HOW DO 10 BILLION CRYSTALS CO-DEFORM?

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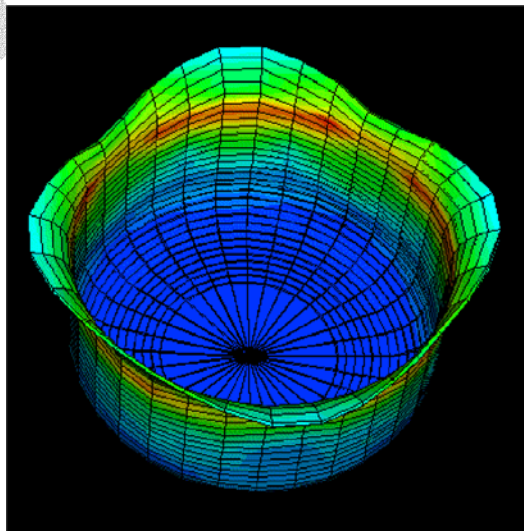
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Report abstract

Crystalline materials reveal highly anisotropic mechanical behavior[1-6]. Examples are metals, geological substances, semiconductors, superconductors, or semi-crystalline polymers. Large scale crystalline anisotropy has four major sources. First, crystals reveal intrinsic elastic *reversible* anisotropy due to the orientation dependence of the atomic bonds. Second, they reveal individual *irreversible* anisotropy due to crystallographic material translations along preferred directions and planes[1-6]. Third, crystalline matter usually occurs in *poly*crystalline form with typically more than 10 billion *interacting* crystals[4-6] each of which has a different orientation, shape, and size[7]. Fourth, crystals undergo re-orientations during loading[1-6]. Our report presents for the first time a method which predicts mechanical anisotropy of polycrystals consisting of huge numbers of grains taking full account of these mechanisms. The novelty of the approach consists in the integration of a small set of spherical crystallographic orientation distribution functions[8,9] into a non-linear finite element model with an elasto-plastic anisotropic constitutive law[10-12]. The method is suited for simulating anisotropical mechanical response of crystalline samples as encountered in materials science, geology, production technology, solid state physics, and civil engineering.

Mechanical anisotropy is a general property of materials which consist of one or more crystals. It proceeds from the intrinsic elastic-plastic anisotropy of each single crystals on the one hand and from the mechanical interaction and re-orientation of the crystals on the other hand (Fig. 1). Anisotropy may be desired such as in many functional materials (promotion of quasi single crystalline superconductivity in high-T_C superconductors or transformer steels) or not desired such as in many partially crystalline thermoplastic polymers.

Figure 1a   Research on anisotropy of materials 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, avoid failure, and minimize elastic back stresses in formed parts. Scientists want to understand the nano- and micromechanics of interacting crystals. Geologists and polymer chemists want to understand the origin of anisotropy in crystalline or partially crystalline material containing large numbers of crystals.
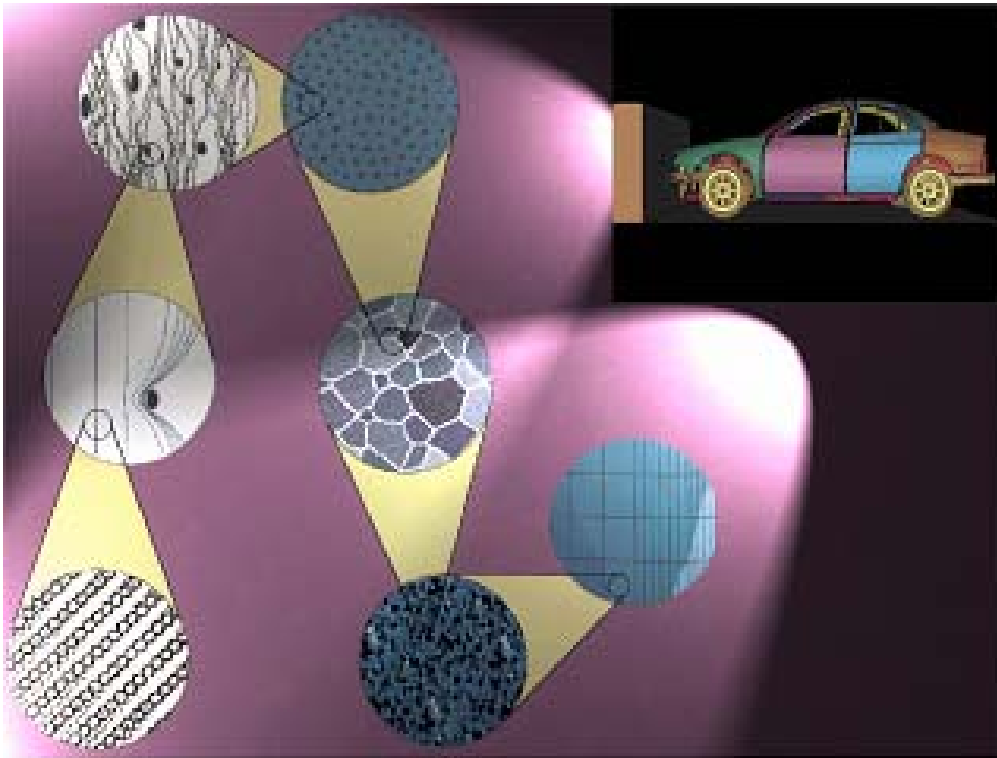
Figure 1b   Research on anisotropy in terms of multiscale modelling.

This progress report is about a new method which is capable of predicting the mechanical anisotropy of polycrystalline material consisting of an arbitrary number of crystals, its origin, and its development under loads. The method takes full account of crystal-scale reversible and irreversible anisotropy, the mechanical interactions among crystals, and their individual re-orientations. The approach can help to better understand and predict the anisotropy of samples consisting of huge numbers (e.g. 10^{10}) of crystals.

Classical crystal elasticity and plasticity finite element models represent excellent tools for simulating the mechanics and re-orientations of crystals under realistic boundary conditions[10-12]. However, these models are limited by the relatively small number of crystals they can handle (usually less than 10^4). This limit is due to the fact that crystal-scale finite element approaches up to now required a *discrete* representation of the crystalline orientation information at each integration point. When dealing with small numbers of crystals discrete mappings of their orientations are achieved by a simple one-to-one approach, where each

Gauss point in the finite element mesh is occupied by one discrete crystallographic orientation. This approach, however, is inappropriate when simulating samples which contain much larger numbers of crystals.

The key challenge of our new approach, therefore, lies in identifying a way of placing orientation *distributions* rather than *discrete* sets of orientations onto a finite element mesh. This new technique is the main topic of this progress report, i.e. we introduce a new efficient method of mapping a *representative* crystallographic orientation distribution, comprising a *huge* number of grains, on the Gauss points of a finite element mesh using a compact mathematical form which permits crystalline re-orientation during loading. For this purpose we use the orientation component method[8,9]. This is a technique of approximating the orientation distribution function of large numbers of crystals in the form of discrete sets of symmetrical spherical central functions which are defined in orientation space. Such functions have individual height and full width at half maximum as a measure for the strength and scatter of the crystallographic orientation component they represent. The mathematical reproduction of the orientation distribution function by component functions can be expressed by the superposition

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

where g is the orientation, $f(g)$ is the orientation distribution function, and F is the volume portion of all randomly oriented crystals (random texture component). The intensity I^c describes the volume fraction of all crystallites belonging to the orientation component c. The orientation density of the component is described by a central function, i.e. its value decreases isotropically with increasing orientation distance $\tilde{\omega}^c = \tilde{\omega}(g^c, g)$ from the maximum. This means that $f^c(g)$ only depends on $\tilde{\omega}^c = \tilde{\omega}(g^c, g)$, but it is independent on the rotation axis $\tilde{n}^c$. In our approach we decompose an initial orientation distribution function by a set of spherical central Gauss functions which are described by

$$f^c(g) = N^c \exp\left(S^c \cos\tilde{\omega}\right) \tag{2}$$

where

$$S^c = \frac{\ln 2}{1 - \cos(b^c/2)} \quad \text{and} \quad N^c = \frac{1}{I_0(S^c) - I_1(S^c)} \tag{3}$$

with $I_l(x)$ being generalized Bessel functions. The value b^c is the full width at half maximum which corresponds to the mean diameter of a spherical component in orientation space. The orientation component method is well suited for an incorporation of orientation distributions into crystallographic finite element methods. This advantage is due to the fact that the method is based on using sets of localized spherical normalized standard functions which are characterized by simple parameters of physical significance (Euler angle triple for the main orientations, volume fractions, full widths at half maximum). Typically only a few orientation components are required to describe the orientation distribution function which in turn can represent the texture of any crystal assembly whatever size it may have.

The second step of the new method is that the orientation component method must now be connected to a suited crystal elasticity and plasticity constitutive model. In our approach we use the large-strain constitutive crystal model suggested by Kalidindi[12]. In this formulation one assumes the stress response at each macroscopic continuum material point to be potentially given by one crystal or by a volume-averaged response of a set of crystals comprising the respective material point. Details of the constitutive law are given in [12].

The third element of our new approach consists in the integration of the orientation component functions into the crystal finite element method. More precisely, the main task of the new concept is to represent sets of spherical Gaussian orientation components on the integration points of a finite element mesh designed for crystalline constitutive laws. This procedure works in two steps: In the first step the discrete preferred orientation g^c (center orientation, mean orientation) is extracted from each of the orientation 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. 2). In the second step, these discrete orientations are re-oriented in such a fashion that their resulting overall distribution reproduces the

texture function which was originally prescribed in the form of a Gaussian orientation component (Fig. 2). In other words the orientation scatter described initially by a texture component function is in the finite element mesh represented by a systematically re-oriented set of orientations, each assigned to one integration point, which reproduces the original spherical scatter prescribed by that 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.
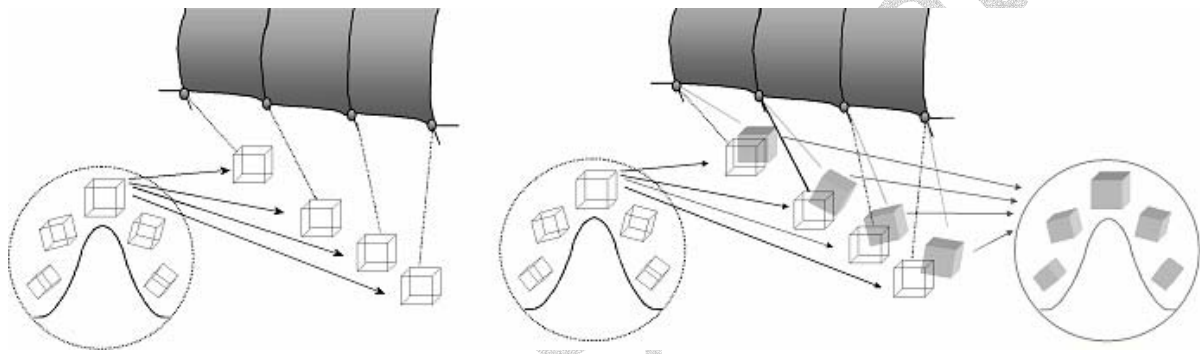

Figure 2 The first step of the decomposition of an orientation component consists in extracting the preferred orientation (center or mean orientation) from the orientation function and assigning it in terms of its respective Euler angle triple, i.e. in the form of a single identical rotation matrix, onto each integration point. In this state the sample is a single crystal. In the second step all orientations are re-oriented to give the initial orientation distribution.

The described allocation and re-orientation procedure is formulated as a weighted sampling Monte Carlo integration scheme in orientation space. Local homogenization allows one to map more than one preferred crystallographic orientation on each integration point and to assign to each of them an individual volume fraction. This means that the procedure of mapping and rotating single orientations in accord with an initial orientation component scatter width is individually conducted for *all* prescribed components as well as for the random background extracted from initial experimental or theoretical data. After decomposing and representing the initial orientation components as a lateral and spherical

single orientation distribution in the mesh, the texture component concept is no longer required in the further procedure. This is due to the fact that during the subsequent crystal finite element simulation each individual orientation originally pertaining to one of the orientation components can undergo an *individual* orientation change. This means that the orientation component method loses its significance during the simulation. In order to avoid confusion one should, therefore, underline that the orientation component method is used to *feed* crystal orientations into finite element simulations on a strictly physical, scaleable, and quantitative basis. The components as such, however, are in their original form as compact functions not tracked during the simulation. It must also be noted that the orientation points which were originally obtained from the components do not represent individual *grains* but portions of an orientation distribution function.
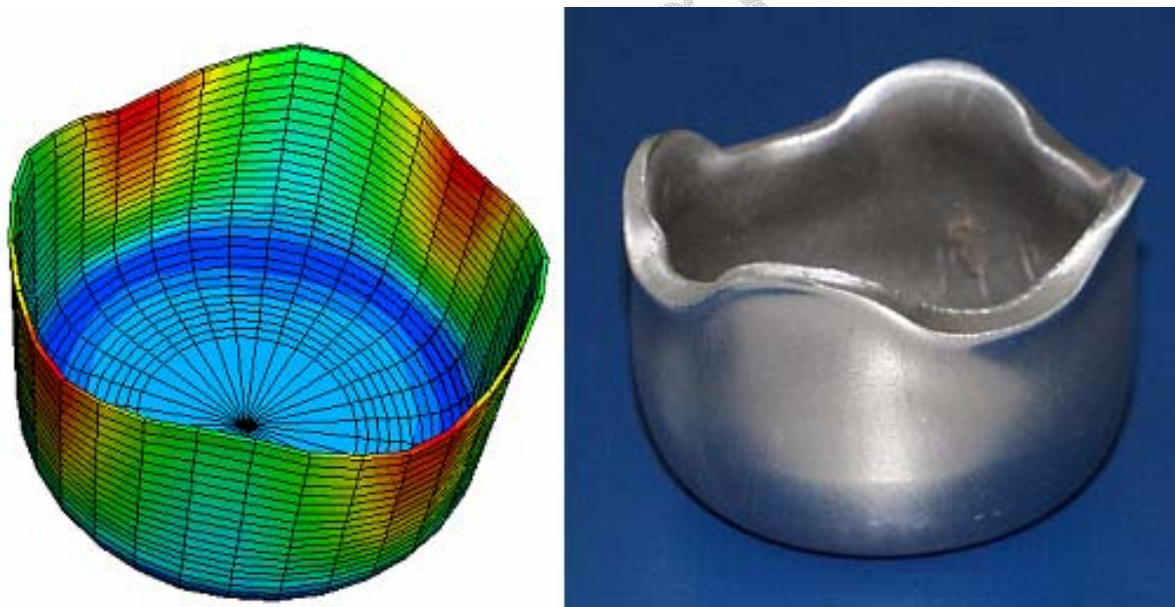

Figure 3 Example of a simulated large strain forming operation (99.99% aluminum) including orientation information and rotation of the crystals during straining. The importance of the crystallographic orientation can be seen from the resulting shape revealing the so called earing phenomenon. The color scheme indicates the wall thickness.
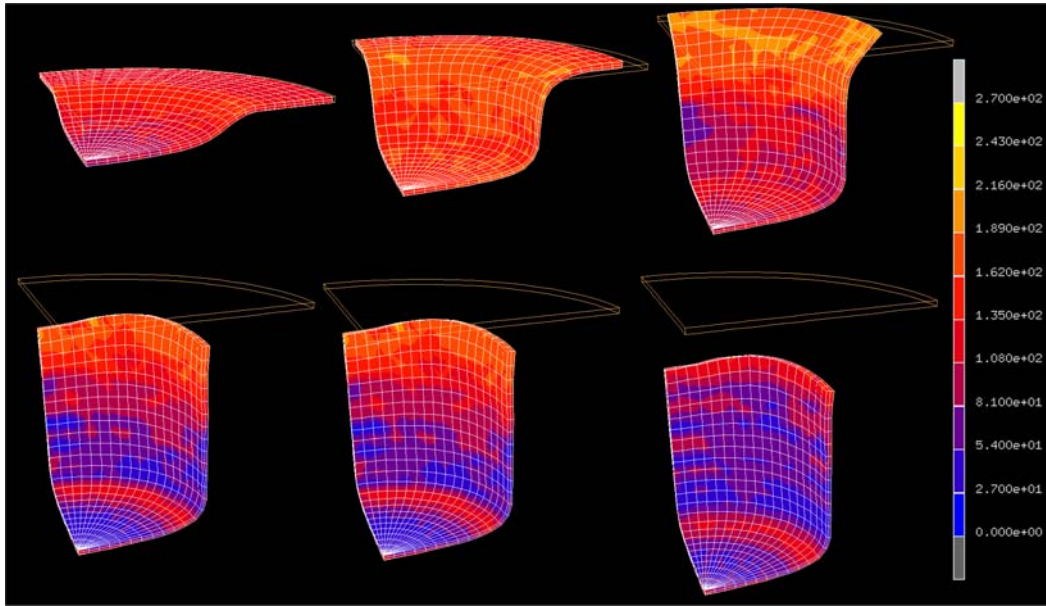
Figure 4 Shape change during drawing of an aluminum sample containing about 10^{10} crystals. The color scheme represents the von Mises equivalent stress.

Fig. 3 shows an example of a cup drawn aluminum sample and a corresponding experiment. The simulation predicts very well the final ear shape and the thickness distribution of the drawn sample. The original sample contained about 10^8 crystals which were all included in the simulation via our new orientation component finite element method. Fig. 4 shows an example of a large strain drawing simulation of an aluminum sheet containing about 10^{10} crystals. The last part of the figure shows details of the elastic spring-back effect, i.e. the elastic–plastic relaxation of the material after removal of the tool.

The current progress report gave an introduction into a novel finite element method which includes and updates orientation distributions in physically based anisotropy simulations. The method is based on feeding spherical orientation functions onto the Gauss points of a finite element mesh which uses a elastic-plastic constitutive law taking full account of single crystalline anisotropy. The major progress of the approach consists in its ability to feed large numbers of crystals in terms of mathematically compact orientation component functions into finite element simulations on a strictly physical, scaleable, and quantitative basis.

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