

Patterns in surface morphologies as signatures for underlying kinetic processes

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The chemical weathering of rocks is a complex phenomenon including a multitude of possible reactions. Mineral surfaces interact with natural water and undergo time-dependent reactive alteration of their morphologies[1]. The characteristic changes in surface topography depend on a large variety of environmental parameters and kinetic processes. Structure and chemical composition of minerals as well as crystallographic orientation of reacting surfaces substantially influence the geometry of morphological features and their kinetic behavior. The shape, spatial organization, and kinematics of these features are ultimately related to the chemical composition of the reacting fluid, temperature, and other environmental factors. Therefore, morphological patterns observed on mineral surfaces can be considered as possible material-specific characteristic signatures of fluid chemistry and related reactions at solid-fluid interfaces.

Decoding signatures from geometry and spatial organization of kinetic surface features requires thorough understanding of their formation mechanisms. The necessary step is the investigation of possible reactions that may happen at different surface sites. We address this issue by using Kinetic Monte Carlo simulations of mineral dissolution where reaction rates are converted into reactive event probabilities and temporal surface evolution is directly observed as modelling output. During the last two decades we developed microkinetic models for dissolution of tectosilicates, phyllosilicates, carbonates, and sulfates[2]. Additionally, we incorporated the influence of pH and background electrolytes on surface speciation of carbonates by using complementary Grand Canonical Monte Carlo simulations[3]. The influence of surface morphology on the kinetic pathways to and from equilibrium is also investigated by using KMC simulations and the kinetic rate laws are re-evaluated and re-derived[4]. In this talk we present the key underlying theoretical concepts establishing the connections between mineral structure, morphological patterns, chemistry of fluids, and process kinetics.

[1] Brantley, Kubicki & White, Eds. (2008), *Kinetics of Water-Rock Interaction*; Springer-Verlag: New York.

[2] Kurganskaya & Rohlfs (2020), *American Journal of Science* 320, 1–26.

[3] Kurganskaya & Churakov (2018), *J. Phys. Chem. C* 122 (51), 29285–29297.

[4] Kurganskaya & Luttge (2021), *ACS Earth Space Chem.* 5 (7), 1657–1673.