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Study of Crystallization Pressure by Molecular Simulation

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The in-pore crystallization of salts is considered one of the major sources of degradation of construction materials, geomaterials, and built heritage. When crystallizing, salts may exert mechanical pressure against the surface of the pore, which can damage materials. Crystallization within the porous network remains one of the most misunderstood phenomena in porous media mechanics. We propose an investigation combining molecular simulations and theoretical development to quantify and clarify the origin of the crystallization pressure at the finest scale.

At thermodynamic equilibrium, crystallization pressure results from the change in the solubility of a crystal as it is compressed. Direct molecular dynamics simulations to compute the solubility of salts are challenging because the time scale of dissolution and precipitation, microseconds or more, is at the limit or beyond computing capabilities. For this reason, we use a thermodynamic integration approach to overcome this issue. With this approach, we can quantify the effect of stress on NaCl solubility, and more specifically the effect of stress anisotropy which has been disregarded so far. We use these results to revisit the existing theory describing crystallization pressure and extend it to account for stress anisotropy. After investigating the case of bulk crystallization, we focus on the effect of confinement by looking at the thermodynamics of a salt solution confined in a nanometric thin film at the interface between two crystals. We conduct molecular simulations to determine how the thickness of the film decreases with the normal pressure exerted by the surrounding crystals. Doing so, we identify the critical pressure threshold at which this wetting film, responsible for the crystal growth, will disappear, providing an upper bound to the crystallization pressure phenomenon.

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