Weighted Voronoi simulation of the dissolution of the Calcite cleavage (104) surface

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Dissolution kinetics of carbonates have been studied extensively, both experimentally and computationally. In AFM measurements, atomic steps moving across the surface were observed [1]. The stepwave model [2] assumes defect-generated steps as the basic mechanism of dissolution of the mineral surface. Kinetic Monte Carlo (KMC) models of the calcite cleavage (104) surface [3] have been established in order to simulate crystal surface evolution. The overall motivation is to improve our ability to predict material fluxes from or to the reacting surfaces in order to quantify the fate of materials in technical or environmental settings. Because modeling approaches are necessarily limited in terms of system size and reaction time, we focus on a new potentially very fast simulation method based on Voronoi diagrams [4].

Using an initial calcite cleavage surface and defect distribution, weighted Voronoi calculations [5] of non-euclidean distance functions are used to determine the surface morphology (**Fig. 1**), as well as the dissolution rate's distribution and statistical heterogeneity [6]. This approach retains basic morphologic and key results in terms of kinetics returned by KMC models. We expect integrated KMC-Voronoi simulations to provide a valuable approach to the problem of material fluxes over large space and time scales.

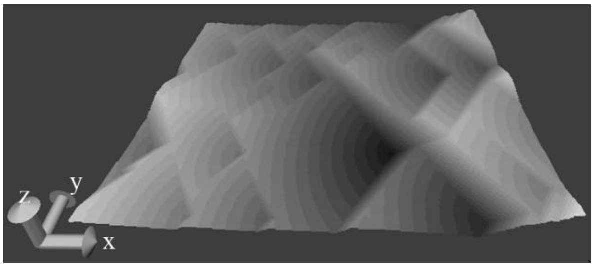

Fig.1: Weighted Voronoi distance map (300x300 units) of a calcite (104) face after dissolution at screws.

[1] Hillner *et al.* (1992) *Ultramicroscopy* **42-44 (2)**, 1387-1393. [2] Lasaga & Luttge (2001) *Science* **291**, 2400-2404. [3] Kurganskaya & Luttge (2016) *J. Phys. Chem. C* **120**, 6482-6492. [4] Voronoi (1908), *J Reine u Angew Math* **133**, 97–178. [5] Aurenhammer (1991), *ACM Comp Surv* **23 (3),** 345-405. [6] Fischer *et al*. (2012), *GCA* **98**, 177-185.