

How crystal surface nanotopography controls surface reactivity

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The variability of the surface reactivity of crystals is a long-standing and important problem, as it is critical for predicting reactive transport. The evolution of dissolving or growing crystal surfaces has been intensively studied using surface sensitive methods, such as AFM or interferometric microscopy, and the mechanistic influence of surface steps and kinks is well known from such investigations. In contrast, more complex surface architectures consisting of overlapping etch pits and fast moving steps are difficult to assess quantitatively in terms of their effective reactivity. However, this surface architecture forms the complex reacting topography at the pore scale and is thus important for the parameterization of reactive transport models.

The present study addresses this issue by quantitatively analyzing the changing surface architecture across length scales. We examine several dozen data sets of a reacting surface that was measured sequentially. This provides a unique sequence of the reacting crystal topography. We use the power spectral density (PSD) method to analyze the nano- and microtopography across scales. The principle of PSD curves is to reduce the dimension of topographic information in order to achieve a cross-scale quantification of its variability. We statistically evaluate this quantification in the frequency domain against the rate distribution of each reaction step using the rate spectrum analysis. The conclusions from the correlation analysis of PSD curves and rate spectra are discussed in this presentation. Temporal stability and variability of specific rate contributors are identified and will provide theoretical support for current reactive transport models.