

Supporting Information

A kinetic Monte Carlo approach to model barite dissolution: the role of reactive site geometry

Inna Kurganskaya ^{1,2,*}, Nikolay Trofimov ¹ and Andreas Luttge ^{1,2,3}

¹ Geology department(FB5), University of Bremen, Klagenfurter Str. 4, 28359 Bremen, Germany; trofimov@uni-bremen.de (N.T.); aluttge@marum.de (A.L.)

² MAPEX—Center for Materials and Processes, University of Bremen, Postfach 330 440, 28334 Bremen, Germany

³ MARUM—Center for Marine Environmental Sciences, University of Bremen, Leobener Str. 8, 28359 Bremen, Germany

*Correspondence: inna.kurganskaya@uni-bremen.de

Contents:

Influence of a system size on etch pit morphology.....2

Figure S1 Influence of a system size on etch pit morphology: Monolayer pits.....2

Figure S2 Influence of a system size on etch pit morphology: Multilayer pits.....3

Step velocity calculations.....3

Figure S3 Step velocity vs distance from the hollow core.....4

Influence of a system size on etch pit morphology

The triangular shape of pits can be clearly visible at systems of sizes 50×50 unit cells. Pits preserve their shape upon growth in size. Figure S1 shows evolution of an etch pit in a system of a size 300×300 unit cells.

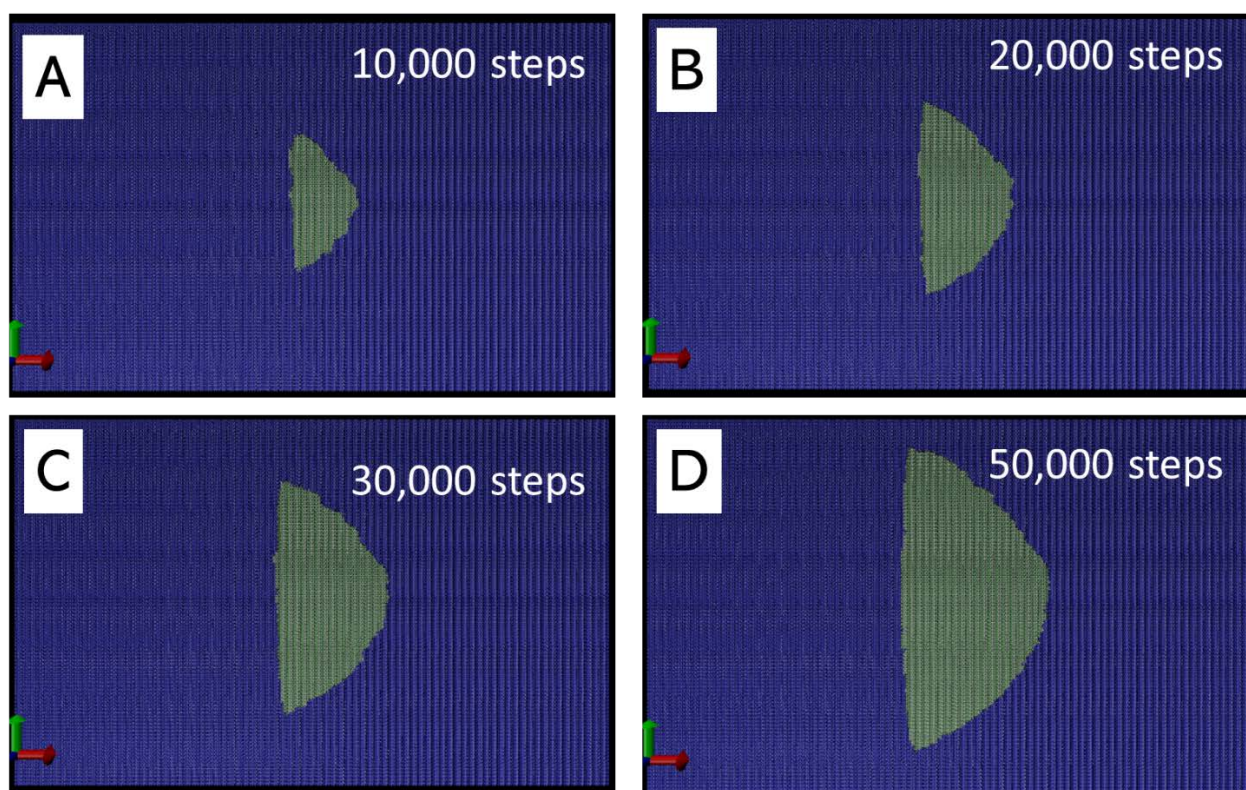


Figure S1. Influence of a system size on etch pit morphology: Monolayer pits. The lateral system size is 300×300 unit cells. (A) 10,000 atoms removed; (B) 20,000 atoms removed; (C) 30,000 atoms removed; (D) 50,000 atoms removed.

Multilayer etch pit morphology can be described as a vertical sequence of triangles rotated by 180° in each consecutive layer. This morphology can be clearly visible at system sizes 100×100 unit cells. Once an etch pit grows in size, the overall morphology is preserved (Figure S2). At bigger sizes (Figure S2C,D) steps appear to be less rough and the overall morphology is more euhedral.

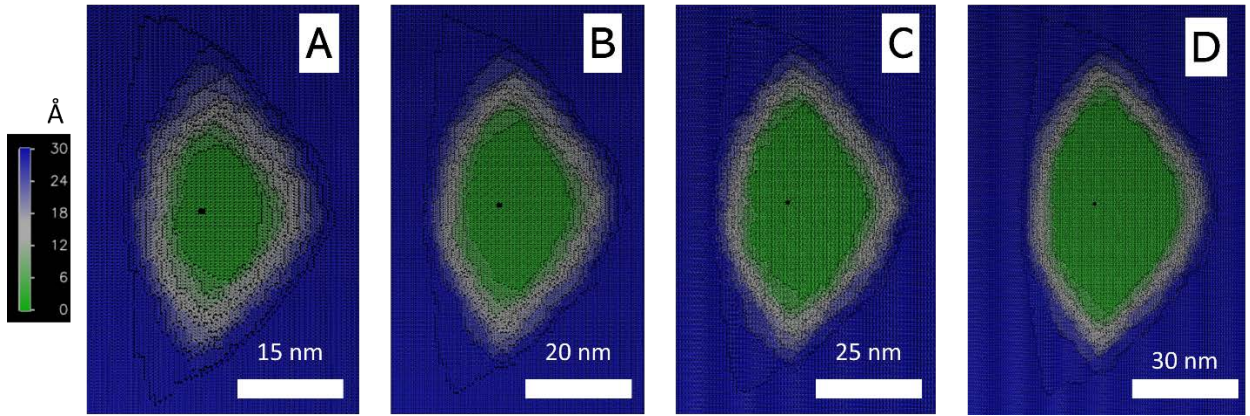


Figure S2. Influence of a system size on etch pit morphology: Multilayer pits. The lateral system size is 300×300 unit cells. (A) 10,000 atoms removed; (B) 20,000 atoms removed; (C) 30,000 atoms removed; (D) 50,000 atoms removed.

Step velocity calculations

The step velocities were calculated as average on 10 measurements at different distances from the hollow core. The measurements were performed on a single monolayer pit (see Methods for more details).

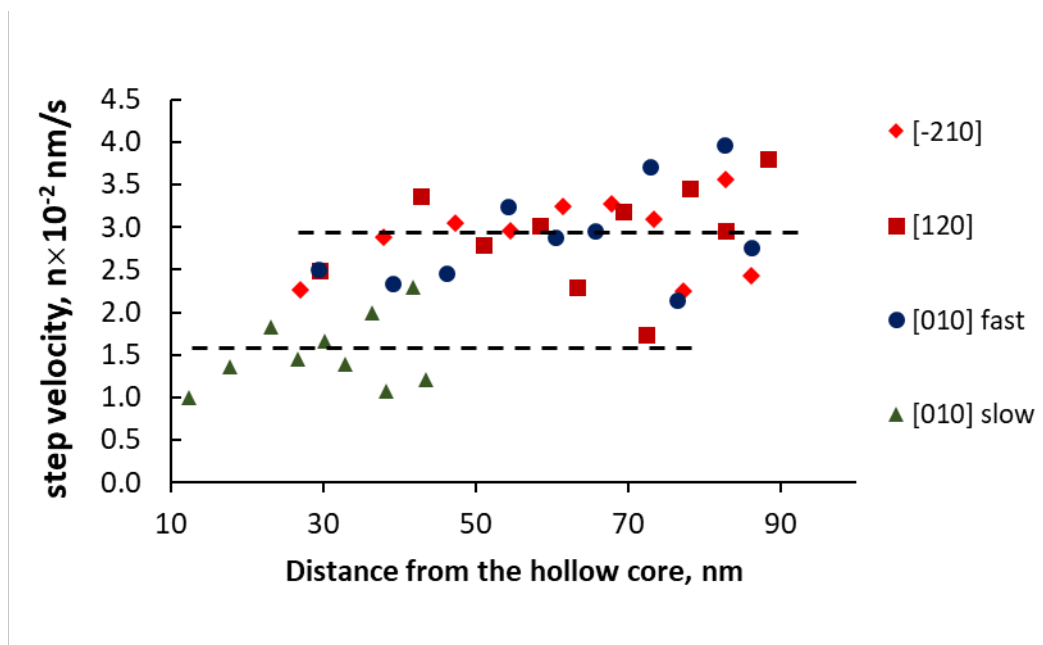


Figure S3. Step velocity as a function on the distance from the hollow core