Interaction of dislocations during mica dissoultion- a Kinetic Monte Carlo Study

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Clay mineral reaction kinetics has a tremendous importance for many natural and man-made systems, examples include oil and gas reservoir rocks (e.g, shales) and nuclear waste disposal sites. However, experimental approaches to study clay mineral reactivity are difficult and time consuming to implement. Particularly, the interpretation of experimental data involve resolving relationships of size, structure, and composition unique to these materials which significantly increase the range of independent physiochemical variables(e.g.temperature, pH) one must explore.

This experimental overhead is a major motivation for studying reaction kinetics of clay minerals by using kinetic Monte Carlo (KMC) simulations. In order to analyze the impact of different types of crystal defects on clay mineral reactivity, we modified an existing KMC sheet silicate model [1]. This new model allows the analysis of both screw and point dislocations. Since point defect distributions yield significant differences in the surface energy of sheet silicates [2], the improved model provides significantly enhanced insight into the reaction kinetics. A key result of this study is the evidence for superimposition of dissolution stepwaves originating from both screw and point dislocations. The analysis of rate components that combine to produce the overall rate and their temporal evolution provides critical insight into the dissolution kinetics of phyllosilicate minerals.

[1] Kurganskaya & Luttge (2013), *GCA*, 545-560 [2] Kuwahara (2008), *Am. Mineral.*, 1028-1033

[2] Barber (2010) ,*Dislocations in minerals*.Dislocations in solids ,207