Post-deformational annealing in crystalline materials
First results of t-T modelling

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Aim of the Study

- Characterize annealing microstructures and learn how to "see through" them.
- Quantify grain boundary energies and mobilities for different grain boundaries on the developing microstructure.

Methods

Field work

Natural samples were collected from the Ballachulish igneous complex in Scotland (Fig.1). The thermal and temporal history of the intrusion and subsequent cooling has been well established (e.g. Holness & Watt, 2001). Here, the temperature effect on a largely undeformed sequence can be studied (see t-T modelling). Samples of quartzite were taken at increasing distance from the contact to get temperature gradient profiles (black lines in Fig.1).

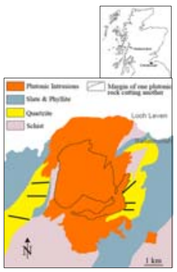


Fig 1. Simplified geologic map of the Ballachulish igneous complex (Scotland).

CL analysis

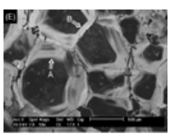


Fig 2. CL image of quartzite.
(Holness, et al., 2001)

Cathodoluminescence analyses provide insight on the grain growth and, in this case, on the t-T history. Each bright band, seen in CL, is interpreted to represent a growth stage. The relative grain boundary energies and mobilities in the sample is given. These analyses will serve as references to the numerical modelling (see below).

EBSD

Electron backscatter diffraction (EBSD) will be used to get a detailed analysis of the boundaries. A complete description of crystallographic orientation and spatial distribution of grains and subgrains will be given. The analyses will be coupled with the numerical modelling system ELLE.

Numerical modelling

Numerical modelling will be preformed using the software ELLE (Jessell, 2001). The crystallographic data obtained with the EBSD is copied into ELLE.
The program will run with different boundary energies allocated. Results will be compared with CL analyses of the samples from the profiles (black lines in fig. 1).

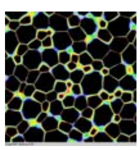
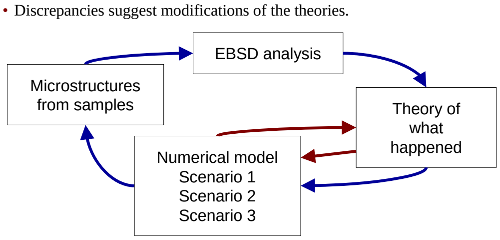


Fig 3. Result from simulation in ELLE of grain boundary sweping. (Jessell, 2001)

Sequence of work

- Microstructures from natural samples are analysed with CL and EBSD.
- These analyses give the relative grain boundary energies which provide starting point for numerical simulations.
- Results from numerical simulationsare compared with microstructures from natural samples.
- Discrepancies suggest modifications of the theories.



References:

Buntebarth, G. (1991) *Thermal models of cooling*. In: *Equilibrium and Kinetics in Contact Metamorphism: The Ballachulish Igneous Complex and its Aureole*. Edited by Voll, G., Topel, J., Pattison, D.R.M and Seifert, F. British Geological Survey.

Holness, M.B., Watt, G.R. (2001) *Quartz recrystallization and fluid flow during contact metamorphism: a cathodoluminescence study.* Geofluids, **1**, 215-228.

Jessell, M.W., Bons, P.D., Evans,L., Barr, T.D. & Stüwe, K. (2001) *Elle: the numerical siulation of metamorphic and deformation microstructures.* Computer Geosci. **27**,17-30.

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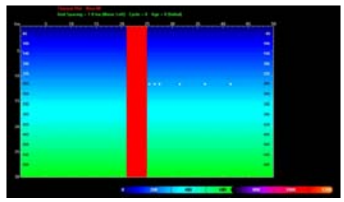
t-T modelling

The time-temperature paths for each sample in a profile from the Ballachulish igneous complex (see Fig. 1), was modelled using the software KWare Heat 3D (www).

In the modelling mesh, the magma intrusion was set as a cylinder of 4 km diameter and infinite length. For simplicity, all wall-rock was given the properties of quartzite. Watch points were set at 1, 2, 3, 7, 12 and 16 km from the contact and at 12 km depth. Grid size is 1 km.

Starting values according to table 1.



Known conditions of the intrusion.

The igneous complex can be approximated as a cylinder of 4 km diameter and infinite length. The pre-intrusion temperature of the metasediments was approximately 250 °C. (Buntebarth, 1991).

Table 1.

Starting values	Rock	Magma 1	Magma 2
k [W m^{-1} K^{-1}]	3.50 (1)	2.66 (1)	3.42 (1)
Cp [J kg^{-1} K^{-1}]	800 (1)	814 (1)	795 (1)
Bulk density [kg m^{-3}]	2700 (1)		
Temperature [°C]		1050 (2)	950 (2)

(1) Physical Properties of Rocks and Minerals, Vol II-2
(2) Buntebarth, 1991

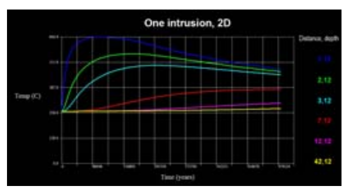
Aim

- To get t-T paths for samples collected, by developing several possible t-T paths to be compared with observed microstructures.

Problem

- 1 or 2 intrusion events
- Conditions

1 intrusion

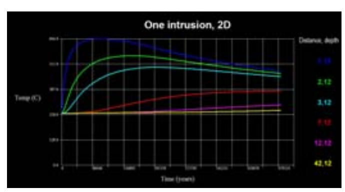


2 intrusions

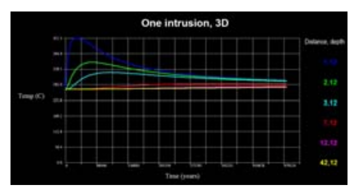
In the model with 2 intrusions the second intrusion occurred just before the central portion of the first magma solidified (Buntebarth, 1991), at about 127 000 years after the first intrusion event.

The effect of adding another intrusion event is most noticeable at greater distances from the contact. At 1 km the maximum temperature (T_{max}) is the same whereas the rest of the watch points T_{max} is increased. Furthermore, T_{max} is reached at a later stage (as would be expected since the volume of magma is increased in the second intrusion).

1 intrusion in 2D

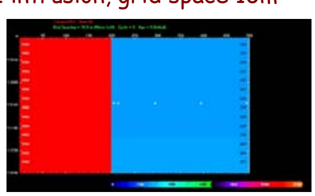


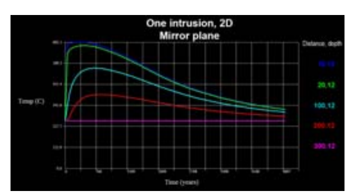
1 intrusion in 3D



Results from modelling 1 intrusion event in 2D and in 3D shows that T_{max} are reached much faster in 3D. In 3D the heat has a larger area to spread. Another difference is that T_{max} is much lower in 3D (452.3 °C vs 644.9 °C).

1 intrusion, grid space 10m





The same conditions as previous models but with 10 m grid spacing. The mesh is mirrored to the left. Watch points are at 10, 20, 100, 200 and 300 m distance from the contact.
In this model, a point at 100 m distance from the contact has T_{max} = 540 °C. This can be compared with T_{mas} = 644.9 °C in the mesh grid of 1 km.