Application of wetting concepts to confined crystal growth and dissolution

Luca Gagliardi[a] and Olivier Pierre-Louis[b]

CNRS, ILM Institut Lumière Matière, Université Claude Bernard Lyon 1 Campus LyonTech-La Doua Batiment Brillouin, 10 rue Ada Byron F-69622 Villeurbanne, France

a. luca.gagliardi@univ-lyon1.fr b. olivier.pierre-louis@univ-lyon1.fr

Crystal growth or dissolution in confinement is characterized by a thin liquid solution film separating the crystal surface from the confining substrate allowing transport of solid units.

We describe the non-equilibrium dynamics within the contact region using a continuum thin film equation. Our model contains many instances typical of nanoscale wetting such as surface tension, hydrodynamics, capillary forces and disjoining pressure (crystal interface-substrate interaction). In addition physical ingredients specific to crystal growth such as attachment-detachment kinetics, bulk diffusion and the presence of an external load are considered to obtain self-consistently in the lubrication limit an evolution equation for the crystal interface.

Based on this model, we study dissolution under a macroscopic load and growth under an applied supersaturation [1]. During dissolution the functional form of the disjoining pressure appears to strongly influence the dynamics. A divergent repulsion leads to a flat contact and to a dissolution rate which increases indefinitely with the applied load. In contrast, a finite repulsion such as that induced by electrostatic interactions, implies a sharp pointy contact shape, and a dissolution rate independent from the applied load. In confined growth we show the generic formation of a single cavity in the contact region, which ultimately leads to the formation of a rim [2]. The results are supported by experiments on $NaClO_3$. This transition appears to be supercritical or subcritical, depending on the functional form of the disjoining pressure and can be hindered by viscosity effects [3]. Finally the model allows to address the problem of the stress generated by a crystal growing in a pore under the effect of a supersaturated environment (crystallization force). We show that we are able to extend our understanding beyond the well known equilibrium thermodynamic description.

[1] L. Gagliardi and Olivier Pierre-Louis. Thin film modeling of crystal dissolution and growth in confinement. *Physical Review E*, 97(1):012802, jan 2018

[2] Felix Kohler, Luca Gagliardi, Olivier Pierre-Louis, and Dag Kristian Dysthe. Cavity formation in confined growing crystals. *Submitted, arXiv:1802.00310*, feb 2018.

[3] L. Gagliardi and Olivier Pierre-Louis. Crystal growth in nano-confinement: Subcritical cavity formation and viscosity effects. *Submitted, arXiv:1803.06269*, mar 2018

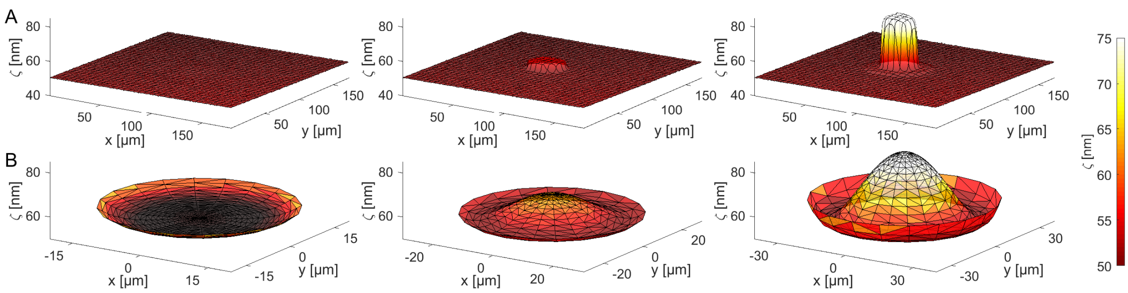

Figure 1: Cavity formation on the confined surface of a $NaClO_3$ crystal. **A**. Experimental data. **B**. Simulation results in an axysimmetric contact.