Geophysical Research Abstracts
Vol. 18, EGU2016-8250, 2016
EGU General Assembly 2016

Towards an integrated numerical simulator for crack-seal vein microstructure: Coupling phase-field with the Discrete Element Method

Simon Virgo (1), Kumar Ankit (2,3), Britta Nestler (2,3), and Janos L. Urai (1)

(1) RWTH Aachen University, Geologie - Endogene Dynamik, Aachen, Germany (s.virgo@ged.rwth-aachen.de), (2) Institute of Materials and Processes, Karlsruhe University of Applied Sciences, Karlsruhe, Germany, (3) Institute of Applied Materials—Computational Materials Science, Karlsruhe Institute of Technology, Karlsruhe, Germany

Crack-seal veins form in a complex interplay of coupled thermal, hydraulic, mechanical and chemical processes. Their formation and cyclic growth involves brittle fracturing and dilatancy, phases of increased fluid flow and the growth of crystals that fill the voids and reestablish the mechanical strength.

Existing numerical models of vein formation focus on selected aspects of the coupled process. Until today, no model exists that is able to use a realistic representation of the fracturing AND sealing processes, simultaneously.

To address this challenge, we propose the bidirectional coupling of two numerical methods that have proven themselves as very powerful to model the fundamental processes acting in crack-seal systems: Phase-field and the Discrete Element Method (DEM).

The phase-field Method was recently successfully extended to model the precipitation of quartz crystals from an aqueous solution and applied to model the sealing of a vein over multiple opening events (Ankit et al., 2013; Ankit et al., 2015a; Ankit et al., 2015b). The advantage over former, purely kinematic approaches is that in phase-field, the crystal growth is modeled based on thermodynamic and kinetic principles. Different driving forces for microstructure evolution, such as chemical bulk free energy, interfacial energy, elastic strain energy and different transport processes, such as mass diffusion and advection, can be coupled and the effect on the evolution process can be studied in 3D.

The Discrete Element Method was already used in several studies to model the fracturing of rocks and the incremental growth of veins by repeated fracturing (Virgo et al., 2013; Virgo et al., 2014). Materials in DEM are represented by volumes of packed spherical particles and the response to the material to stress is modeled by interaction of the particles with their nearest neighbours. For rocks, in 3D, the method provides a realistic brittle failure behaviour.

Exchange Routines are being developed that translate the spatial domain of the model from DEM to the phase-field and vice versa. This will allow the fracturing process to be modeled with DEM and the sealing processes to be modeled with phase-field approach. With this bidirectional coupling, the strengths of these two numerical methods will be combined into a unified model of iterative crack-seal that will be able to model the complex feedback mechanisms between fracturing and sealing processes and assess the influence of thermal, mechanical, chemical and hydraulic parameters on the evolution of vein microstructures.

References:

Ankit, K., Nestler, B., Selzer, M., and Reichardt, M., 2013, Phase-field study of grain boundary tracking behavior in crack-seal microstructures: Contributions to Mineralogy and Petrology, v. 166, no. 6, p. 1709–1723

Ankit, K., Selzer, M., Hilgers, C., and Nestler, B., 2015a, Phase-field modeling of fracture cementation processes in 3-D: Journal of Petroleum Science Research, v. 4, no. 2, p. 79–96

Ankit, K., Urai, J.L., and Nestler, B., 2015b, Microstructural evolution in bitaxial crack-seal veins: A phase-field study: Journal of Geophysical Research: Solid Earth, v. 120, no. 5, p. 3096–3118.

Virgo, S., Abe, S., and Urai, J.L., 2013, Extension fracture propagation in rocks with veins: Insight into the crack-seal process using Discrete Element Method modeling: Journal of Geophysical Research: Solid Earth, v. 118, no. 10

Virgo, S., Abe, S., and Urai, J.L., 2014, The evolution of crack seal vein and fracture networks in an evolving stress field: Insights from Discrete Element Models of fracture sealing: Journal of Geophysical Research: Solid Earth, p. 2014JB011520