XXI ICTAM, 15–21 August 2004, Warsaw, Poland

MODELING THE CRYSTALLOGRAPHIC TEXTURE EVOLUTION BASED ON THE MAXIMUM ENTROPY METHOD

Thomas Böhlke, Albrecht Bertram
Institute of Mechanics, Otto-von-Guericke-University Magdeburg, PO box 4120, D-39016 Magdeburg, Germany

Summary We present a new approach for modeling the texture induced anisotropy that is based on a tensorial Fourier expansion of the crystallite orientation distribution function (CODF). The general evolution equations for the Fourier coefficients are derived. By this approach the texture evolution can be described by modeling some low order Fourier coefficients and by estimating the higher order coefficients based on the maximum entropy method. It is shown that such a low dimensional approach of the CODF yields a reasonable description of the texture evolution and represents a versatile alternative to classical mixture theories (Taylor, Sachs).

INTRODUCTION

The distribution of crystal orientations is an important microstructural feature which affects the overall properties of polycrystalline metals. If this distribution is inhomogeneous, the material has a crystallographic texture. Such a texture influences the overall elastic and the overall viscoplastic behavior as well as the non-mechanical properties of a polycrystal. The distribution of crystal orientations can be described by correlation functions. In texture analysis, the one-point correlation function is called crystallite orientation distribution function. It specifies the volume fraction of crystals having a specific orientation. A crystal orientation can be identified by a proper orthogonal tensor.
Phenomenological models seem to be generally unable to adequately represent the evolution of the crystallite orientation distribution. Therefore, if the evolving texture has to be taken into account in the context of finite element simulations, e.g. of deep drawing processes, in most cases mixture theories (Taylor, Sachs) are applied. In these cases, the texture evolution is described by a system of (algebro-) differential equations. The dimension of such a system is in between 300 - 10000. Hence, at each integration point of the finite element mesh, large systems of differential equations have to be integrated. This fact considerably limits the number of degrees of freedom that can be handled by standard finite element codes. Therefore, there is a need for homogenization strategies which allow to condense the number of degrees of freedom and nevertheless accurately describe the crystallite orientation distribution function.

ELEMENTARY BOUNDS

In the present work, the viscoplastic properties of a textured aggregate of face-centered cubic (fcc) crystals are considered. The advantage of a viscoplastic modeling is that on both scales, the grain scale as well as on the macro scale, the constitutive equations are given by potential relations. Furthermore, the methods of statistical continuum mechanics allow to bound the macroscopic potentials. In the most simple case, the one-point correlation function of crystal orientations is taken into account, which contains only the volume fraction information of the microstructural features. The corresponding bounds are called elementary bounds.

COORDINATE-FREE REPRESENTATION OF A CRYSTALLOGRAPHIC TEXTURE

There exist different approaches for the representation of the CODF. The classical representation by generalized harmonic functions was introduced by Bunge (1965) and Roe (1965). Later on, Adams et al. (1992) introduced a tensorial Fourier expansion of the CODF (see also, Zheng and Fu, 2001). Both representations are principally equivalent. The advantage of the tensorial representation is that it is coordinate-free. Therefore, the texture coefficients that occur in the tensorial representation can be used as micro-mechanically defined and measurable internal variables in continuum mechanics (Böhlke and Bertram, 2003). The general evolution equations for the Fourier coefficients are derived. The evolution equations contain only microscopic parameters and depend on the current CODF. If only a limited number of texture coefficients is taken into account, then the CODF has to be estimated based on these coefficients in order to specify the evolution equation.

MAXIMUM ENTROPY METHOD

How to estimate the CODF, if a fixed number of leading tensorial Fourier coefficients is known? The estimate has to be consistent in the way that it is nonnegative and normalized. Such a type of a problem is usually called moment problem. Moment problems are well known in statistical mechanics and other areas of science. The estimate of a distribution function based on incomplete data is not unique. One way to single out a solution of the aforementioned problem is to maximize the (information-theoretic) entropy of the CODF. In this contribution the moment problem is stated in terms of tensorial texture coefficients. It is shown that the so called crystallographic exponential family, here introduced with tensorial coefficients, solves the moment problem. The tensor-valued functions, which have to be solved in order to specify the exponential form have been formulated for all tensor ranks that occur in the tensorial Fourier expansion (Böhlke, 2004).

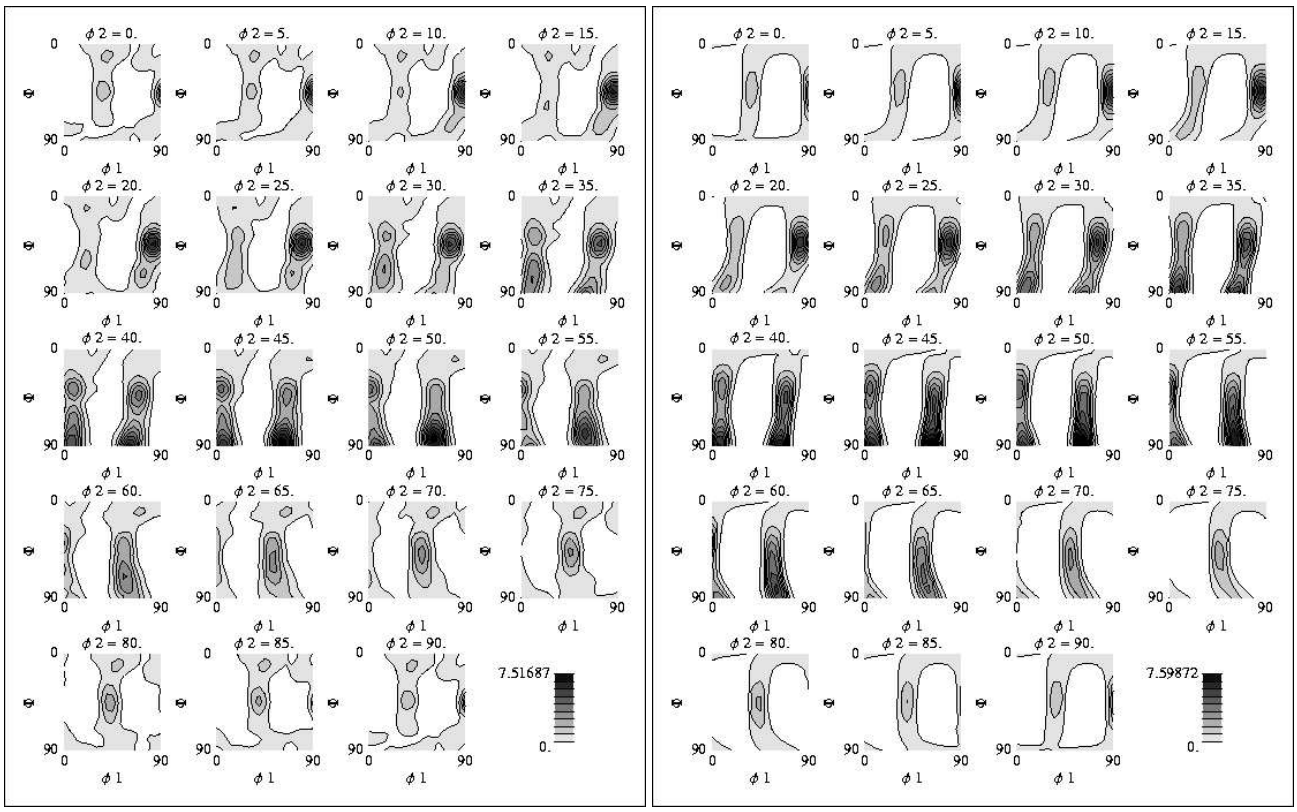

Figure 1. Left: Prediction of the classical formulation of the Taylor model with 1000 discrete crystal orientations. Right: Suggested model based on 22 internal variables (texture coefficients).

The numerical solution of the governing equations is obtained by a combination of an adaptive integration scheme on the orientation space and Newton's method.

If the evolution equations for the texture coefficients are combined with the maximum entropy estimate of the CODF, then it is possible to model the time evolution of the CODF. In this case a much smaller number of internal variables is needed compared to the classical formulation of the Taylor model. Fig. 1 shows a representation of the CODF in the Euler angle space for a simple shear deformation of an initially uniform orientation distribution. The left figure shows the CODF predicted by the Taylor model based on 1000 discrete crystal orientations, i.e. 3000 internal variables describing the orientation distribution. The right figure shows the predicted final CODF based on the 4th- and 6th-order texture coefficients and the maximum entropy method. The 4th-order tensorial coefficient contains 9 independent components and the 6th-order coefficient has 13 independent components.

References

Adams, B., Boehler, J., Guidi, M., Onat, E., 1992. Group theory and representation of microstructure and mechanical behavior of polycrystals. J. Mech. Phys. Solids 40 (4), 723–737.

Böhlke, T., 2004. Application of the maximum entropy method in texture analysis. To appear in: Computational Materials Science .

Böhlke, T., Bertram, A., 2003. Modeling of deformation induced anisotropy in free-end torsion. Int. J. Plast. 19, 1867–1884.

Bunge, H.-J., 1965. Zur Darstellung allgemeiner Texturen. Z. Metallkde. 56, 872–874.

Roe, R., 1965. Description of crystalline orientation of polycrystalline materials. III. General solution to pole figure inversion. J. Appl. Phys. 36, 2024–2031.

Zheng, Q.-S., Fu, Y.-B., 2001. Orientation distribution functions for microstructures of heterogeneous materials: II Crystal Distribution functions and irreducible tensors restricted by various material symmetries. Appl. Math. Mech. 22 (8), 885–903.