A kinetic Monte Carlo approach to study Plagioclase dissolution Mechanisms

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Solid-fluid interaction is an ubiquitous process on the Earth surface and in the Earth's crust. This process controls material fluxes in any geochemical environment involving fluids and represents a particular importance for toxic/hazardous material adsorption/desorption on mineral surfaces. Feldspar minerals represent the most abundant mineral group in the earth continental crust.

There have been plenty of exprimental studies on plagioclase dissolution in the last decades, including studies of the entire albite-anorthite solid solution series at different environmental conditions[1]. The influence of the composition and degree of Si/Al order onto dissolution mechanisms is an important problem that can be answered by using compuational modelling. A Kinetic Monte Carlo (KMC) model developed by Zhang and Luttge [2] yielded plagioclase surface evolution with restrictions in ordering coefficients and nm scale size. We develop this model further, by using a new generation model that incorporates long-range bond order effects shown to be important for silicates, such as quartz [3].

This new model is aimed at understanding mechanisms of plagioclase dissolution under far from equilibrium conditions with special focus on alumina/silica order disorder and alumina content as well as role of lattice defects. We present the new results showing mechanistic influence of plagioclase composition and order onto the interface structure and material fluxes of the dissolving surfaces.

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