

Diversity of mineral dissolution scenarios at the nanoscale: mechanistic insights from Monte Carlo simulations

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Reactive and sorptive properties of mineral surfaces at the nano- to micro-scale depend on a large number of factors: internal crystal structure and chemical composition, lattice defects, crystal face orientation and periodic bond chain structure, chemical composition of the intact fluid and the fluid transport regime. Minerals in rock assemblages are subjected to the spatial confinement that imposes restrictions to mineral grain sizes and material transport, giving rise to a variety of complex dissolution-reprecipitation scenarios. This complexity has tremendous importance for the fate of the systems composed of nano- to micro-size objects, such as mineral grains and pore walls, as well as microorganisms that introduce even more specific and complex feedback into the overall microcosm.

We would like to present our mechanistic insight into mineral dissolution at the nano- to micro-scale for carbonates[1], quartz[2], phyllosilicates[2], specific to mineral faces and environmental conditions. This work is based on the system-specific Kinetic Monte Carlo models developed with connection to the ab initio and Grand Canonical Monte Carlo studies of mineral-fluid interfaces. A special attention is given to calcite-magnesite solid solution series showing unique compositional and system size effects on the dissolution dynamics. Comparison of the material fluxes obtained in the simulations to their experimental analogues showed that intrinsic dissolution variance persists across the scales[4]. These observations impose new methodological requirements for the modelling of mass transport through the mineral assemblages and the predictability of the overall system's behavior.

[1] Kurganskaya & Churakov (2018) *Phys. Chem. C* **122**, 29285–29297. [2] Kurganskaya & Luttge (2013) *J. Phys. Chem. C* **117**, 24894–24906, [3] Kurganskaya & Luttge (2013) *Geochim. Cosmochim. Acta* **120**, 545–560. [4] Fischer *et al.* (2014) *Appl. Geochem.* **43**, 132–157. [5] Luttge *et al.* (2013) *Elements* **9**, 183–188.