A stochastic approach to study dissolution of carbonates

I. KURGANSKAYA[1], A. LUTTGE*[1,2] AND C. FISCHER[1,2]

[1]Rice University, Earth Science Department, 6100 Main Street, Houston, TX, 70005, US
[2]MARUM,Klagenfurter Straße, D-28359, Bremen, Germany
*correspondence: aluttge@marum.de

Carbonate dissolution-precipitation reactions have a large importance for natural and man-made processes: accumulation of marine sediments, oil reservoir formation, growth of skeletons and shells of marine organisms, karst formation, rock cavitation, failrue due to the CO_2 injection, etc. Thus, understanding of carbonate-water interaction is critical for our ability to predict and influence behavior of many geological and geochemical systems.

Mechanisms and rates of carbonate dissolution have been extensively investigated using experimental approaches. Studies of surface topography at the micro-scale revealed complex dissolution kinetics controlled by surface structure. Another remarkable finding was a substantial rate variation [1,2], attributed to inhomogeneous spatio-temporal distributions of reactive sites[2]. The aim of this study is to explain and predict complex carbonate dissolution kinetics and identify the sources of this rate variance. In order to reach this goal, we employ a Kinetic Monte Carlo (KMC) method as a tool capable to explore mechanistic links between the dissolution reaction at the molecular and microscopic levels. Previously Liang et al.[3] used KMC to demonstrate how different orientations and energetics of steps and kink sites induce step velocity anisotropy. In this study we extend this approach further by applying it to the large systems involving linear crystal defects. Here we demonstrate kinetic effects caused by the interaction of surface features: steps and kinks (Fig.1). We also compare our simulation results with experimental AFM and VSI data.

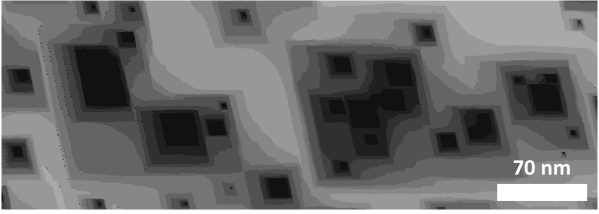

Fig. 1. Dissolving calcite surface (KMC simulations).

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