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Quantitative modeling of quartz vein sealing

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Mineral precipitation significantly effects many aspects of fluid-rock interaction across all length scales, as the dynamical change of permeability, of mechanical interaction and redistribution of dissolved material. The hydrothermal growth of quartz establishes one of the most important mineralization processes in fractures. Tectonically caused fracturing, deformation and fluid transport leaves clear detectable traces in the microstructure of the mineralized veins. As these patterns give hints on the deformation history and the fluid pathways through former fracture networks, accurate spatio-temporal modeling of vein mineralization is of special interest, and the objective of this study. Due to the intricate polycrystalline geometries involved, the underlying physical processes like diffusion, advection and crystal growth have to be captured at the grain scale.

To this end, we adapt a thermodynamically consistent phase-field model (PFM), which combines a kinetic growth law and mass transport equations with irreversible thermodynamics of interfaces and bulk phases. Each grain in the simulation domain is captured by a phase field with individual orientation given by three Euler angles. The model evolves in discrete time steps using a finite difference algorithm on a regular grid, optimized for large grain assemblies. The underlying processes are highly nonlinear, and for geological samples, boundary conditions as well as many of the physical parameters are not precisely known. One motivation in this study is to validate the adequately parameterized model vs. hydrothermal experiments under defined (p,T,c) conditions. Different from former approaches in vein growth simulation, the PFM is configured using thermodynamic data from established geochemical models. Previously conducted batch flow experiments of hydrothermal quartz growth were analyzed with electron backscatter diffraction (EBSD) and used to calibrate the unknown kinetic anisotropy parameters. In the simulations, we study the sealing of syntaxial veins of 300 microns aperture by epitaxial overgrowth of preexisting grains from the rock surface. Results from 3D simulations conducted in the limit of low Damköhler numbers explain the observed transition regime in competitive crystal growth for blocky-elongate veins. The initial formation of quartz crystal bridges, especially pronounced in the regime of low supersaturation, is observed. The morphological evolution of micro-ensembles of grain neighbourhoods from the rock sample compares well to that of the simulations. To juxtapose larger polycrystal domains, the variation of grain number, texture and porosity as function of scaled distance from the initial wall is calculated. Velocity profiles from solutions of the isothermal incompressible Navier-Stokes equation are used to record permeability evolution and to evaluate deviations from the cubic law. Both, the geometry of the microstructure and the permeability of the flow pathway, are used as upscaling parameters for larger scale (fracture scale) simulations.