Kinetic Monte Carlo study on dissolution kinetics of different sheet silicate octahedral structures

J. SCHABERNACK[1]*, E. MACKE[1], M. PETER[1], I. KURGANSKAYA[2], C. FISCHER[1] AND A. LUTTGE[1]

[1]MARUM / FB 5 – Geowissenschaften, Universität Bremen; Klagenfurter Str. GEO, D-28359 Bremen, Germany (*correspondence: jschaber.uni-bremen.de)

[2]Universtät Bern, Institute of Geological Sciences, Baltzerstr. 3, CH-3012 Bern

Sheet silicates play a key role in many natural processes, such as weathering and diagenesis. They are widely used for important industrial applications, e.g. as materials for thermal and electronic insulators, additives to paint and cosmetics, and other purposes that exploit their unique structural properties. New materials are currently designed with certain properties mainly by heuristic methods. Due to the increasing speed and decreasing cost of computational resources, predictive numerical models can play a key role in the design process. Thus, different structural and chemical properties and their impact on the overall material performance can be investigated without the need for complex and time-consuming experiments.

In this work we systematically study the influence of muscovite and phlogopite chemical composition and structure on dissolution kinetics as a first step towards a predictive model applicable to the more complex sheet silicate structures. We choose these two minerals because of their principal difference in terms of crystal structure: the dioctahedral occupation of the octahedral layer in muscovite versus the trioctahedral occupation of the phologpite octahedral layer. In order to observe differences in dissolution mechanisms and evolution of dislocations on atomic level, we used kinetic Monte Carlo (KMC) simulations, modifying a existing successful model [1] to develop a model for phlogopite. We compare model results with experimental and analytical studies [2] in order to validate simulation results and improve the new code, and analyze model results of using phlogopite versus muscovite. We discuss these results in terms of an improved mechanistic understanding of the dissolution kinetics of sheet silicates at the atomic scale.

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