Integration of solvent parameters in kMC dissolution modeling

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One of the main challenges in the modeling of dissolution processes is the matching of time and length scales in computational and experimental studies. Due to limited computational resources, important properties on a molecular level have to be omitted in modern kinetic Monte Carlo (kMC) approaches that are able to predict both overall dissolution rates and structural features of dissolving crystalline surfaces by using a proper parametrization [1].

Figure 1:
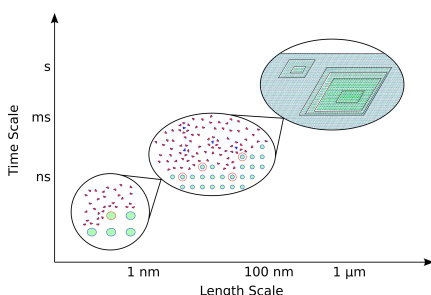
Dissolution modeling as a multiscale challenge.

In this contribution we focus on the way how to parametrize modern kMC dissolution studies by proposing fitting functions that are integrated into the dissolution event rates. These functions are based on insights from molecular scale and allow to introduce solvent based properties like the pH to fast kMC models that do not simulate the solvent itself. Since the approach pays respect to different surface site geometries, it is able to indicate the impact of solvent properties on both the overall dissolution rate as well as the etch pit forming mechanisms.

Eventually, a well proven parametrization scheme for mesoscale dissolution modeling may possibly help to simulate the dissolution of materials in conditions and settings that are difficult to manage in the laboratory.

[1] Kurganskaya & Luttge (2013), *J. Phys. Chem. C* **117**, 24894 – 24906.