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Weighted Voronoi calculations in crystal surface morphology: a fast approach

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We explore a new and very fast method for the simulation of the reaction kinetics of a dissolving crystal, capable of being used for much larger systems than established kinetic Monte Carlo simulations, which are limited in spatial system size. We calculate Voronoi distance maps that are based on a non-Euclidean distance function corresponding to the crystal lattice, weighted additively in relation to stochastic etch pit depths.

The dissolution of an initially flat Kossel crystal surface served as an example to show that a sequence of Voronoi calculations can predict dissolution kinetics based on the information about the distribution of screw defects.

KMC-parameterized weighted Voronoi distance maps show the evolution of reacting (dissolving) crystal surfaces with sufficient detail to enable analysis of rate maps, rate spectra, and surface roughness data. The calculation time-saving efficiency of these Voronoi simulations provides an opportunity for the reactivity analysis of larger systems. Thus, the upscaling of reaction rates in larger systems could benefit from the application of Voronoi techniques.