Project 5

Dislocation scale modelling in Halite and Olivine

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Aims & objectives

Multiscale modelling and computation is becoming one of the most active research areas in materials science. This evolution is driven by the rapid growth in available computing power and by the development of many innovative algorithms and techniques. In mineral physics, the issue of mantle and crust rheology, controlled by the deformation of mineral assemblages, can be addressed by this new approach. In contrast to thermodynamic properties like the equation of state, which are fully determined at the atomic length scale, mechanical properties are inherently multiscale; they depend on the interrelationship between processes operating at the scale of the atom, the crystal, the rock and the whole planet. Moreover, these different scales are often strongly coupled to each other, which makes the problem even more challenging.

Mechanical properties of real materials are controlled by crystal defects such as point defects, dislocations, stacking faults and grain boundaries. Taken individually, these defects can be described at the fundamental level through their atomic and electronic structures, which can be found by solving the Schrödinger equation. First-principles calculations and molecular dynamics are used to address such problems. At the scale of a grain, the mechanical properties are often the result of the collective behaviour of these defects in response to the loading conditions. Newly developed three-dimensional dislocation dynamics simulation techniques are aimed to take these interactions between defects into account to provide insights about single-crystal plasticity.

The aim of this IP is to use dislocation-scale modelling on two materials of interest for the CRP: halite and olivine in order to provide physical constraints to modelling the spatial distribution of dislocations within grains and their evolution to produce subgrain structure (IP1), and to experimentalists observing dislocations in their deformed samples (AP1 & AP2). The deformation and stress fields observed in the numerical (IP4 & IP6) and physical (IP2 & IP3) grain scale experiments will in turn provide the boundary conditions for our modelling.