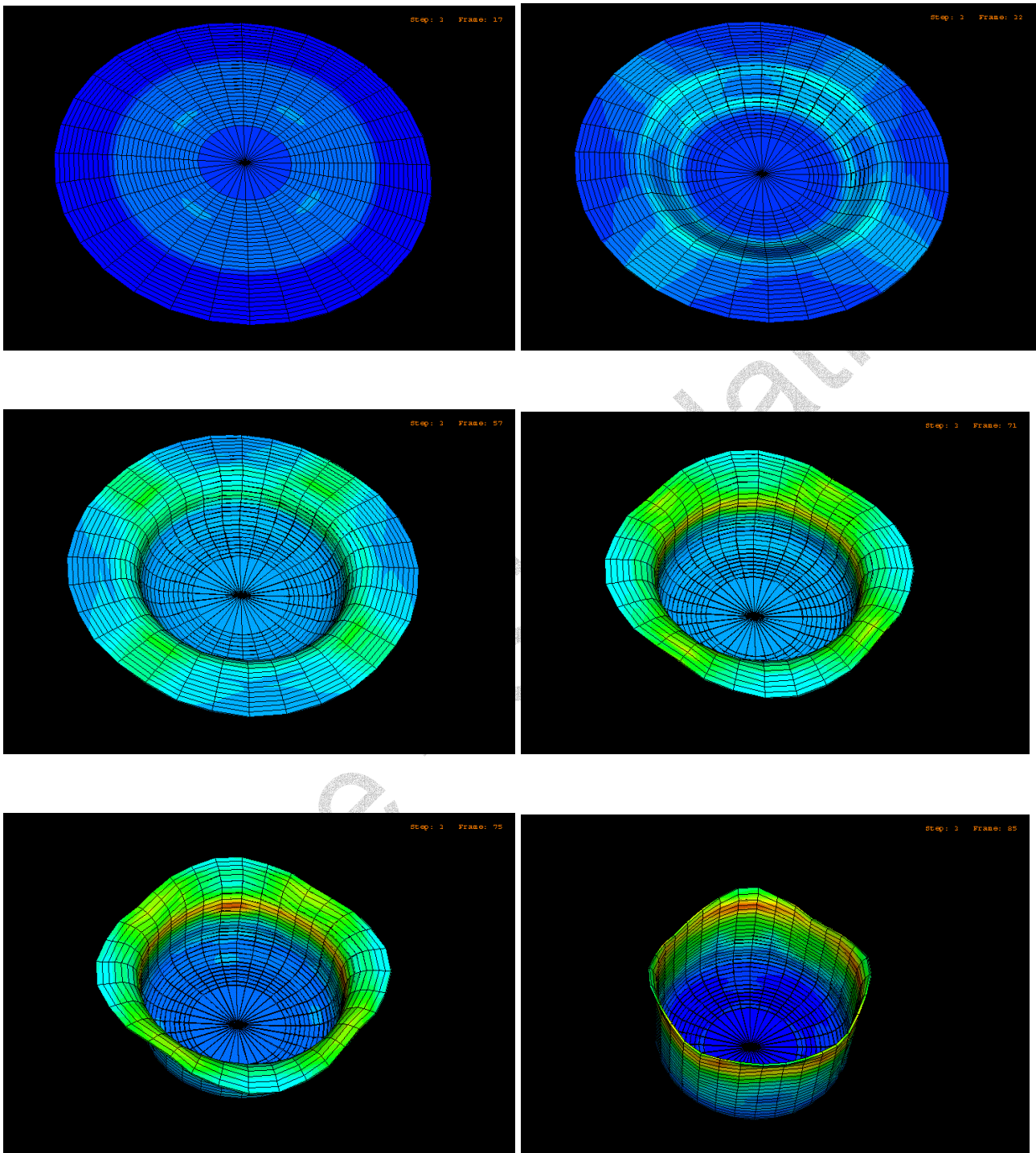


Fig. 6. Sequences from a deep drawing simulation obtained by the texture component crystal plasticity finite element method.

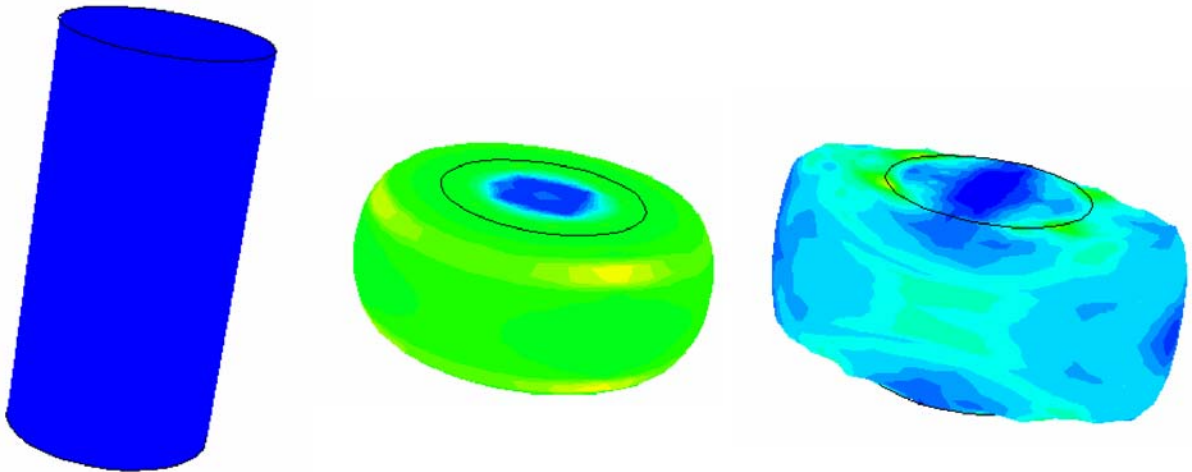


Fig. 7. Simulation obtained by the texture component crystal plasticity finite element method.

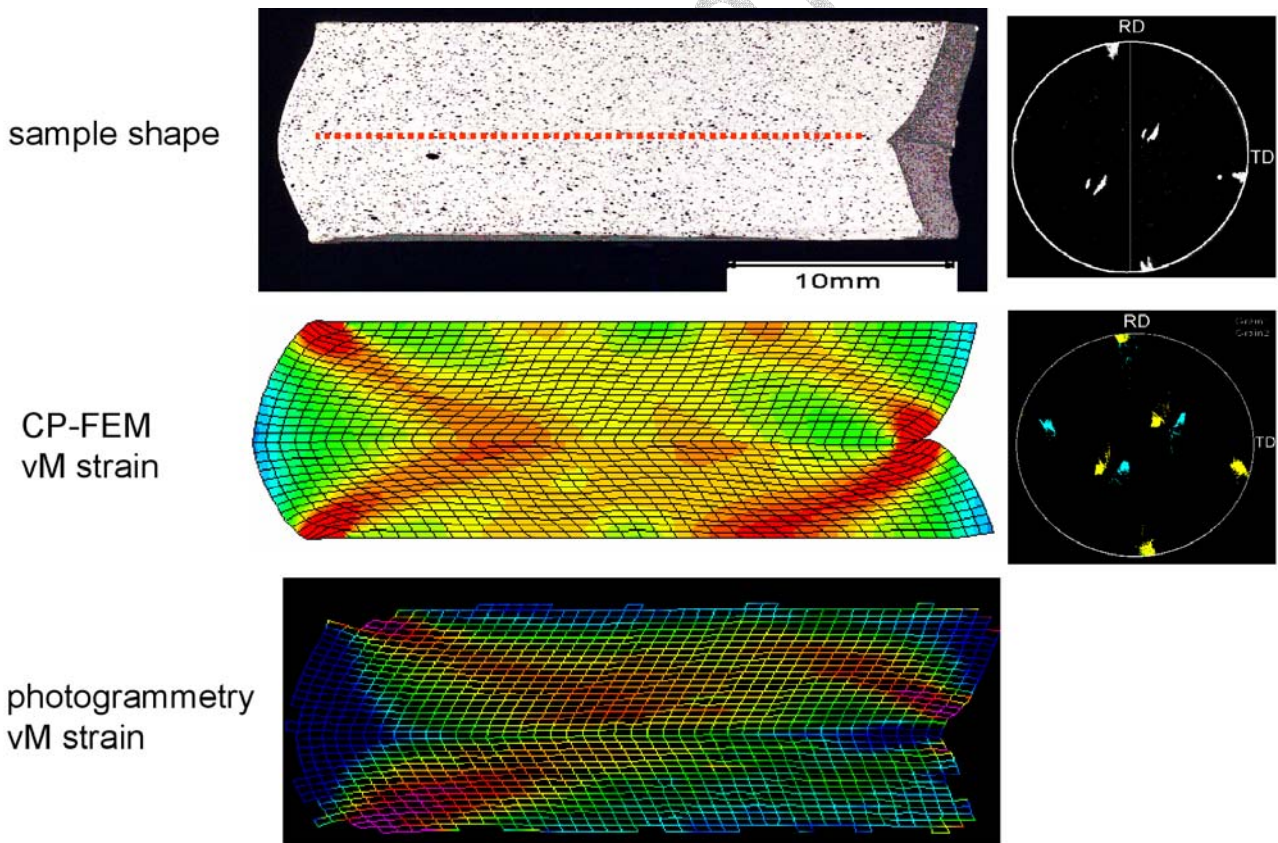


Fig. 8. Experiment and simulation obtained by the texture component crystal plasticity finite element method.

4. Summary

Discrete crystallographic spherical Bessel-Gauss-type texture component functions which represent an efficient and compact method of describing orientation distributions in textured polycrystalline materials have been integrated for the first time into finite element modeling. The validity of the method and of the computational procedure have been verified by comparing earing predictions with corresponding experimental results. The new approach, which is referred to as *texture component crystal plasticity finite element method* (TCCP-FEM), represents a highly efficient way of predicting plastic anisotropy of textured polycrystals at the industrial scale.

Raabe - Simulation



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