

Visual simulation of crystal growth and development of sector zoning in hydrothermal quartz

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Crystal growth in the natural environment is a poorly understood process. Recent measurements of chemical impurities preserved within natural crystals offer important clues toward understanding morphologic evolution during crystal growth. In natural hydrothermal quartz crystals, internal chemical heterogeneities define sector zones as individual growth faces trap different amounts of impurities. The concentration of impurities is a sensitive indicator of the kinetics of crystal growth and thus can serve as a speedometer of the growth rate of individual faces. We present a visual simulation that illustrates the morphologic evolution of a quartz crystal as it grows from hydrothermal solution. We show how growth on different crystal faces leads to chemically distinguishable sector zones inside a single crystal. Our simulations can generate the large differences in impurity concentrations across sharp sector zone boundaries that are observed in natural crystals. Our results constrain the relative growth rates of individual faces during crystal growth in the hydrothermal environment.

Surface charge development at the interface of nanocrystalline-anatase and aqueous solutions

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Oxide and oxyhydroxide crystals with nanometer-scale dimensions are common in natural systems near the Earth's surface, arising from chemical weathering and biomineralization processes. These nanometer-sized particles display novel, size-dependent properties which may dramatically impact geochemical processes; including, enhanced adsorption of ions, and regulating the mobility and bioavailability of ions. Consequently, models predicting the behavior of ions in the environment require quantification of size-dependent mineral-surface properties.

The surface properties of nanocrystalline-anatase in aqueous NaCl solutions were investigated utilizing various characterization techniques, and experimental and modeling studies. A suite of anatase samples ranging in size from 3.5 to 200nm in diameter were characterized by BET, XRD and HR-TEM. Further characterization of the 3.5nm sample was conducted utilizing SANS, U-SAXS and Laser diffraction analyses. Potentiometric titrations and electrophoretic mobility studies were completed, to investigate the size-dependence of surface charge development, and the pH_{znpc} and IEP values of the nanometer anatase particles. The two experimental techniques were matched as closely as the different procedures permitted. Titrations were performed in NaCl media at ionic strengths from 0.005 to 0.3 molality, at 25°C. The surface charge of the anatase was enhanced with increasing ionic strength. Moreover, the experimental data suggests that the pH_{znpc} values increase with decreasing particle size.

The experimental results were rationalized using the 1-pK and MUSIC surface complexation models, in combination with a basic Stern-layer representation of electrical double layer (EDL) structure. Modeling of the diffuse layer of the EDL of the smallest particles at the lower ionic strengths accounts for the spherical symmetry of the diffuse portion of the EDL.

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