project 3

The role of grain boundaries in substructure development

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Aims & objectives

The microstructural development of a mineral or metal aggregate, the subject of this CRP, is the result of a complex interplay of substructure-building elements (e.g. dislocations, tilt walls, grain boundaries) and the processes that act on or with them (e.g. dislocation glide, grain boundary migration). Subgrain boundaries and grain boundaries play a crucial role in microstructural development, and therefore the physical and chemical properties of a crystalline material:

- They form the boundaries between crystallographically and mineralogicaly relatively homogeneous volumes (the grains and subgrains).
- They are chemically distinct from the (sub) grains they separate, possibly containing fluids and carrying incompatible components.
- They are physically distinct and may provide weak planes for grain boundary sliding as well as preferred pathways for diffusion of fluids and (trace) elements, or even advective flow of fluids.
- By their migration through a grain aggregate they play a crucial role in the mechanical recovery of the material, by destroying piled-up dislocations and other lattice defects, destroying or interacting with other boundaries and by redistributing second phases (e.g. particle drag).
- Because of the important role of grain boundaries, this IP will be fully dedicated to the experimental analysis of the properties and behaviour of grain boundaries. The IP will address three questions:

How does grain boundary behaviour affect the smaller-scale substructure?

Substructure development is a two-way multi-scale process: large-scale-down and small-scale-up. At the smallest scale, substructure development is driven by processes like vacancy diffusion, creation, movement and annihilation of dislocations (IP 5) and the nucleation of new (sub)grains (IP 1 & 2). Grain boundaries influence these processes as nucleation and annihilation sites. The objective of this IP is to determine indicative structures for the interaction of grain boundaries with smaller-scale substructures and to quantify the interaction between the two, as a function of boundary conditions.

How can grain boundary behaviour be quantified to develop algorithms for the numerical modelling of microstructural development?

To successfully model substructure development (IP 4 & 6) it is necessary to understand the properties and behaviour of grain boundaries, and to be able to describe these in terms of algorithms. For example, the velocity magnitude and direction of a migrating grain boundary must be described in terms of the grain boundary morphology (e.g. curvature), its chemical and physical properties (fluid content, trace element content, width, etc.), the properties of the phases on either side (mineral type, lattice orientation), the state of these phases (e.g. dislocation density) and the boundary conditions or extrinsic variables (stress state, pressure, temperature). The objective is to develop (in collaboration with IP 4 & 6) evolution equations for the front-tracking and material transfer modules within the model Elle that describe the migration of grain boundaries and physico-chemical interaction with the solid phases.

How does grain boundary behaviour affect the mechanical and rheological properties of a crystalline aggregate?

The role of grain boundary properties and behaviour in the mechanical properties of materials remains poorly understood and is therefore often oversimplified. For example (e.g. Regenauer-Lieb & Yuen, 2003), the role of recrystallisation on the rheology of rocks is often described by a grain-size (g) term in the flow law (de/dt=f(s,g)). The important effect of water on the rheology is then described by a separate equation (de/dt=f(s,XH2O)). This ignores the fact that the presence of water directly influences the mobility of grain boundaries and therefore the grain size term: g=f(de/dt,s,XH2O,etc.). This effect may be greater than the effect of water on dislocation activity. The objective is to quantify the dynamics of grain boundaries and their effect on rheology and mechanical properties, through their modification of the substructure of a crystalline material. Particular attention will be given to the presence of fluids on grain boundaries (see Urai and Jessell, 2001), as this is of crucial importance to the behaviour of crust and mantle.

To achieve the above objectives, this IP will carry out a detailed experimental study of the behaviour and properties of grain boundaries, focussing on the mineral halite and other salts.