Prediction of porosity evolution in polycrystalline material: A kinetic Monte Carlo study using the rate spectra concept

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Quantitative predictability of porosity evolution as a result of water-rock interaction is of great interest in multiple disciplines of Earth science. Related data are required as input parameters in reactive transport models dealing with challenges such as CO_2 sequestration, extraction of thermal energy, and reservoir rock diagenesis. Crystal surface reactivity is an important but not constant bounding condition for the dynamic evolution of porosity. Dynamic systems can be successfully simulated using Kinetic Monte Carlo (KMC) methods. KMC calculations cover large enough intervals of both length- and time scales that are sufficient to address the evolution of reacting crystal domains appropriately. Here we utilize KMC simulations to study the evolution of reaction rates and surface pores in crystalline structures built-up of domains characterized by constant surface reaction energies but having varying defect densities. For the first time, we apply the rate spectra concept [1] to KMC results in order to analyse systematically the rate contributors in the frequency domain of rate datasets [2]. We discuss simulation results with respect to both, inheritance and passivation of initial reactivity in polycrystalline material. We furthermore highlight implications that result from the observed variability in pore volume and distribution with great potential for many interesting applications.

[1] Fischer et al. (2012), *GCA*, **98**, 177-185 [2] Fischer et al (2014), *Appl Geoch* **43**, 132-157