Application of molecular dynamics simulations to the study of the growth of minerals from solution.

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The nucleation and growth of crystals from supersaturated solution is one of the fundamental processes in chemistry. In many cases, the morphology and chemico-physical properties of a mineral can be determined by the growth conditions such as solvent, supersaturation, temperature, pressure and impurities. Unfortunately, the growth process occurs on a very thin layer at the crystal-solution interface and is rather difficult to characterize its atomistic details with the standard spectroscopic techniques.

A giant leap forward has been made two decades ago with the introduction of atomic force microscopy (AFM) that allows the real-time study of the growth process on the nanometer scale. A natural complement to this technique is molecular modeling that can be used for the interpretation of the AFM images in term of surface structure and energetic. The molecular dynamics approach is of particular interest in this respect as it allows to take fully into account the influence of entropy and solvation on the growth kinetics. In this presentation, the latest applications of molecular dynamics simulations to the study of minerals growing from solution will be reviewed and some examples will be discussed in detail to illustrate the advantages and disadvantages of this method.