A stochastic multiscale approach to model dissolution of silicates

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The dissolution kinetics of silicates is one of the most important fundamental problems in modern geochemistry and environmental sciences. A large amount of kinetic data are now available from published laboratory experiments, both from macroscopic dissolution of mineral powders and microscopic observations of reacted surface topography using atomic force microscopy (AFM) and optical interferometry (VSI). The size of the systems studied range from nm (AFM) to microns and cm (VSI and powder experiments). During the last few decades, quantum mechanical and Molecular Dynamics-based calculations have also substantially expanded our knowledge of molecular-level reaction mechanisms involving the mineral surface. Kinetic Monte Carlo methods have traditionally been used to connect atomic scale surface reactions with their phenomenological, macroscopic result, e.g., etch pit formation and step movement [1] or etch pit growth and coalescence [2].

Our goal is to understand the mechanistic relationship between surface site reactivity, explored by molecular level calculations, and macroscopic surface kinetics, observed in the laboratory. We present a new kinetic Monte Carlo model of silicate dissolution based on the most important findings from *ab initio*, DFT calculations and MD simulations. We discuss key problems related to model parameterization, optimization, and verification of results from experimental data. These model systems have scales on the order of microns, and are thus direcly comparable to AFM and VSI data.

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[2] Meakin P. and Rosso K. (2008), J. Phys. Chem., 129, 204106.