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The Calcite 104 cleavage surface simulated with weighted Voronoi methods

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The dissolution and precipitation behavior of carbonate minerals is not only industrially interesting, but also of huge environmental and climatic importance. However, so far, there is a gap between established simulation methods like kMC, which are limited in their spatial system size, and experimental data which usually covers a much larger scale.

A new and extremely fast approach to modeling Calcite dissolution, based on computational geometry, namely the concepts of Voronoi diagrams and non-euclidean distance functions, is introduced to attempt to close that gap.

A software partitioning the Calcite 104 cleavage surface into Voronoi cells generated by screw defect outcrops was developed. Height was described as a function of distance, via the detour of using the stepwave model velocities, which are functions of distance to the nearest defect. Etch pit coalescence was described algorithmically as the interaction of nearest neighbors sharing a Voronoi diagram segment. This led to larger pit areas enveloping the smaller single etch pit.

Despite the anisotropy of the crystal lattice, the generated Voronoi surfaces were sufficiently similar to kMC simulation results to meaningfully compare rate maps, rate spectra, and surface roughness. Key morphological features seen in kMC simulations were retained in the Voronoi distance map, which proves the general suitability of the new method to predict surface reactivity.