Microstructure Physics
and
Metal Forming
Prof. Dr. D. Raabe

Theory and Simulation
Dr. F. Roters

Development of a Grain Fragmentation Criterion and its Validation using Crystal Plasticity FEM Simulations

F. Roters, Z. Zhao, D. Raabe

Max-Planck-Institut für
Eisenforschung GmbH
Düsseldorf/Germany

Motivation

During plastic deformation of polycrystals the grains tend to change their orientation. However, in certain cases the grains do not rotate homogeneously but local orientation gradients are developed. These orientation gradients can finally lead to severe fragmentation of the originally homogeneous grains. Grain fragmentation is of great interest for several reasons:

- Local orientation gradients are connected with high numbers of geometrically necessary dislocations. These dislocations have great impact on local properties such as flow stress and hardening.
- Areas of high local orientation gradients are preferred nucleation sites for static primary recrystallisation.
- Grain interaction is an important factor during texture evolution. Therefore a quantification is necessary to improve classical homogenization theories for predicting plastic anisotropy.

It is therefore the aim of the presented studies to develop a simple analytic treatment to predict the fragmentation tendency as a function of orientation and strain path, crystal neighborhood, and grain size and form. The predictions of this criterion are than checked by crystal plasticity FEM simulation.

The Criterion for Grain Fragmentation

Based on an approach of Klein and Bunge flow field theory can be used to develope a criterion to predict grain fragmentation. While the flow field itself [1] gives information on the reorientation rate of a certain grain orientation (figure 1) the divergence of the flow field can be used as a measure of grain fragmentation tendency (figure 2). In this context negative values for the divergence mean that an orientation is stable and does not rotate at all. Zero divergence means that the grain rotates homogeneously and positive values mean that the tendency of fragmentation is the higher the values are.

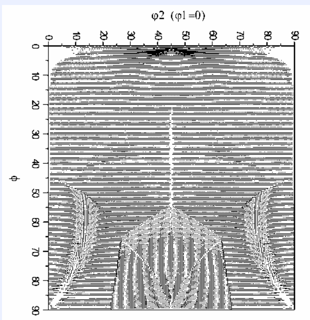


Figure 1: Flow field of BCC crystal
48 slip systems
„pancacke model“ [2]

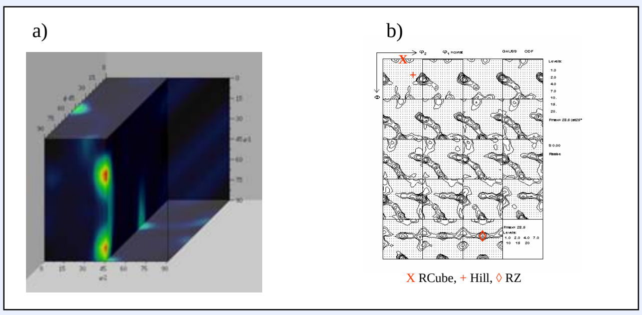


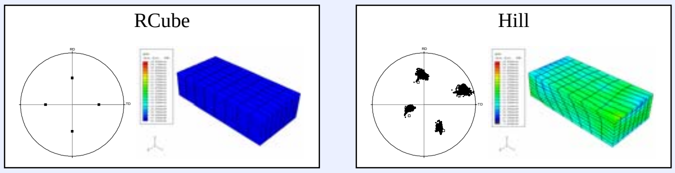
Figure 2: Divergence of the flow field as shown in figure 1
a) 3D representation in Euler space
b) 2D sections of the Euler space

Literature

1. H. Klein, E. Dahlem, C. Esling, H. Bunge in “Theoretical Methods of Texture Analysis”, DGM Informatoionsgesellschaft (1987), 259 – 272
2. P. v. Houtte: in Proc. 6th Int. Conf. On “Texture of Materials” (ICOTOM 6) Iron and Steel Inst. of Japan (1981) 428

Single crystals

It can be seen from figure 2 that under plain strain compression certain orientations like RCube should be completely stable while others like Hill should rotate homogenously or like RZ should be fragmentized. To check this predictions crystal plasticity FEM simulations where carried out.



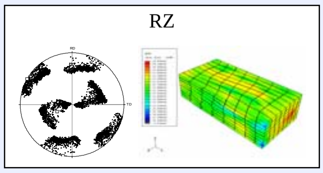


Figure 3: Results of a plain strain compression simulation for three different initial orientations. Pole figures show the orientation at every integration point. Colour in FE plots represents misorientation from original orientation.

Bicrystals

The single crystal simulations quiet nicely support the predictions of the chosen criterion for the fragmentation tendency. However, one might object, that the situation in a polycrystal aggregate would be totally different. In a polycrystal every grain has to deform in accordance with its neighbors. Therefore as a first step we performed bicrystal simulations, where one crystal is completely surrounded by another one. This setup (figure 4) can be used to study the influence of a neighboring grain on the fragmentation of the center grain (figure 5).

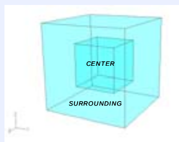


Figure 4: Geometrical setup of the bicrystal calculations

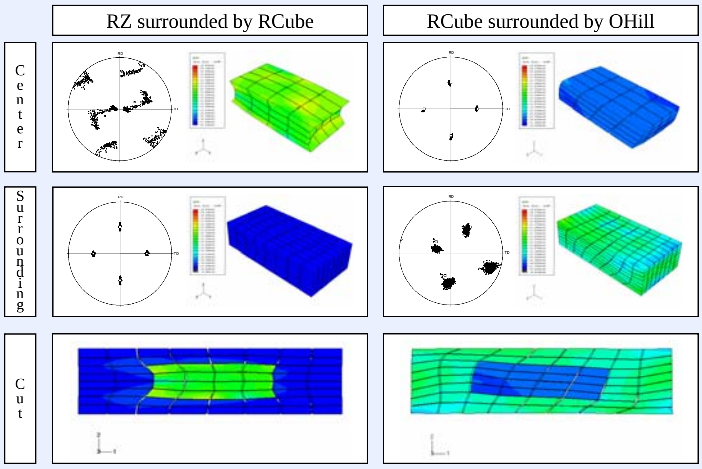


Figure 5: Results of a plain strain compression simulation for two different bicrystal configurations. Pole figures show the orientation at every integration point. Colour in FE plots represents misorientation from original orientation.

Conclusions and outlook

It was shown, that the divergence of the flow field can be used as a measure for grain fragmentation tendency. Even though the neighborhood is neglected by this method it can be shown at least for bicrystal configurations that the predictions are still qualitatively correct. In the future more realistic grain surroundings have to be checked. For the use in statistical models a quantitative measure for grain fragmentation tendency has to be defined.