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How can computer models help us understand mineral forming processes?

Luca Valentini
Department of Geosciences, University of Padua, Padua, Italy (luca.valentini@unipd.it)

The birth (and death) of minerals is controlled by a series of basic physical and chemical processes such as nucleation, growth, dissolution, diffusion and adsorption, which normally occur over time and length scales that are not easily accessible to common experimental investigation methods. However, reconciling these microscopic processes with macroscopic observations may represent a key to the interpretation of the geological archive as well as to optimizing the engineering of geomaterials based on the exploitation of mineral resources.
Motivated by this need, an overview of commonly used numerical techniques for the simulation of mineral forming processes, and their relevant input parameter, is provided, with the aim of assessing the potential and limitations of specific computational tools in different scenarios.
The scope and suitability of methods such as Molecular Dynamics, Kinetic Modelling, Cellular Automata, Monte Carlo and Population Balance are illustrated, with a brief introduction of the theoretical principles, followed by examples of applications to specific case studies.
Challenges and future perspective, with emphasis on multiscale modelling, are discussed.