Is it possible to compute a reliable macroscopic dissolution rate from molecular measurements?

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The macroscopic dissolution rate of minerals is generally deduced from solution chemistry experiments, where the rate is derived from the increase of the concentration in a liquid where the material dissolves. Thanks to atomic force microscopy, a microscopic dissolution rate can also be inferred from the dynamics of molecular events, among which the atomic step migration are the dominant ones. Unfortunately, both hardly ever agree, even qualitatively. In the worst cases, orders of magnitude separate the two. Besides a general theory linking the kinetics at the two scales is still lacking.

We present here AFM microscopic dissolution rates of gypsum in quantitative agreement with macroscopic rates. This unusual agreement has been obtained in taking care of two features.

First, the force applied by the AFM tip on the surface has been seen to increase the solubility of the mineral, thereby introducing a bias, so we have always worked with a constant and low applied force. Secondly we have clearly identified the driving molecular mechanism, namely the migrations of rough steps, which have often been neglected in former studies. This result shows that the analysis of the topographic changes during the dissolution of a mineral may permit to deduce a reliable macroscopic dissolution rate (fig. 1).

Preliminary use of this methodology for the measurement of the dissolution and precipitation rates of calcite, and the investigation of the influence of organic ligands on these phenomena will also be presented.

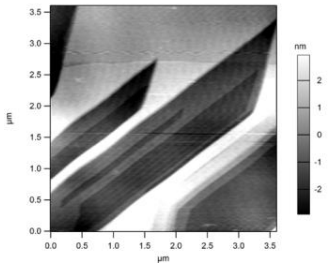

FIG. 1: AFM images of the dissolving cleavage surface of a gypsum single crystal.