

2. State of the art, preliminary work / Stand der Forschung, eigene Vorarbeiten

Introduction:

In this project, we will simulate microstructural evolution during deformation in rocks, in order to better understand the link between deformation processes and the resulting microstructures. Our aim is to improve the use of microstructures in tectonites as tools to determine:

- a) the conditions at which the tectonites formed and deformed (e.g. temperature, sense of shear, strain rate, stress, steady state);
- b) the processes responsible for the formation of the microstructures (e.g. dislocation creep, pressure solution, etc.).

Optimal use of microstructures as such tools is only achieved when we know how and how much specific processes and combinations of processes affect and interact with the geometry of developing microstructures, the rheology of the deforming rock and the development of rheological instabilities. Only then can we determine and quantify which microstructures are indicative for certain processes and coupling between processes, and the conditions at which these operated.

To achieve these goals, we will use and further develop "ELLE", which is a numerical modelling environment designed to simulate microstructural evolution by multiple, competing and interacting deformation and metamorphic processes. The numerical simulations will be compared with, and complemented by *in-situ* experiments with organic rock analogues and by observations on natural tectonites. Out of the vast range of deformation microstructures and processes, we will focus on medium to high temperature ductile deformation, particularly in high strain zones.

With this project we intend to strengthen the position of the Mainz Tectonophysics Laboratory as a key member of the international ELLE group (collaborators in Australia, Austria, Germany, Norway, Korea, U.S.A and U.K.) and as a prominent research centre for microstructural studies, which will enhance our chances for future European Community funding.

2.1 State of the art / Stand der Forschung

Microstructures, as visible in thin sections, are an important tool for geologists. For the study of deformation of rocks, microstructures are widely used to unravel deformation phases, deformation conditions and mechanisms and to some extent to estimate the intensity or amount of deformation or finite strain (e.g. Zwart 1963, Groshong 1988, Knipe 1989, Hirth & Tullis 1992, Passchier & Trouw 1996). To properly interpret microstructures, it is vital to know *how* they form, but despite over a century of microstructural studies, both in naturally deformed rocks and experiments, our knowledge of microstructural development is still largely qualitative and empirical. Three main problems are:

- Firstly, the number of potentially useful microstructures is very large and each forms by different mechanisms and conditions. So far, only a limited number of these structures has been

investigated in detail. Although many microstructures have been studied in detail (see overview in Passchier & Trouw 1996), others remain under-utilised. For example, Heilbronner (2001) showed that the misorientation distribution contains information of the deformation regime. The misorientation distribution describes the variations in crystallographic orientation between (sub-) grains.

- Secondly, geological microstructures develop over long time scales and at high pressure and temperature. This precludes direct observation of their formation in experiments or in nature. Rocks can be deformed experimentally, but at exaggerated strain rates and therefore often at adjusted (unrealistic) pressure, temperature and differential stresses. Scaling to geological rates and conditions can be problematic, and since samples are deformed in thick pressure vessels, observation of microstructures is restricted to the beginning and end state of an experiment (e.g. Schmid et al. 1987, Hirth & Tullis 1992). In-situ experiments with organic and salt analogue materials have provided invaluable insight in microstructural development as deforming samples can be observed under a microscope throughout an experiment (Urai 1987, Means 1989, Herwegh & Handy 1998, Bons & Jessell 1999). However, a problem remains to "translate" the observations of deforming analogue materials to real rock forming minerals, since their rheology can differ significantly from real rocks. In summary, direct observations of the formation of deformation microstructures in rocks are lacking.
- Thirdly, the complexity of simultaneously operating processes that act on a microstructure has so far proven to be inhibitive for analytical or numerical modelling of full microstructural development. The fundamentals of many operating processes are well known (e.g. Frost & Ashby 1982, Poirier 1985, Schmid et al. 1999) and numerous single-process numerical models have been published. Such numerical models can be divided into several different types of models, such as, for instance, finite element codes to model viscous deformation (Barr & Houseman 1996), finite difference codes to model lattice rotation (Zhang & Wilson 1997) and node network codes to model grain boundary migration (Bons & Urai 1992, Bons et al. 2001) and fibre growth (Bons 2001, Koehn et al. 2000; 2001). However, these models usually neglect the influence of other concurrent or interacting processes, which is obviously a problem in complex systems such as rocks. For example, numerical models exist to model crystallographic preferred orientations by lattice rotation in isolation (e.g. Lister et al. 1978, Zhang & Wilson 1997), but Jessell & Lister (1990) showed that adding grain boundary migration to the model can strongly alter the resulting crystallographic preferred orientation.

Summarising, there is a wealth of knowledge on individual processes that may operate in rocks during ductile deformation, but there remains a need to determine and quantify how each one of these processes and combinations of several coupled processes affect the microstructure and can therefore be recognised from a microstructure.

The possibilities for quantified microstructural analysis have been expanded significantly over the past decade, especially with the advent of computerised image analysis (see review Bons & Jessell 1996). The "Automated Achsenverteilungs Analyse" or AAVA is a particularly promising technique that is simultaneously developed by several workers (Heilbronner & Pauli 1993, Stöckhert & Duyster 1999, Fueten 1997, Fueten & Goodchild 2001). All versions of this technique involve the acquisition of a series of digital images of a thin section, taken at various angles between polariser(s) and thin section. The series of images is then converted to digital maps of *c*-axes orientations (for appropriate minerals), mineral type, grain boundaries, etc.. Only with such digitised versions of the microstructure is it possible to systematically, accurately and quickly measure a variety of microstructural parameters, such as size, shape and orientation of each individual grain, grain boundary morphology, and general statistical parameters, such as mean grain size, grain size

distribution, etc.. This technique is likely to soon become standard in microstructural analysis. A complete "package" can be purchased from Fueten (Appendix 9.2).

Once we have a better understanding of how processes affect microstructural development, it will be possible to:

- 1) delineate which specific microstructural indicators can be used to assess the activity of specific processes and their interaction;
- 2) quantify the effect of these processes, the conditions at which they operated (P, T, σ , strain rate) and their magnitude (finite strain, duration);
- 3) determine the interaction between rheology and microstructure under different PT-fluid conditions;
- 4) and finally recognise whether a microstructure reflects steady state or is in a state of transition.

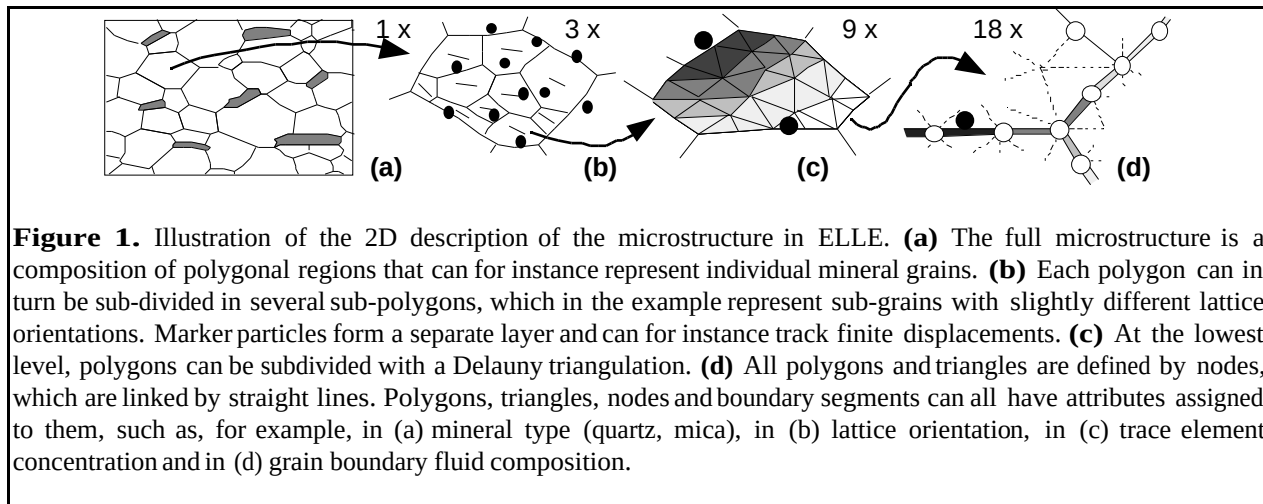
Clearly, this would greatly improve the usefulness of microstructures for geological tectonic and metamorphic studies. Better understanding of the rheological behaviour will also benefit large scale geophysical modelling of e. g. mountain building and deformation in crust and mantle.

2.2 Preliminary work / Eigene Vorarbeiten

The applicants Bons and Passchier have devoted much of their research efforts over the past years to the topics described in the previous section, resulting in several dozens of peer-reviewed publications (see Appendix 9.4), a widely used text book (Passchier & Trouw 1996) and a web-based course (Jessell & Bons 2000) on deformation microstructures. The current proposal is based on a decade of microstructural investigations in which numerical modelling played a central role, but of course linked with field studies and analogue experiments. Main themes in this work, all involving numerical models, were properties of polyphase materials (Bons & Cox 1994, Tóth et al 1994), grain growth (Bons & Urai 1992, Bons et al. 2001), vein and fringe growth (Bons 2001, Hilgers et al. 2001, Koehn et al. 2000; 2001), formation of crystallographic and grain shape fabrics (Passchier 1987; 1990, Bons & den Brok 2000), boudinage and delta-clasts (Passchier et al. 1993, Bons et al. 1997). Bons was one of the initiators of the ELLE project (Jessell et al. 2001) and has introduced the program into the Tectonophysics group in Mainz, where it was used for the DFG-funded and DAAD supported PhD-research of Sandra Piazzolo (GRK 392/1, D/98/27425). The latter project in particular forms a solid base for the successful execution of the proposed project.

Both Bons and Passchier have extensively combined field studies and numerical modelling with laboratory experiments with rock analogues (Passchier & Sokoutis 1993, Bons & Urai 1994; 1996, Bons & Jessell 1997; 1999, den Brok et al. 1998a&b; 1999). Image analysis has by now become a standard tool in microstructural studies and features prominently in this proposal. The applicants have been active in this field by developing programs for automated optical strain analysis of in-situ deformation experiments (Bons et al. 1993, Bons & Jessell 1995). based on this experience, Bons was invited for a review on image analysis in (micro-) structural analysis of deformation structures (Bons & Jessell 1996).

The proposed project, the questions to be addressed and the methods to use, follow from the work described above, especially the DFG-funded PhD-project by Piazzolo. The outlined experience and publication record of the applicants are a guarantee for a the feasibility and a successful completion of the project, as well as the rapid dissemination of the results in international journals.



The program ELLE

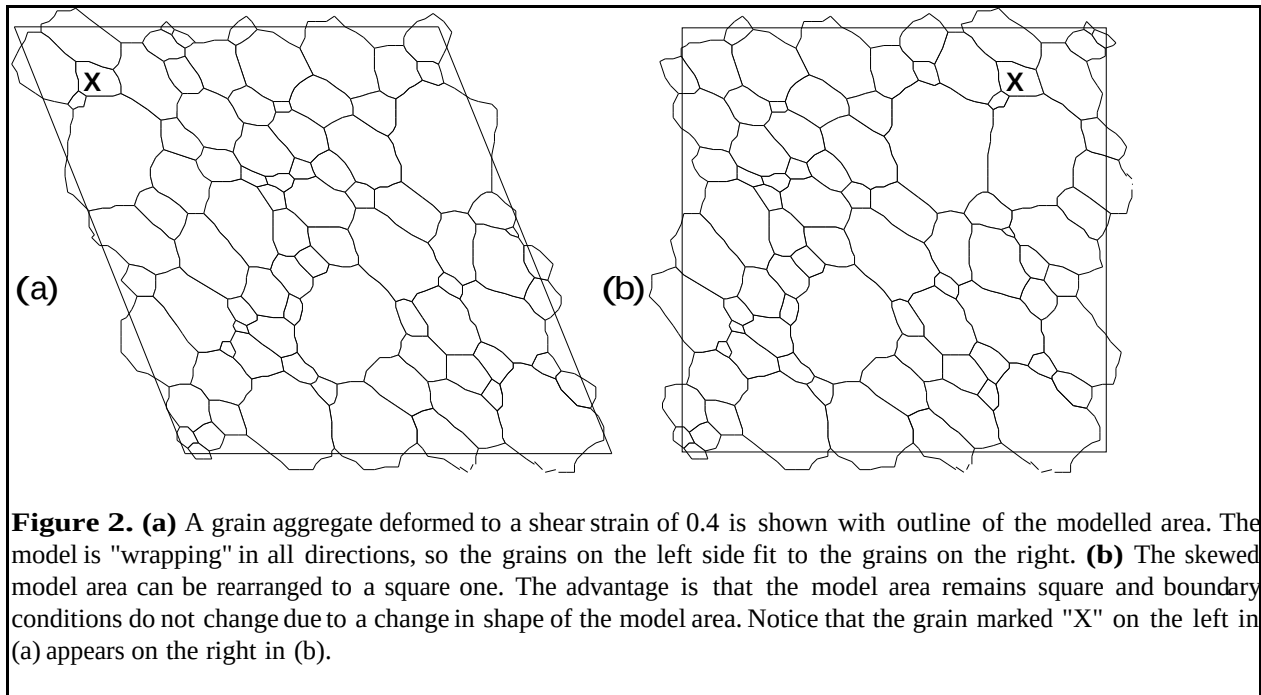
The growing speed and capacity of computers has rapidly increased the ease and power of numerical modelling. Recently, a new approach was taken with the development of the numerical model ELLE (Evans 2000) by Mark Jessell, Terence Barr, Paul Bons and Kurt Stüwe, originally all at Monash University (Melbourne, Australia). As one of the applicants (Bons) was from the start involved in the making of ELLE and, more recently, Bons and Piazzolo have further developed ELLE in the Tectonophysics Laboratory in Mainz, we present the description of the model here under "Eigene Vorarbeiten", although it should be clear that this work was in collaboration with colleagues outside the Mainz Tectonophysics group.

ELLE was developed in order to provide a modelling environment that can simulate the effects of multiple simultaneously operating metamorphic and deformation processes on microstructural development (Jessell et al. 2001, Evans 2000, Evans et al. 2000, Bons et al. 2001, Piazzolo et al. *in review*). This is achieved by:

- 1) A flexible finite-element based description (in 2D) of the microstructure, where triangular and polygonal regions and their boundaries can be assigned a range of properties, such as mineral type, lattice orientation, trace element concentration, etc. for regions, and fluid content, grain boundary width, surface energy, etc. for boundaries (Fig. 1). A separate layer of "particles" or material points is used to track finite strain and is used for the modelling of trace-element diffusion.
- 2) A modular program architecture, where each process is programmed as a separate module. This greatly simplifies the programming and allows the various collaborators to contribute modules that are added to the ever expanding library.
- 3) A central "shell" or "mother" program that repeatedly passes the microstructure (a data file) to successive process modules that operate on the microstructure. Each module performs a calculation or modifies the microstructure by a small amount only, simulating the operation of a process during a small time increment.
- 4) The data are contained in a file (a "snap shot" of the evolving microstructure) that is continuously modified slightly by the process modules. Visualisation and analysis modules use stored series of these files for interpretation and visualisation in the form of images or movies.

Two additional features of the program ELLE, which are particularly relevant to this project, are:

- a) The simulated area is a unit-cell with repetitive ("wrapping") boundaries (Fig. 2). With this feature, it is possible to simulate simple shear deformation to arbitrarily high finite strain, as the model area does not change in outer shape and hence, boundary conditions remain constant.
- b) Stresses needed to deform the "sample" are calculated and recorded using a finite-element module (Barr & Houseman 1996). It is thus possible to track the changing stresses as a microstructure evolves. A run with ELLE can thus be regarded as a creep experiment and the physical rheological effects of microstructural development can be studied as well as the microstructure itself.



Currently, a comprehensive set of process modules is already available for the modelling of solid state ductile deformation by crystal plastic deformation processes (Evans et al. 2000, Piazzolo et al. *in review*). The library of modules for ELLE is not yet complete, but rapidly expanding. The main available modules are:

1. BASIL for finite element stress - velocity field/strain rate calculations in cohesive heterogeneous linear or power-law viscous materials (Barr & Houseman 1996).
2. OOF, an object-oriented finite difference module for stress-elastic strain calculations in heterogeneous linear elastic materials, incorporating full crystallographic elastic anisotropy.
3. TBH, a module to simulate lattice rotation according to the Taylor-Bishop-Hill theory (Lister et al. 1978, Jessell & Lister 1990).
4. A module for surface energy driven grain boundary migration, which incorporates lattice controlled anisotropy in grain boundary energy (Bons et al. 2001).
5. A module for internal energy driven grain boundary migration, with internal energies, for instance, calculated from the work factor derived from the TBH-module (Piazzolo et al. 1999).
6. Modules for lattice and grain boundary diffusion.
7. Modules for the simulation of subgrain formation or the nucleation of new grains (Piazzolo et al. 1999).

An examples of an ELLE run that employs most of these modules is shown in figure 3. The paper by Piazzolo et al. (*in review*) accompanies this application. Auxiliary data to this paper, in the form of movies can be viewed on: http://www.uni-mainz.de/FB/Geo/Geologie/tecto/elle_movies.

More information on ELLE can be found on: <http://orion.earth.monash.edu.au/Research/Elle/>.

A listing of all publications based on the ELLE and related modelling software is given in Appendix 9.3.

The program ELLE has been installed on computers (PC) in the Tectonophysics laboratory in Mainz under the supervision of Bons. We thus have gained the necessary experience with the running of the program and its operating system (LINUX) to immediately start the project. The current state of the ELLE software package is such that simulations can start immediately once the project commences and the research assistant is introduced in the operation of the program.

From the start, ELLE modelling has been compared with in-situ experiments with rock analogues in transparent deformation cells (cf Means 1989). This comparison is an important way to test and develop ELLE (Fig. 4). Bons and Passchier have used analogue experiments extensively and the Tectonophysics laboratory is well equipped for these experiments.

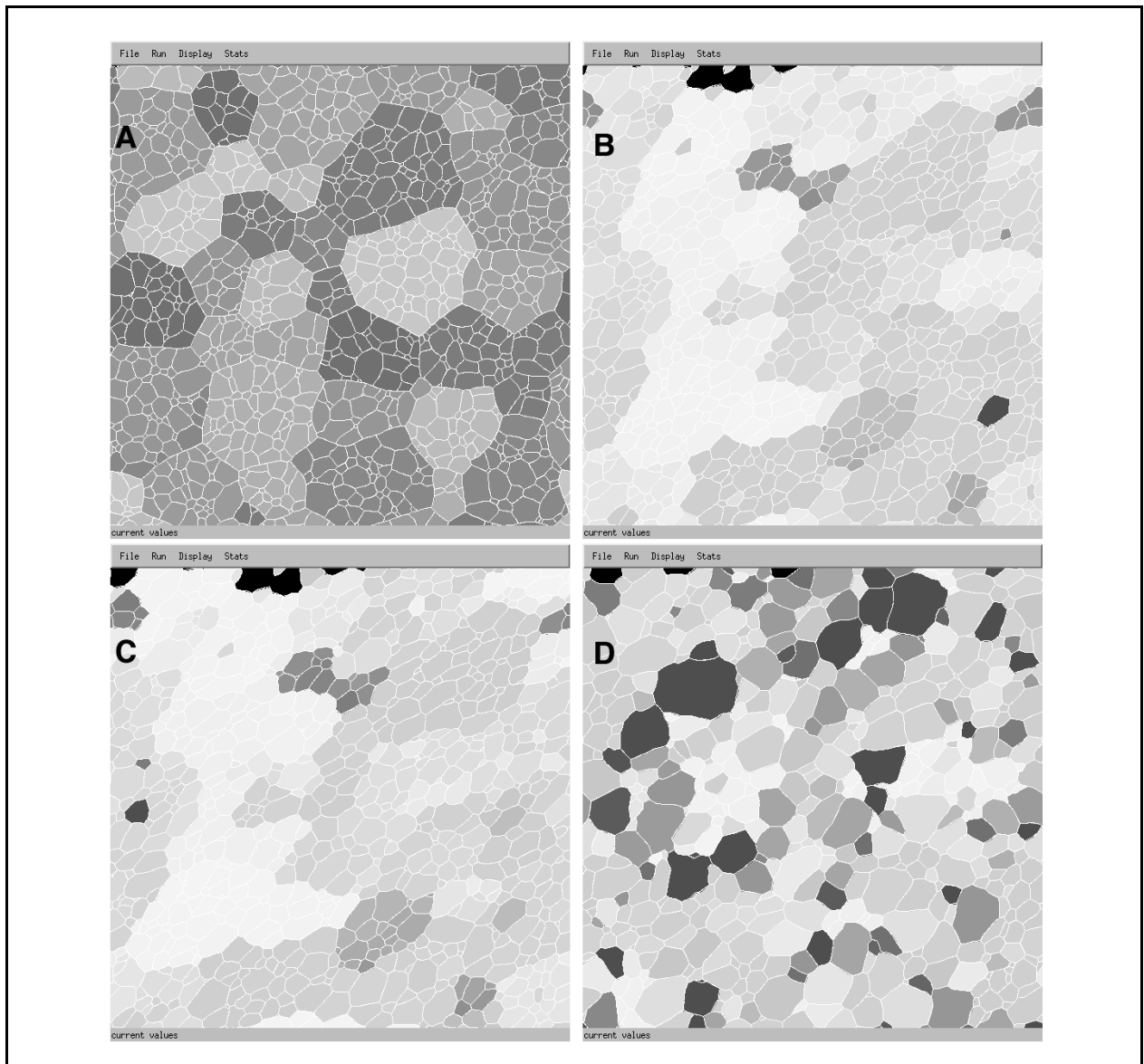


Figure 3. Example of a simulation with ELLE of a deforming monomineralic grain aggregate, in which most of the modules mentioned in the text above occurred, except elastic strain and diffusion. Grey scales reflect the internal energy (dark = low, bright = high). An initial foam texture (a) was deformed to a shear strain of 0.7 (b & c) and then left to anneal.
For quicktime movies, see: http://www.uni-mainz.de/FB/Geo/Geologie/tecto/elle_movies.

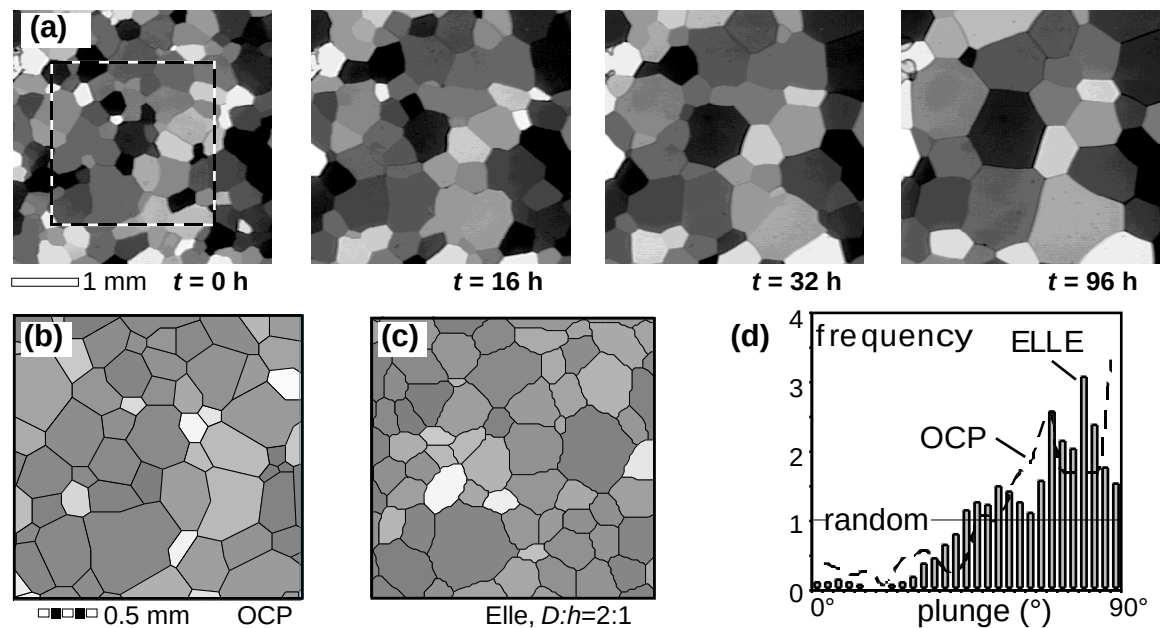


Figure 4. Example of a comparison of ELLE modelling with an in-situ analogue experiment with octachloropropane (OCP). **(a)** Four images of grain growth in a thin sheet of OCP. **(b)** Drawing of outlined area in OCP-sample, with shading reflecting plunge of the c-axis (bright = shallow). **(c)** ELLE simulation of grain growth in a material as OCP (but not exactly the same sample as (a)). Shading as in (b). Notice the similarity in texture. **(d)** Comparison of crystallographic preferred orientation in the OCP sample and the ELLE model, both giving mostly steeply plunging c-axes (from Bons et al. 2001).

3. Goals and work schedule / Ziele und Arbeitsprogramm

3.1 Goals / Ziele

General aims

In this project we will aim to determine and quantify:

1. microstructural indicators of relative contribution of acting processes (e.g. slow sub grain rotation, high grain boundary mobility);
2. microstructural indicators of metamorphic and tectonic conditions (e.g. temperature, pressure, strain rate);
3. microstructural indicators of the amount of deformation (finite strain) and related to that;
4. microstructural indicators of steady-state, or changes in conditions (e.g. fluctuating strain rate);

5. how and under which conditions instabilities form (e.g. shear bands);

The project should result in better understanding of microstructural evolution in rocks and provide the geological community with improved and more quantitative tools for microstructural interpretation.

Remarks on feasibility of method and philosophy of approach

At all times we will critically assess the validity of our numerical simulations by comparing outcomes with observations on real deformed rocks and with in-situ experiments with (organic) rock analogues under carefully controlled conditions (Fig. 4). However, numerical modelling has the highest priority and is the main technique to be used in this project with most of the time devoted to it.

Numerical modelling is a powerful tool, but should always be carefully scrutinised. It is clear that a visual similarity between a microstructure in a thin section and a numerical model does not by itself mean that the model is right or meaningful. Producing realistic microstructures is certainly our aim, but it does not stop there. Our aim is to understand *why* and *how* such microstructures form and how individual parameters play a role. A problem that is immediately encountered in this type of modelling is the paucity of published data on individual parameters, such as values of grain boundary mobility, critical resolved shear stresses, grain boundary energies, etc. for rock-forming minerals. A numerical model like ELLE is, however, also suited to deal with this problem, as one is free to choose and vary values of different parameters and investigate the outcome. This way, ELLE can actually be used to constrain the values, sometimes in absolute terms, sometimes relative to other parameters (in the form of ratios or dimensionless scaling parameters). Rephrased in practical terms: even if absolute geological values of a parameter are poorly known, one can investigate what the effect of changing this parameter would have on a microstructure. The feasibility to do this with ELLE is shown by the study of Piazzolo et al. (*in review*)

3.2 Work schedule / Arbeitsprogramm

As stated before, we will restrict ourselves to the investigation of medium- to high temperature microstructures, as most ELLE routines for this are already available or close to completion. We will start with the modelling of monomineralic aggregates, particularly quartzite. Having gained enough experience with this, we may proceed to polymineralic systems, in particular the system granite - gneiss - mylonite with quartz + feldspar $\pm$ mica. Although ELLE is also intended for the simulation of metamorphic reactions, we will not include these in the current aims.

A. Dynamic recrystallisation. Dynamic recrystallisation produces a microstructure that is determined by the balance between various driving forces that drive grain boundary migration (internal strain energy and grain boundary surface energy), lattice rotation and the formation of sub-grains that may develop into grains. Following on from the pilot study of Piazzolo et al. (*in review*), we will carry out a systematic investigation of the effect of the various parameters that play a role (Table 1) and will try to determine which particular (combinations of) microstructures are indicative for particular conditions of deformation, as expressed in the form of active deformation processes and values of the relevant parameters. The outcomes will be compared with experimental results and natural microstructures, such as the microstructural classification of Hirth & Tullis (1992) and Stipp et al. (*in press*)

1.	Processes that play a role in dynamic recrystallisation:	grain boundary migration, recovery, sub-grain formation by rotation, nucleation or bulging, recovery, strain, lattice rotation, etc.
2.	Parameters that play a role in dynamic recrystallisation:	grain boundary energy, dislocation energy, dislocation density, grain boundary mobility, dislocation creation and annihilation rate, temperature, critical resolved shear stresses, strain rate, stress, etc.
3.	Possible microstructural indicators, measurable in thin section:	grain size, grain shape, grain size distribution, grain shape preferred orientation, lattice preferred orientation, serrateness of grain boundaries, etc.

Table 1. Processes, parameters and microstructural aspects that play a role in dynamic recrystallisation

B. Instabilities and localisation. Whereas many models for microstructural development use a simplification for the stress/strain rate distribution (typical the constant strain rate or Taylor approach), ELLE can model variable stress and strain rate within a sample (using the module BASIL). We will systematically investigate the effect on localisation of deformation in a grain aggregate as a function of strain-dependent flow laws (hardening/softening) and dynamic recrystallisation.

C. Steady state and the effect of changing conditions. Stresses and strain rates are not constant over time. Yet we have very scant knowledge of how to recognise changes in deformation conditions and the rate at which microstructures equilibrate to achieve a steady state (Jessell & Lister 1991). Arbitrarily high finite strains can be achieved with ELLE, and we will utilise this to run series of simulations where stress/strain rate is stepped up/down and the evolving microstructure will be studied. Main questions to be answered here are:

- (1) how much strain/time is needed to achieve a steady state microstructure?
- (2) Is it possible to distinguish a non-steady-state from a steady-state microstructure?

D. Comparison with thin sections and in-situ analogue experiments. At all stages, we will compare the modelling results with natural microstructures as described in the literature and from our own collection and other field-based research activities. In-situ experiments with rock analogues, using the well-equipped Tectonophysics Laboratory, are important as a means to test ELLE-routines under well-controlled conditions (Fig. 4). Comparison of ELLE-results with microstructures in thin sections and experiments will be greatly improved by the automated microstructural analysis technique of F. Fueten (Fueten 1997, Fueten & Goodchild 2001, appendix 9.2). With this technique it will be possible to automatically, systematically and quantitatively measure a range of microstructural parameters that are also output by ELLE.

In practical terms, the research program will be carried out as follows:

First half 2002:

- Appointment of postdoctoral assistant ⁽¹⁾.
- Introduction of postdoc to program ELLE, including 1 month visit to main programmer, Lynn Evans, at Monash University, Melbourne Australia.
- Systematic literature search to establish data base of known values of all relevant parameters (e.g. grain boundary mobility, grain boundary surface energy).
- Checking (debugging), modification of available routines & writing of remaining necessary routines. This stage does not yet involve any significant programming in the "core" of ELLE.
- First exploratory test runs to explore "parameter space" (Table 1) and design of final simulation program for theme A (Dynamic recrystallisation).

Second half 2002:

- Execution ^(2, 3) and data processing ⁽⁴⁾ of the simulation program for theme A (Dynamic recrystallisation).
- Selection and design of routines needed for theme B (Instabilities and localisation), debugging & testing. This follows on from theme A as it needs insight into how different processes directly or indirectly lead to time/strain dependent changes in rheology (hardening and softening)
- Purchase & installation of microstructural analysis equipment and software of Fueten (theme D).

First half 2003:

- Execution of simulation program for theme B (Instabilities and localisation).
- Evaluation of results so far and consideration of the need for modifications and additions to the "core" of the ELLE program.
- Building on from results of, and experience with themes A and B, design and start execution of simulation series for theme C (Steady state and the effect of changing conditions). By this stage, routines must have been optimised to allow long experimental runs to very high finite strain.
- Comparison of modelling results with natural examples and *in-situ* deformation experiments with rock analogues ⁽⁵⁾.
- Determining whether a third year is needed for the project and if so, write extension proposal.

Second half 2003:

- Last simulations and final data processing for themes A-C and submission of manuscripts to journals (typically Computers & Geosciences, Journal of Structural Geology, Tectonophysics, or on-line journals such as Journal of the Virtual Explorer, etc.).
- Planning future work, direction and projects with the program ELLE.
- Comparison of modelling results with natural examples and *in-situ* deformation experiments with rock analogues.

2004:

The work in the third year (subject to extension application, to be submitted 2003) depends very much on the progress achieved during the first two years. It is expected that at this stage:

- The expanded library of routines can and will be applied to other minerals (in particular olivine) to address microstructural developments in rocks other than quartzite in shear zones.
- Application of ELLE to polymineralic rocks, in particular to study the transition of granite to gneiss or mylonite.
- The implementation of diffusional mass transfer (pressure solution) in ELLE is currently undertaken in collaboration with Oslo (not subject of this proposal). If successful, the effect of the competition of diffusional mass transfer with other deformation mechanisms will be investigated at this stage.

Notes on the above research plan

1) ELLE is by now a large and complicated program. Therefore, this project requires a full-time dedicated person with strong numerical skills and experience with rock mechanics. *The high level of expertise required for this project makes it vital that an assistant of postdoctoral level is available for the project.*

2) Designing, writing and testing modules and simulations is the most time consuming step in this work, as well as processing the results. Actual running of simulations takes time (up to a week per simulation), but takes place in the background and does not use much time of the researcher. Once a set of runs is designed, tested and running, other work can be done.

3) Programming and testing of simulations can be done on a desktop PC, running under LINUX. Actual runs are done on faster UNIX machines. For this we have access to computers at the ZDV of Mainz University and we have an ongoing agreement for use of computers at Monash University (Melbourne, Australia), which can be accessed from Mainz.

4) Output of the program ELLE mainly comes in the form of microstructural maps that show grain shapes, but also maps of stress, strain, strain rate, dislocation density, lattice orientation and a variety of other parameters. Extensive, but often simple data processing is needed, which can in part be carried out by a undergraduate-level research assistant (HiWi).

5) It is foreseen that *in-situ* experiments with rock analogue are carried out for comparison with ELLE simulations. The Tectonophysics laboratory has all the equipment and expertise needed for this. Such experiments are ideally suited for "Diplom"-projects and it we will try to attract students to carry out this part of the work, in close connection with the proposed project. Prof Spiers (Utrecht University, The Netherlands) has expressed interest in sending Utrecht students to Mainz to do (part of) their MSc-research projects in this area.

Travel, conference and workshop visits

We intend to present results at the following international conferences:

- Gordon Conference on Rock Deformation, Italy, May 2002 (Passchier is invited speaker).
- Deformation mechanism, Tectonics and Rheology Conference, St. Malo (France), Spring 2003.
- European Geophysical Union (EGU) or European Union of Geologists (EUG) conference, Spring 2003.
- American Geophysical Union (AGU) Meeting in San Fransisco, December 2002 or 2003.

The international ELLE-group holds a workshop meeting every 1-2 years. These workshops play an important role in the development of the program and it is vital for the project to attend these meetings. The next workshop is tentatively planned to take place in Estonia in Summer 2002, organised by Dr Soesoo (Tartu University, Estonia) and Bons.

Close collaboration with other members of the ELLE group needs to be maintained, by form of the workshops and bilateral visits. Two one-week visits to collaborators in Europe (UK, Austria, Norway, Estonia) are planned for each year.

The ELLE group currently has one professional full-time programmer (Lynn Evans), based at Monash University, Melbourne, Australia. To efficiently and quickly learn the program ELLE, the assistant postdoc will have to make a training visit to Monash University, early in the project.

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