# Phase-Field Modelling and Computation of Fracture in Multiphase Materials

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Polycrystalline materials are widely used in engineering and material science applications, e.g. automobile, aerospace or renewable energy. The actual microstructure of the material at meso- and microscopic scales has a tremendous effect on the mechanical properties of the material and especially on the fracture toughness. Since fracture is the major failure mechanism in most construction materials, it is vital to analyze and to understand the fracture performance of polycrystals at the meso- and microscopic level. There are two main types of fracture observed in failed polycrystalline materials: intergranular and transgranular. The intergranular fracture follows the grain structure where the cracks mainly propagate along the grain boundaries. Transgranular fracture is associated with the cracks which mainly go through the grains interior. The competition between intergranular and transgranular cracking depends on the relation between the grain boundary energy (excess of energy at the boundary between two grains compared to the bulk energy of the grains) and the free surface energy (excess of energy of the free surface compared to the bulk energy of the grains). The studies in the literature have shown that the crack path strongly depends on local differences in toughness (grain interior versus grain boundaries), which significantly influences the macroscopic response of the entire structure. Hence, understanding microstructural effects in polycrystals is crucial to predict the damage mechanisms and requires considering a full complexity of the phenomena in mesoscale. In general, conventional methods (such as the extended finite element method (XFEM), cohesive zone models (CZM) or Linear elastic fracture mechanics (LEFM)) cannot capture all details of the defects in polycrystals (such as inter- and transgranular fracture) which is a major challenging task to study.

Nowadays, the phase-field method has established as one of the promising tools for the description of crack propagation in different kinds of materials. While phase-field approaches to describe crack evolution in solids are well-developed [1, 2], generalization to fracture in polycrystalline materials is still a challenging task. In particular, the multiphase-field theory is a perfect tool to study the crack propagation in polycrystalline media, because the interface energy between any pair of grains and surface energy are the natural input parameters for the model [3].

The main purpose of this study is to develop a comprehensive multiphase-field model for fracture in a multiphase system. Theoretical analysis is complemented with developments in computational modeling of the fracture phenomena. The model is implemented inside the open source software project OpenPhase to solve some examples in three-dimensions. The model reproduces well different cases. It is shown that how the competition between intergranular and transgranular cracking depends on the relation between the grain boundary energy and the free surface energy.

## References

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