Defect distribution and dissolution morphologies on low-index surfaces of α-quartz.

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Dissolution of mineral surfaces is a ubiquitous geochemical process. The morphology of dissolving mineral surfaces is often complex because of the influence of defects. Common mechanisms of surface dissolution include the etching of extended defects (pitting), and step-wise dissolution. The contribution of a given dissolution mechanism to surface morphology depends on the distribution of defects (such as dislocations and pores) and steps on the surface in question. The contributions of different kinds of defects can interact and produce a topography that is difficult to characterize quantitatively using standard methods. The present work aims to 1) analyze the morphological differences that arise from changes in the distribution of emerging defects on the prismatic (100) and rhombohedral (101) surfaces of α-quartz, and 2) beyond standard analyses, apply scaling concepts and wavelet analysis to the characterization of such surfaces.

The dissolution of the prismatic quartz face in 0.01 M KOH solution at 400-500 K is dominated by pits centered on dislocation sites. The recurrent emergence and pitting of dislocations produced an increasingly rough surface morphology with time on all length scales observed (1 – 90 microns). Dissolution on the rhombohedral face proceeds mostly through step-wise dissolution on the small scale (1-10 microns). Only on large length scales (50-90 microns) did extended defects contribute to the surface morphology. As a result, the roughness of the rhombohedral surface stayed stable on the ≤ 1 μm scale throughout the reaction, and reached its saturation value on the 10-90 μm scale within 60 hours of the reaction.

Fast kinetic Monte Carlo models for defect controlled dissolution of multiple etch pits

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Kinetic Monte Carlo models have been developed to simulate the dissolution of etch pits under the control of multiple dislocations and point defects. Simulations like that shown in figure 1 required the development of fast algorithms for large systems. The computer models are being used in conjunction with laboratory experiments to develop a better understanding of the formation of geometrically complex surfaces during dissolution.

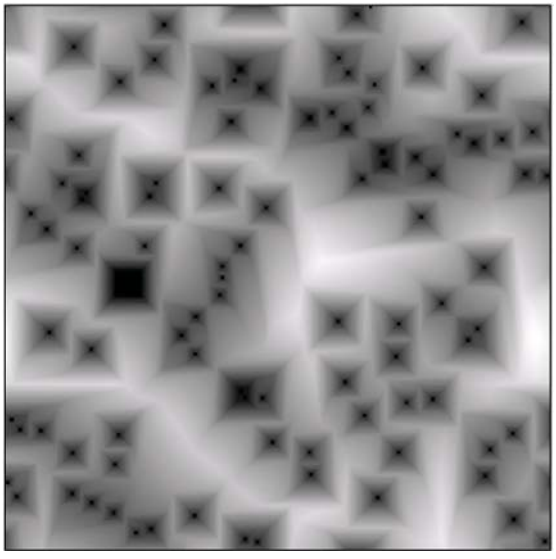

Figure 1: Cubic lattice model simulation of the dissolution of a mineral surface controlled by 100 screw dislocations in an area of 2048 × 2048 lattice units.