Mechanisms of quartz dissolution at the micro-scale: an insight from Kinetic Monte Carlo simulations

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Quartz is one of the most important rock-forming minerals in the Earth's crust and terrestrial sediments. Dissolution of quartz-bearing rocks drives many geological processes from hydrothermal ore deposition to soil formation. Quartz dissolution is a very slow process and experimental laboratory studies at low T conditions are difficult or even impossible. Modeling techniques can help to overcome this limitation. However, the correct application of modeling results to "real-world" systems is often problematic. Since most modern studies of silicate-water interface operate at the molecular level direct upscaling of these data is problematic due to the complexity of the crystal surface and a large number of rate-controlling parameters. Thus, our goal is to understand the effects of molecular reactions on dissolution patterns observed in experiments. In our previous study we developed a KMC model for silicate dissolution that was parameterized by using ab initio data [1]. Then, we applied the calculations to predict the surface structure of a dissolving quartz crystal at the nm to micron scale (Fig. 1), where the dissolution process can be observed as a result of the interaction between reactive surface features, such as kinks, steps and etch pits. Here, we will discuss our KMC simulation results in terms of the kinematic stepwave model [2]. We will show that the use of our approach can explain important controls of the quartz dissolution realted to spatio-temporal changes of surface reactivity distribution.

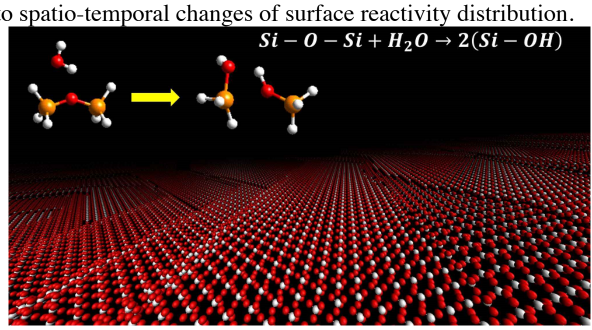

Fig. 1. The quartz dissolution process: hydrolysis of individual bonds leads to the formation of stepwaves and etch pits.

[1] I. Kurganskaya and A. Luttge (2013) *J.Phys.Chem.C* **117**, 24894-24906 ; [2] A.C. Lasaga and A. Luttge (2001), *Science* **291** (5512), 2400-2404.