Crystal dissolution studied by a combination of kinetic Monte Carlo and Voronoi methods

RICARDA D. ROHLFS[1], CORNELIUS FISCHER[12], INNA KURGANSKAYA[2] AND ANDREAS LUTTGE[12]

[1]Universität Bremen, Abt. Mineralogie, Marum; Klagenfurter Str., D-28359 Bremen

[2]Rice University, Earth Science Dept, 6100 Main Street, Houston, TX 77005, USA

Kinetic Monte Carlo (KMC) methods have been extensively used for the study of crystal dissolution and surface reactivity. The latter is heterogeneously distributed. Step waves and etch pits generate complex surface topographies. Crystal defects are an important contributing factor to the surface evolution. To quantify rate contributions, the concept of rate spectra is used [1]. Using KMC, (synthetic) rate spectra can be calculated.

Voronoi diagrams as a means of partitioning a surface plane are a well-known concept from geometry [2]. A set of generating points is defined and generates regions which are closer to one generating point than to any other. Voronoi diagrams can also be weighted by defining the distance differently and assigning weight to different generating points. Voronoi diagrams are often applied to describe natural or technical systems, e.g., crystal growth [3].

In this study of a dissolving Kossel crystal surface, etch pit development was modeled with KMC. Results are compared to weighted Voronoi diagrams that use defect outcrops, i.e., etch pit centers as the set of generating points. A combined approach of KMC and Voronoi geometry is used to examine the heterogeneous surface reactivity and resulting dissolution rate spectra.

Here, our rate results generated by KMC simulations are used for weighting the Voronoi diagrams. The overall aim of this study is to predict surface reactivity by using geometrical methods and combining them with established KMC simulation techniques and the rate spectra concept.

[1] Fischer et al (2012), *GCA* **98**, 177-185. [2] Voronoi (1908), *J Reine u Angew Math* **133**, 97–178. [3] Aurenhammer (1991), ACM Comp Surv **23** (**3**), 345-405.