

Control of Silicate-Fluid Interactions by Nanoporous Interfacial Systems

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Our ability to reliably predict the mechanisms and kinetics of dissolution of silicate materials constitutes a prominent challenge to our understanding of a range of (bio)geochemical and industrial processes involved in mineral weathering and soil formation, nutrient cycling in the critical zone, urban infrastructure durability and nuclear waste disposal safety.

How are the dissolution mechanisms and kinetics affected by the formation of nanoporous phases at the reacting interface between fluid and silicate minerals, cements and glasses? To answer this question, we combined advanced analytical methods allowing direct observation of the interfacial dissolution-reprecipitation reactions (using feldspars as model silicate minerals) with high-performance atomistic simulations of silica nanopores.

We measured the properties of the porous amorphous silica layers forming at the fluid-mineral interface by using *in-situ* and/or surface sensitive techniques including synchrotron-based grazing-incidence small-angle X-ray scattering (GISAXS), X-ray reflectivity (XRR), transmission electron microscopy (TEM) and vertical scanning interferometry (VSI). We investigated the mobility of water and alkali ions through model nanoporous systems by molecular dynamics (MD) modeling. We generated relevant water-silica-ions interactions by including the effect of negative surface charge. We evaluated the ability of single cylindrical silica nanopores to sustain concentration gradients by estimating their permeability and salt rejection capabilities. Our results support the analogy of such systems with semi-permeable membranes or nanofluidic diodes, which may ultimately explain the ability of nanoporous interfacial layers to modulate fluid-mineral interactions.