

# Micro-Mesoscale Analysis of Crack Initiation and Propagation in Metallic Polycrystals

Torsten Luther and Carsten Könke

Institute of Structural Mechanics,  
Bauhaus-University Weimar, D-99423 Weimar, Germany

**Abstract.** Durability analysis in engineering is predominantly based on numerical simulations of macroscopic damage behaviour using phenomenological fracture models. But the true mechanisms of crack initiation and various crack propagation can only be discovered by considering of localized damage phenomena on meso and macro scale.

For metallic polycrystals we can assume that crack propagation on meso-scale ( $10^{-3}\text{m}$  -  $10^{-6}\text{m}$ ) occurs mainly along grain boundaries and depends strongly on atomic debonding on microscale ( $10^{-6}\text{m}$  -  $10^{-10}\text{m}$ ). The mutual dependence can be investigated by a multiscale analysis obtaining finally a reasonable macroscopic damage model based on micromechanical features. Our current work is focused on micro and meso models for damage analysis in metallic polycrystals and the parameter transfer between both scales.

On microscale we investigate the atomic debonding along grain boundaries between arbitrary oriented crystal lattices referring to the quasicontinuum (QC) method by Tadmor [1]. This method couples a continuum mechanical approach with material models based on interatomic potentials. Therefore the underlying atomic patterns of crystal material are considered explicitly. The main idea of the QC method is to refine the spatial discretization up to single atoms in these regions where high strain gradients must be represented. In other regions the behaviour of groups of atoms is represented by one representative atom. This fact allows for significant savings in computational effort compared to pure atomic simulations, such as molecular dynamic simulations.

Our mesoscale model describing the polycrystal material structure is based on a Voronoi cell geometry, wherein each cell is assigned to a single crystal. Both, crystal orientation and material properties are distributed in a statistical manner. To simulate crack propagation we apply a cohesive zone model (CZM) on the interface along grain boundaries. In future work the goal is to determine the constitutive relations for this CZM from QC simulations performed on a representative volume element and homogenized to the mesoscale model.

## References

- 1 Tadmor, E.B. (1996): *The Quasicontinuum Method*. Ph.D. Thesis, Brown University.