Geophysical Research Abstracts
Vol. 15, EGU2013-1645, 2013
EGU General Assembly 2013

A three-dimensional phase-field study of grain boundary tracking behavior in crack-seal microstructures

Kumar Ankit, Britta Nestler, and Michael Selzer
Karlsruhe Institute of Technology (KIT), IAM-ZBS, Haid-und-Neu-Str. 7, 76131 Karlsruhe, Germany
(kumar.ankit@hs-karlsruhe.de)

The mechanism by which vein formation occurs is a widely debated topic with chief assertions related to growing crystals-fracture wall surface interaction, degree of super-saturation and fluid-flow pathways. Amidst the debate, an important question is what causes the grain boundaries to curve/bend, a feature commonly observed in natural crack-seal microstructures. Therefore, with a view to amend the current understanding of the vein-growth mechanism, we present a 3D multi-phase-field model to explain the dynamics of crystals precipitating from a super-saturated solution in a progressively widening fracture. Since the present model equations are derived on the basis of general thermodynamic and kinetic principles and relies on interfacial energy minimization, complicated moving boundary problems such as microstructure evolution on a large scale, can be dealt with ease [1,2]. A systematic simulation study of the influence of different boundary conditions (free growth and crack-sealing) on growing crystals highlights the importance of anisotropy in surface energy in free-growth as well as crack-sealing conditions; a factor overlooked in the previous models.

To define the crystal symmetry, we consider the anisotropy in surface energy to simulate crystals (with flat facets and sharp corners) possessing different orientations and study the resulting growth competition to deduce a consistent orientation selection rule in the free-growth regime. From the crack-sealing simulations, we co-relate the grain boundary tracking behavior and the relative rates of crack opening and trajectory, initial grain size and wall roughness. Further, the formation of curved grain boundaries in crack-sealing conditions as an imprint of anisotropy in surface energy of growing crystals and coupling with wall rock is elucidated. We also identify the ‘mixed-mode’ growth of crystals in crack-sealing conditions, characterized by formation of curved as well as straight grain boundaries and decrease in grain boundary tracking behavior. Finally, it is concluded that within the complete crack-seal regime, the propensity to form curved boundaries is higher if wall roughness is not sufficiently high to suppress facet formation.

References

[1] B. Nestler, H. Garcke, B. Stinner, 2005. Multicomponent alloy solidification: Phase-field modeling and simulations. *Phys. Rev. E* 71, 041609.

[2] B. Nestler, M. Reichardt, M. Selzer, 2008. Massive multi-phase-field simulations: methods to compute large grain system. In: Hirsch, J., Skrotzki, B., Gottstein, G. (Eds.), *Proceedings of the 11th International Conference on Aluminium Alloys* Aachen, Germany, pp. 1251-1255.