Experimental Modelling Techniques

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All previous chapters deal with observations of microstructures in rocks, and conclusions that can be drawn from those observations. However, no science is complete without some degree of experimental work to test ideas and theories. Unfortunately, geology is a difficult subject to study by experimental techniques; most geological deformation processes are too slow to model in laboratory experiments; they occur at extreme pressure and temperature, and at a scale too large for experimental reproduction. To overcome this problem, two types of experimental work have been set up to date.

Analogue experiments use materials that are easier and faster to deform than real rocks, but which give results that can be compared with microstructures in rocks. Such experiments are carried out in small presses, usually at atmospheric pressure and low temperature, and even under the microscope. They can reveal the sequence of development of microstructures, and even movies can be made.

Numerical experiments are done on the development of all kinds of microstructures, on the grain scale and beyond. Several examples of such studies are discussed.

In this chapter, we restrict ourselves to experiments on actual microstructures, and do not treat the extensive work on large scale structures, thrust belts, orogenesis, granite intrusion and other crustal and mantle processes.

11.1 Introduction

As we discussed in previous chapters, microtectonics is mostly concerned with the interpretation of geometries in thin section formed by solid-state deformation. Our understanding of the way in which microstructures develop is mainly based on careful observation of fabrics from simple tectonic settings in various stages of development. The only way to test such interpretations unequivocally would be to carry out experiments identical to the deformation processes in the rock. Obviously, this is generally impossible because of the pressure and temperature conditions required, and especially because of the very slow rate of natural deformation processes in rocks. There are, however, ways to get around this problem. At least three different approaches are possible: (1) experimental deformation of rocks at high pressure and temperature, and at high strain rate; (2) experimental deformation of rock analogues at low pressure and temperature and at high strain rate; (3) numerical experiments.

Deformation experiments on rocks and minerals are possible at pressures equivalent to those in the crust for samples on mm–cm scale in special high-pressure deformation rigs (e.g. Rowe and Rutter 1990; Rutter and Neumann 1995; Kohlstedt et al. 1995; Gleason and Tullis 1995; Post and Tullis 1999; Brodie and Rutter 2000; Laurent et al. 2000; Mauler et al. 2000; Pieri et al. 2001; Heilbronner and Tullis 2002; Orzol et al. 2003). In these rigs, brittle and even ductile deformation structures can be produced by implementation of a high confining pressure and high temperature. Since samples cannot be deformed at natural strain rates, deformation is done at excessively high temperature and high strain rate to activate similar deformation mechanisms as in the geological environment under consideration (Chap. 3). Deformation of cylindrical specimens can be implemented to low strain by axial compression or to high strain in torsion. Samples used are either real rocks, or artificial rocks produced through sintering of a mineral powder.

The advantage of this type of experiments is that they give information on flow parameters of natural rocks, (Sect. 3.14) and on the generation of certain small-scale structures. A disadvantage is that only the initial and deformed state of the fabric can be studied, and that the intermediate stages and the actual deformation process cannot be observed during the experiment. In this chapter, we mainly concentrate on analogue and numerical experiments, which are better suited to study the development of microstructures.

11.2 Experimental Deformation of Analogue Materials

Since the 19th century, simple experiments have been set up with materials other than rocks with the aim to increase understanding of rock deformation through the deformation of analogue materials such as clay, sand, bee's wax and paraffin wax. Analogue materials have a different rheology than that of real rocks, but they deform at low pressure and temperature and at high enough strain rate to follow development of structures *in situ*. Although analogue materials deform much faster than rocks, they can form structures that are similar to those formed in rocks such as thrust fault systems, tension gashes, diapirs, but also microstructures such as shear zones, folds, mantled porphyroclasts and mineral fish. This means that analogue experiments are suitable as pilot experiments to create ideas for the interpretation of structures in rocks. It is also possible in some cases to use such experiments as an equivalent of a real rock experiment, provided the model and the original can be scaled in a proper way (Twiss and Moores 1992, p 437). If materials can be found such that length scales, velocities, forces and accelerations in the material can be scaled to that of the real rock, direct comparisons can be made. The main difficulties involved in such scaling are, however, that the rheological properties of real rocks are incompletely understood, that only a limited number of analogue materials and rheologies are available, and that gravity is equal in the real world and in the model (Twiss and Moores 1992).

11.3 Large-Scale Analogue Modelling

In large-scale modelling, cm–m scale machines are used to deform volumes of analogue material. Such studies are mostly directed to m–100 km scale geological features, but here we only discuss some of the types of experiments that have been used to model microstructures. The simplest type of device is similar to that shown schematically in Fig. 11.2 in which simple shear, pure shear and general flow in plain strain can be realised (Figs. 2.1, 11.1, Video 11.2a–d; e.g. Ramberg 1955; Mancktelow 1988a; Sokoutis 1990; Piazolo et al. 2001; Zulauf et al. 2003). A disadvantage of this type of machine is that only a limited finite strain can be reached; once the walls of the machine approach each other, the experiment must be stopped (Piazolo et al. 2001; Video 11.2a–d). High strain as in mylonites cannot be produced. To overcome this problem, another type of deformation rig called a circular or torsion rig can be used. In a torsion rig, a ring-shaped sample is deformed and very high strains can be reached. A disadvantage of the circular rig is that sample preparation is more difficult, and that flow cannot be homogeneous simple or pure shear as in a square shear box; material deforms along curved flow lines and with a strain rate and stress gradient from the inside to the outside of the ring (Fig. 11.1b). Both types of deformation rigs can be filled with clay, salt-mica aggregates (Williams and Price 1990; Williams and Jiang 2001), paraffin wax (Mancktelow 1988b), or with polymers and derived complex materials (McClay 1976; Zulauf and Zulauf 2004; Hailemariam and Mulugeta 1998; Weijermars 1986;

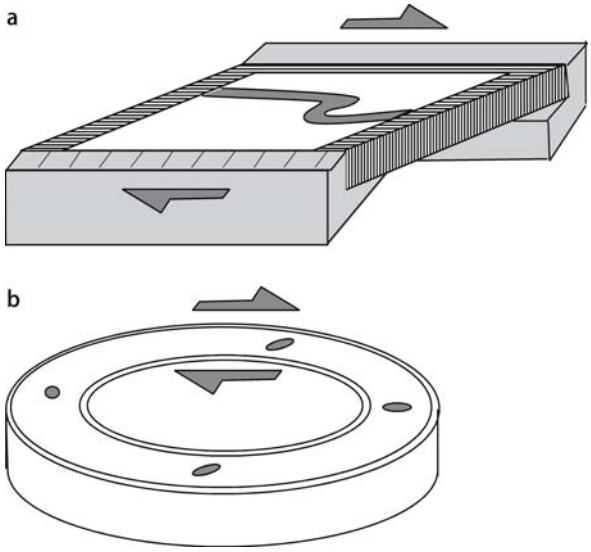


Fig. 11.1. a Simplified drawing of an analogue deformation rig for simple shear deformation. **b** Annular deformation rig for high strain experiments

ten Grotenhuis et al. 2002). Complex initial geometries can be set up such as rigid objects with mantles, multilayers and shear bands. Experiments are usually done at atmospheric pressure and room temperature and at strain rates between 10^{-1} and 10^{-6} s^{-1}. Observations are made at the surface of the sample if the material is not transparent, or by serial sectioning after an experiment is done. Three dimensional studies can be made by using transparent materials such as honey or polydimethysiloxane (PDMS; Weijermars 1986), or by using a rig that can be fitted in an X-ray tomograph (Coletta et al. 1991; Guillier et al. 1995).

Large-scale analogue modelling has been used for microtectonic studies in the following fields; mantled porphyroclasts (Passchier 1994; Piazolo and Paschier 2002b; Passchier and Sokoutis 1993; Passchier et al. 1993; ten Brink and Passchier 1995; ten Brink 1996), foliation refraction (Treagus and Sokoutis 1992); folding and boudinage of foliations (Williams and Price 1990), mineral fish (Pennacchioni et al. 2000; Ceriani et al. 2003), preferred orientation of phenocrysts (Ghosh and Ramberg 1976; Fernandez 1987, 1988; Arbaret et al. 1996, 2001; Ildefonse et al. 1992a,b;

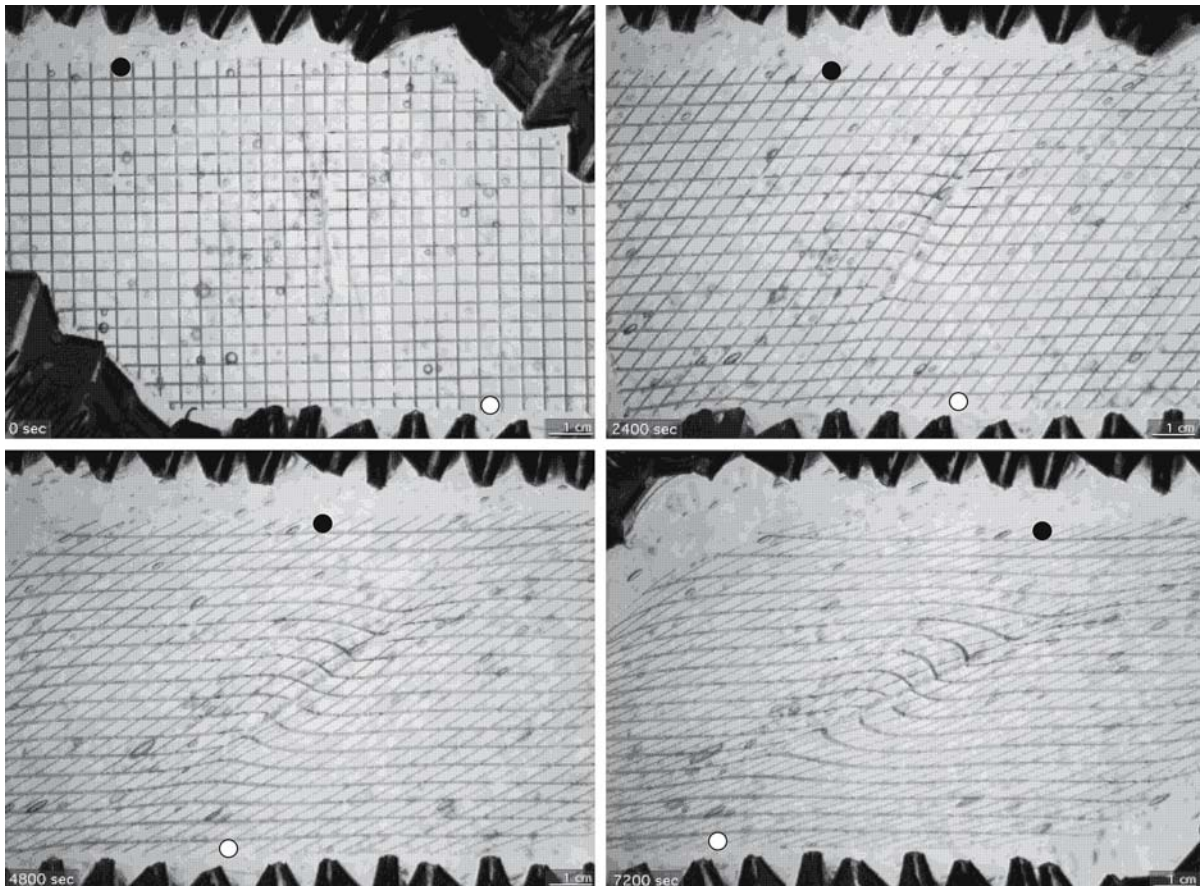


Fig. 11.2. Example of a shear box experiment using a transparent putty, polydimethylsiloxane, and a vertical fault filled with a lubricant in the centre of the box. Dextral shear in the shearbox leads to ductile deformation of the putty and deformation of the grid. The fault is active during this ductile flow, and this leads to development of flanking folds (see also ◉Video 11.2a–d). The experiment is shown at 0, 2 400, 4 800 and 7 200 seconds. *Shaded spheres* indicate marker points on the grid. (Experiment and photographs by Vincent Heesakkers, Mainz)

Ildefonse and Mancktelow 1993; Piazolo et al. 2002; Marques and Coelho 2001, 2002, 2003), folding and boudinage (Kidan and Cosgrove 1996; Kobberger and Zulauf 1995). All these experiments have been designed to model structures at a scale larger than the real objects, and have provided many new ideas on development of microstructures. Disadvantages are that real scaling is difficult because of the limited number of experimental materials available and technical problems of sample preparation. Advantages are the fast, cheap way in which true 3D-experiments can be realised and the possibility to study complex systems.

11.4 Micro-Analogue Modelling

11.4.1 Introduction

Large-scale analogue modelling is suitable for the study of larger, polycrystalline microstructures since they treat rocks as fluids and ignore processes on the crystal scale. Small, crystal scale processes can also be modelled by analogue studies using crystalline analogue materials such as camphor, nitrates and ice which can be deformed in a ductile way by dislocation- or diffusion creep at atmospheric pressure and temperatures between –10 and 300 °C, usually at strain rates between 10^{-2} and 10^{-6} s^{-1}. Such materials can be pressed or ground into thin slabs, which can be placed between glass slides, and deformed under the microscope. In this way, the development of microstructures can be directly observed. Small-scale crystalline analogue experiments are therefore an important tool in research and teaching. Three main types of apparatus have been developed for rock analogue experiments; a linear deformation rig, a torsion rig, and a triaxial press.

11.4.2 Linear Rig

In the linear rig (Fig. 11.3a), a thin sample of analogue material is mounted between two glass slides, usually similar slides as used for thin section preparation (Fig. 11.3b–d,

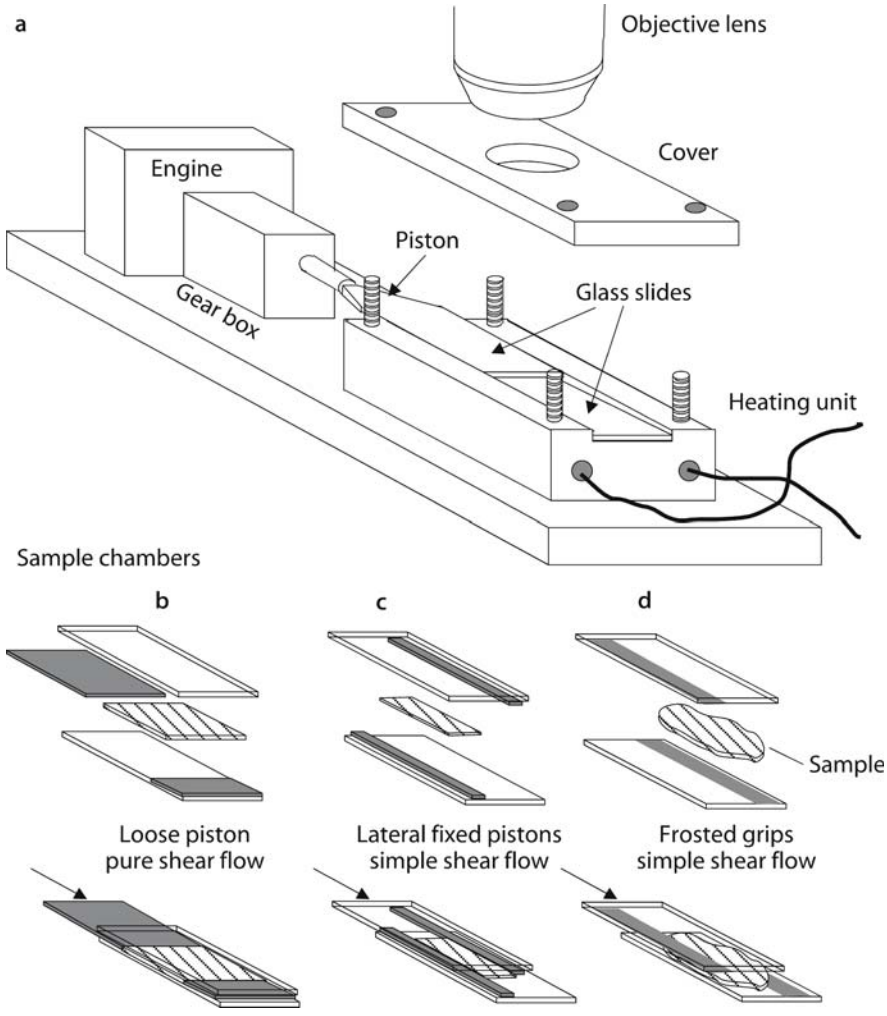


Fig. 11.3.
a Schematic drawing of a linear deformation rig used to deform analogue material. **b–d** Three setups of specimen chambers for the rig. The analogue material is deformed in experiments by movement of a piston **b** or of one of the two glass plates (**c**, **d**); arrangement of the pistons determines how the material is deformed, either in bulk pure shear or simple shear flow

Video 11.3; Means and Xia 1981; Wilson 1984; Burg et al. 1986; Means 1989). The sample can be deformed in coaxial or non-coaxial flow by the geometric arrangement of pistons. Pure shear deformation can be initiated by pressing a thin metal piston (at least 70 µm thick, otherwise the piston will buckle) between the glass slides against the sample (Fig. 11.3a), or by 'frosting' both glass slides at front or back with silicon carbide powder; the sample will remain attached to the frosted part of the glass, and will slide past the untreated glass, especially if the latter is lubricated with silicone grease (Fig. 11.3d). With this setup, samples as thin as 30 µm can be deformed. Simple shear can be initiated by the use of indented piston grips glued onto the glass plates (Fig. 11.3c), or frosted grips (Fig. 11.3d). General non-coaxial flow can be generated with obliquely mounted grips or pistons. The choice of thickness for the sample depends on the amount of detail that is required, and the birefringence of the mineral; minerals like ice and camphor have low birefringence and can be studied in relatively thick samples that are easy to prepare. In such thick samples, it may be difficult to resolve small grains, grain boundaries and other small details. Materials with higher birefringence can be studied in thin sections with frosted grips; this has the advantage that a similar view as a thin section is obtained and that small details can be studied. Disadvantages are difficult sample preparation and the possibility that friction of the sample against the glass plates causes deviations or distortions. The sample and glass slides are contained in a metal frame, which can be heated and kept within a certain temperature range with a thermocouple and a temperature control unit. The sample is deformed by displacement of a piston or one of the glass slides at a constant rate by a small motor (Fig. 11.3a); different strain rates are realised by the use of a range of gearboxes. The deforming sample is observed through a microscope and can be monitored with a camera or video equipment. It is even possible to carry out experiments under conditions of controlled confining pressure by sealing the entire deformation rig inside a small pressure vessel that fits under a microscope (Bauer et al. 2000b).

11.4.3 Torsion Rig

The torsion rig (Fig. 11.4a) deforms a sample between two glass slides (Fig. 11.4b, Video 11.4). Each glass slide has a ring-shaped frosted grip, one of small and one of large diameter. When one of the glass slides rotates, a ring-shaped part of the sample is deformed between the

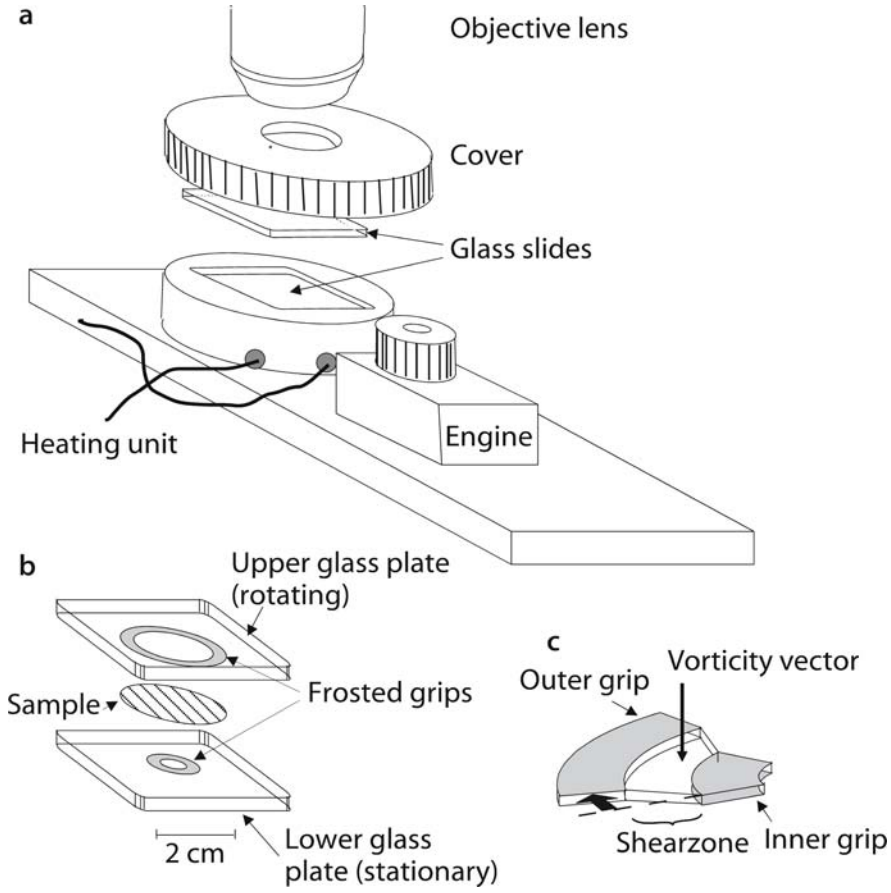


Fig. 11.4.
a Schematic drawing of a torsion deformation rig used to deform analogue material. **b** Setup of the specimen chamber for this rig; analogue material is deformed in torsion between two glass plates that rotate with respect to each other. Presence of frosted grips on the glass causes a small ring-shaped part of the sample to deform in non-coaxial flow. **c** Detail of the ring-shaped deforming part of the sample. (**b** and **c** courtesy C. ten Brink)

two frosted grips (Fig. 11.4b,c). The rotating glass slide is fixed in part of the metal frame of the rig, and both are driven by an engine as described above (Fig. 11.4).

The advantage of the torsion rig is that very high finite shear strain (exceeding 100) can be reached; in the linear rig, shear strains are limited to values of 5–10. In mylonites, shear strain values exceeding 10 are common, and may be required for the development of characteristic structures. A disadvantage of the torsion rig is that the deforming sample is circular and therefore does not deform in simple shear; in fact, there is a strain rate and stress gradient from inside to outside in the ring-shaped part of the deforming sample (Passchier and Sokoutis 1993; Masuda et al. 1995b). However, the gradient is accurately known and such gradients may also occur in natural shear zones.

11.4.4 Triaxial Rig

A triaxial deformation rig (Bons 1993) can be used to determine the rheology of analogue materials. Small columns of analogue material are compressed by a weight and the shortening rate is monitored. Normally, a confining pressure is applied using compressed air. The data are used to determine stress-strain rate curves. Such experiments are done at different temperatures and loads and the results can be used to determine the rheology of the material. Pure materials or mixtures can both be measured. It is not possible, however, to observe the deforming sample in the triaxial rigs that are presently available.

11.4.5 Marker Particles

During development of structures in analogue experiments, deformation is usually inhomogeneous. Besides observation of developing structures, the analogue experimental setup also allows detailed monitoring of gradients of inhomogeneous deformation over the sample. This is realised by insertion of fine silicon carbide powder in the sample (1 000-grid powder, normally used for preparation of thin sections). This powder does not react with the sample material and does not seem to interfere with the deformation process on the scale of observation. The particles act therefore as passive material points (Sect. 2.2; Figs. 2.1, 2.2); structures like grain boundaries cannot be used as markers since they may migrate through the material (Fig. 11.5). If photographs or video images of a deforming sample at various stages of development are combined, the positions of individual particles can be compared and used to reconstruct local deformation (Figs. 11.5, 11.6, Video 11.6b, 11.7b). If the position of at least three particles is known in two subsequent stages of the experiment, finite strain, vorticity and area change can all be determined (Figs. 11.7, 11.8, Video 11.7; Sect. 2.6; Box 4.8). The position of particles must be digitised and can be processed with a computer. Bons et al. (1993) presented a computer program that can process data on positions of particles into contours of strain, vorticity and area change.

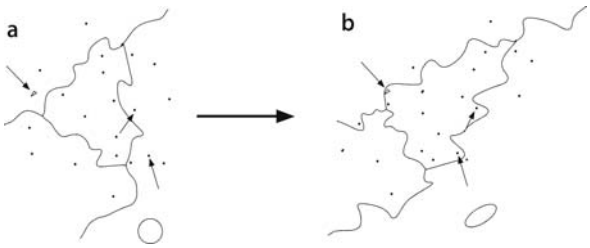


Fig. 11.5. Schematic drawing of marker particles in an analogue material that shows grain boundary migration during deformation. In **b** the marker particles have an arrangement other than in **a** because of deformation of the aggregate. Grain boundaries do not show the same deformation because they have migrated. Marker particles indicated by *arrows* have passed from one grain to another. The position of marker particles before and after this deformation step can be used to reconstruct maps of deformation and deformation gradient in the sample as shown in Fig. 11.8

11.4.6 Examples of Analogue Experiments

A large number of experiments has been carried out with analogue materials (Fig. 11.6). The materials that have been mostly used are octochloropropane (OCP – Fig. 11.6; Jessell 1986; Ree 1990, 1991, 2000; ten Brink and Passchier 1995; Bons and Jessell 1999; Nam et al. 1999), biphenyl, paradichlorobenzene (Means 1980), camphor (Urai et al. 1980; Urai and Humphreys 1981), naphthalene (Blumenfeld and Wilson 1991), norcamphor, benzamide (Herwegh and Handy 1996, 1998; Herwegh et al. 1997, 2000; Rosenberg and Handy 2001; Walte et al. 2003), sodium nitrate (Tungatt and Humphreys 1981a,b), ammonium nitrate (McLaren and Fitz Gerald 2000), paraffin wax (Abbassi and Mancktelow 1992; Mancktelow and Abbassi 1992; Chatterjee 1994; Rossetti et al. 1999; Hafner and Passchier 2000) and ice (Wilson 1982, 1994; Burg et al. 1986; Wilson et al. 1986; Wilson and Zhang 1994; Wilson and Marmo 2000; Wilson and Sim 2002). Effects that have been studied include melt-forming and melt migration processes (Park and Means 1996; Rosenberg and Handy 2001; Walte et al. 2003), fluid migration during deformation (Bauer et al. 2000a), the development of steady state fabrics (Ree 1990, 1991), shape preferred orientation (Herwegh and Handy 1998), lattice-preferred orientation and dynamic recrystallisation mechanisms (Jessell 1986), the influence of temperature and finite strain on these processes (Jessell 1986; Herwegh and Handy 1996), the development of low and high angle grain boundaries and their classification (Means and Ree 1988), grain boundary migration (Means and Jessell 1986; Ngoc Nam et al. 1999), grain boundary sliding and void development (Ree 1994), the development of shear band cleavage (Passier 1991; Chatterjee

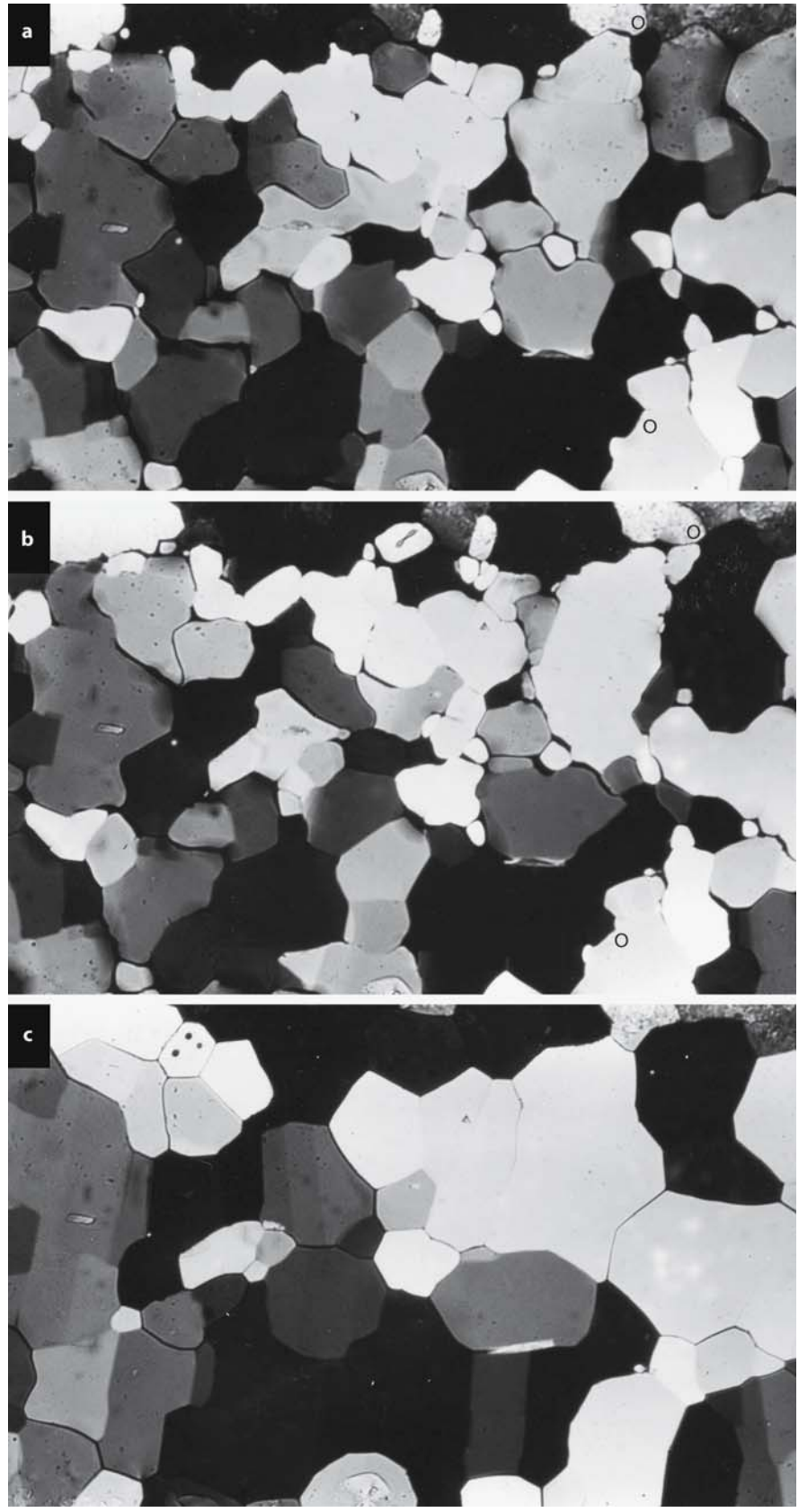


Fig. 11.6.
Examples of a deformation experiment using a sample of octachloropropane (OCP), which is deforming in simple shear in a linear deformation rig (dextral sense of shear). The sample has already undergone a shear strain of 1.7 at stage **a**. Between **a** and **b** a shear strain of approximately 0.1 has accumulated, as shown by the displacement of two marker points indicated by *circles* at *top* and *bottom right*. Due to this extra shear stain, the shape of the grains has changed and grain boundaries have migrated in **b**. After step **b** the experiment was stopped. **c** Shows the same area as **b**, but after 16 h of static recrystallisation. A polygonal fabric has developed in response to grain boundary area reduction (GBAR); grain boundaries have become relatively straight and there is evidence for grain growth. Subgrain boundaries developed in some grains. Unpublished experiment by J-H. Ree. Part of this experiment was published in Means (1989). Width of view 2.1 mm. CPL. (Photographs courtesy J-H. Ree)

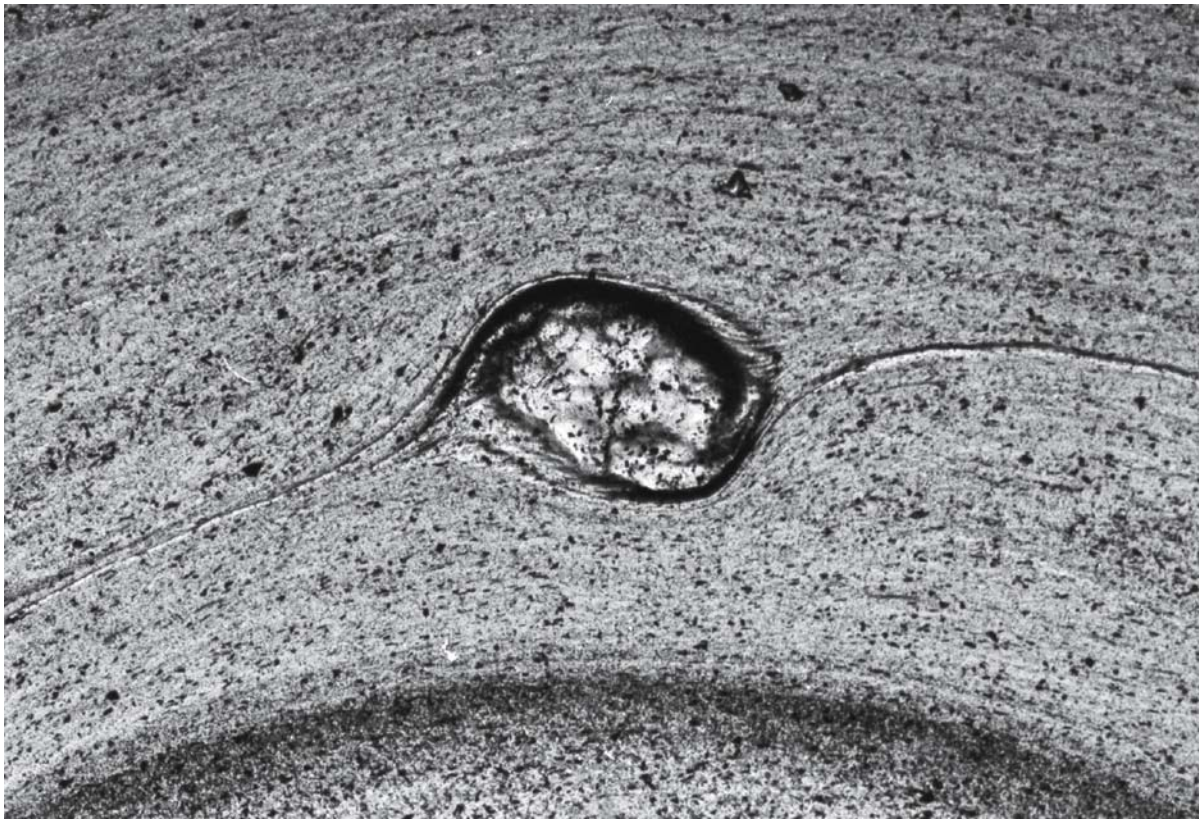


Fig. 11.7. Example of a δ-type mantled porphyroclast developed in a rock analogue experiment in a torsion rig (ten Brink and Passchier 1995). A square polycrystalline aggregate of camphor was embedded in a matrix of octachloropropane (OCP), and both were deformed together at 60 °C and a shear strain rate of 2.6×10^{-3} s^{-1}. Camphor is stronger than OCP at these conditions, and the camphor object rotated in response to non-coaxial flow in the OCP matrix. In the rim of the camphor object, fine-grained material is produced, probably by recrystallisation. This caused development of a fine-grained camphor mantle that deformed into δ-type wings. The entire evolution of this mantled porphyroclast could be studied under the microscope. *Black dots* in the matrix are grains of silicon carbide that act as marker particles. Figure 11.8 shows some results of the analysis of displacement of these marker particles. The curved shape of the wings is due to the circular shape of the specimen chamber (Fig. 11.4). The *dark rim* at the *bottom* of the photograph is the inner grip of the rig (Fig. 11.4). Shear strain in the matrix $\gamma = 94$. Width of view 5 mm. PPL. See also Video 11.7a. (Photograph courtesy C. ten Brink)

1994; Hafner and Passchier 2000), deformation twinning (Blumenfeld and Wilson 1991), the development of mantled porphyroclasts and the effect of a second phase on deformation patterns (Figs. 11.7, 11.8; Bons 1993; ten Brink and Passchier 1995). A review of analogue modelling and a list of the most commonly used analogue experimental materials is given by Means (1989). Some examples of results of analogue experiments in a linear rig are shown in Fig. 11.6 and Video 11.6a–e and of experiments in a torsion rig in Figs. 11.7, 11.8 and Video 11. 7a,b.

11.5 Numerical Modelling

11.5.1 Introduction

Numerical experiments are realised by using computer programs to model deformation. Many techniques of numerical modelling have been used to study deformation in rocks on the scale of the thin section (see Jessell and Bons 2002 for a review). Here, we describe some methods that model the development of geometries of geological microstructures, since this closely approaches the theme of the book. Many relatively simple but useful programs have been developed to study specific geometric processes in rocks, without giving the "virtual materials" true rheological properties. This kind of modelling starts with simple homogeneous deformation that can be modelled in any drawing program (stretching, tilting, rotating), through programs that model simple geological geometries. Examples are flow around rigid objects using analytical equations (Passchier 1987a; Bons et al. 1997; Ramsay and Lisle 2000) and programs for fringe growth (Etchecopar and Malavieille 1987; Kanagawa 1996; Bons 2001; Köhn et al. 2000, 2001a,b; Hilgers et al. 2001; Nollet et al. 2005). Examples of this type of modelling are given in Fig. 6.23 and Videos 6.23, 6.27.

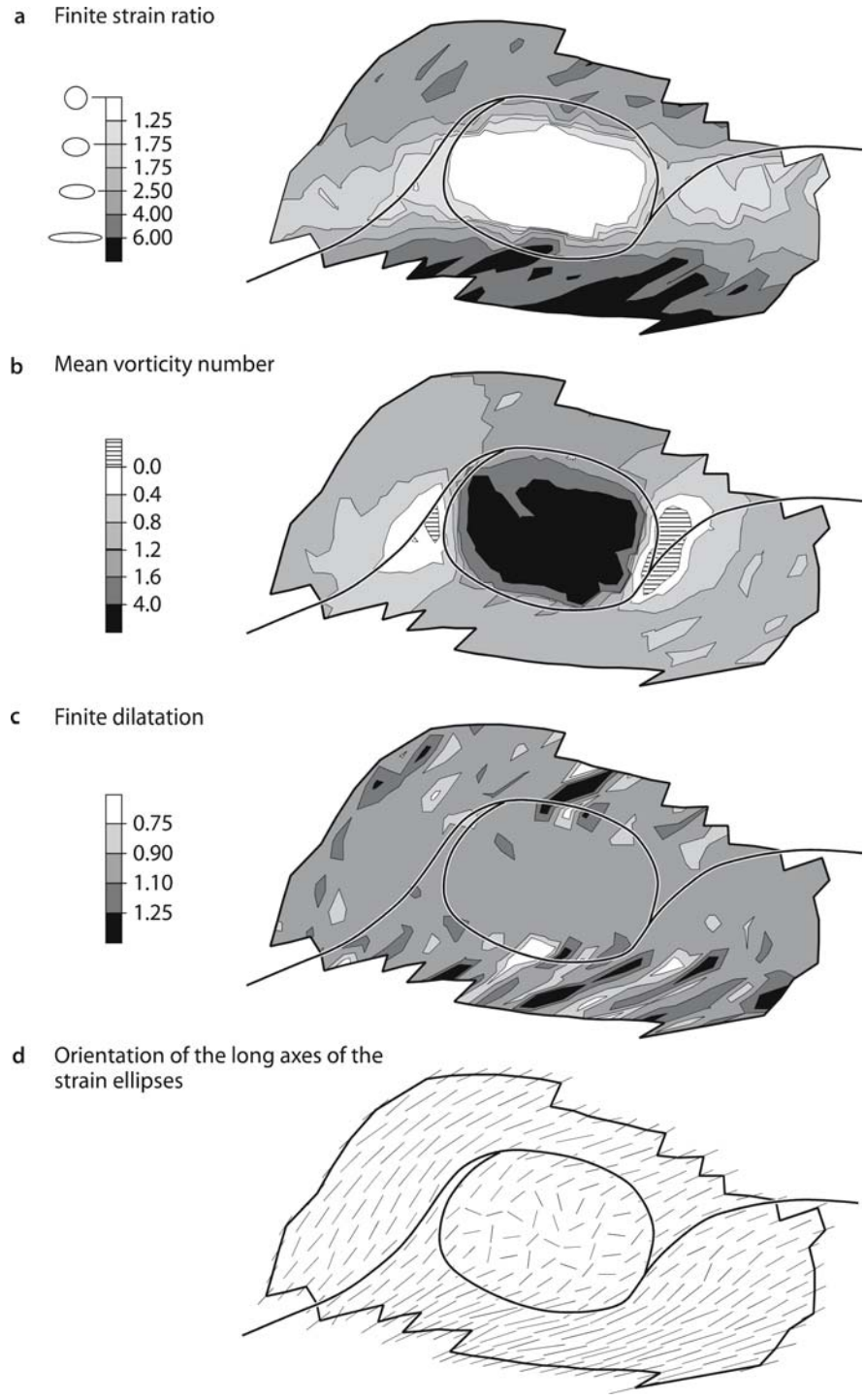


Fig. 11.8.
Example of the use of marker particles to analyse the deformation pattern in an experiment in the torsion rig. The experiment was on development of δ-type mantled porphyroclasts using a core object of camphor in a matrix of octachloropropane, as shown in Fig. 11.7. The drawings are maps of the four components of finite deformation, determined from displacement of marker particles. The contour of a developed camphor δ-type mantled porphyroclast is shown in each diagram. (After ten Brink and Passchier 1995)

11.5.2 Finite Element and Finite Difference Modelling

In *finite element* and *finite difference* modelling (Press et al. 1992, 2002; Gersenfeld 1999; Ramsay and Lisle 2000), deformation in a volume of material is approximated by subdividing space into a number of elements with specific rheological properties. The internal deformation is then calculated for imposed external stresses or external strain rates. In both cases, a *grid* of points or *nodes* is defined linked by lines, which build elements, usually triangles. Within an element the deformation is set to be homogeneous. In the original finite difference method all elements have the same size and are arranged

in a regular grid (for example square or cubic in 3D). The solution of e.g. a diffusion problem on such a grid is relatively straightforward. Therefore finite difference models are widely used in the Earth Sciences. These models have the disadvantage that all elements have the same size so that complex shapes need a very high resolution and thus an enormous amount of elements. In the finite element method elements can have different sizes so that it is easier to model complex shapes. In homogeneous areas of a model material elements can be large whereas they are small in heterogeneous areas. The disadvantage of finite element models is that they are not easy to write and need a large amount of computational time.

If the network of elements in a finite difference or finite element model is dense enough, groups of triangles can be made to coincide with structures to be modelled such as layers, folds, clasts etc. Commercially available finite difference and finite element programs use different mathematical paths to simulate both the elastic and ductile deformation by deformation of the triangles in the grid. Specific rheological properties can be defined for each of the triangles. Applied forces or boundary restraints are transmitted to the grid and from these external conditions, stress conditions are calculated for each node of the triangles in the grid. The programs then calculate, based on specified rheological properties, how each of the triangles is going to deform in a certain time step. Once all triangles are "deformed" during one time step, stresses at nodes are recalculated and the next time step is realised. Modelling therefore consists of loading the model with a stress field, and running a large number of small deformation steps which change the shape of the triangles until a finite deformation can be seen. This method can be applied in 3D, but modelling is commonly done in 2D because of the high price of 3D software and the long calculation time needed for 3D modelling. Modelling of this type is very useful to study the development of simple structures, e.g. rotation of a hard porphyroclast in a soft matrix, or folding of a hard layer in a soft matrix. However, it is difficult to work with faults or other brittle features, and only relatively small strains can be realised since triangles of the mesh should not become too flat. The latter problem can be overcome by recalculating the mesh, but this can introduce errors in the modelling.

Examples of the application of finite difference modelling to microstructural studies are given in Wilson and Zhang (1994), Zhang et al. (1996) and Passchier and Druguet (2002) (Fig. 11.9). Examples of finite element modelling on viscous flow around objects are Bjørnerud and Zhang (1994, 1995), Bons et al. (1997), Kenkmann and Dresen (1998), Pennacchioni et al. (2000), Biermeier et al. (2001), Treagus and Lan (2000, 2003, 2004). Below we give examples of finite element modelling embedded in a special environment.

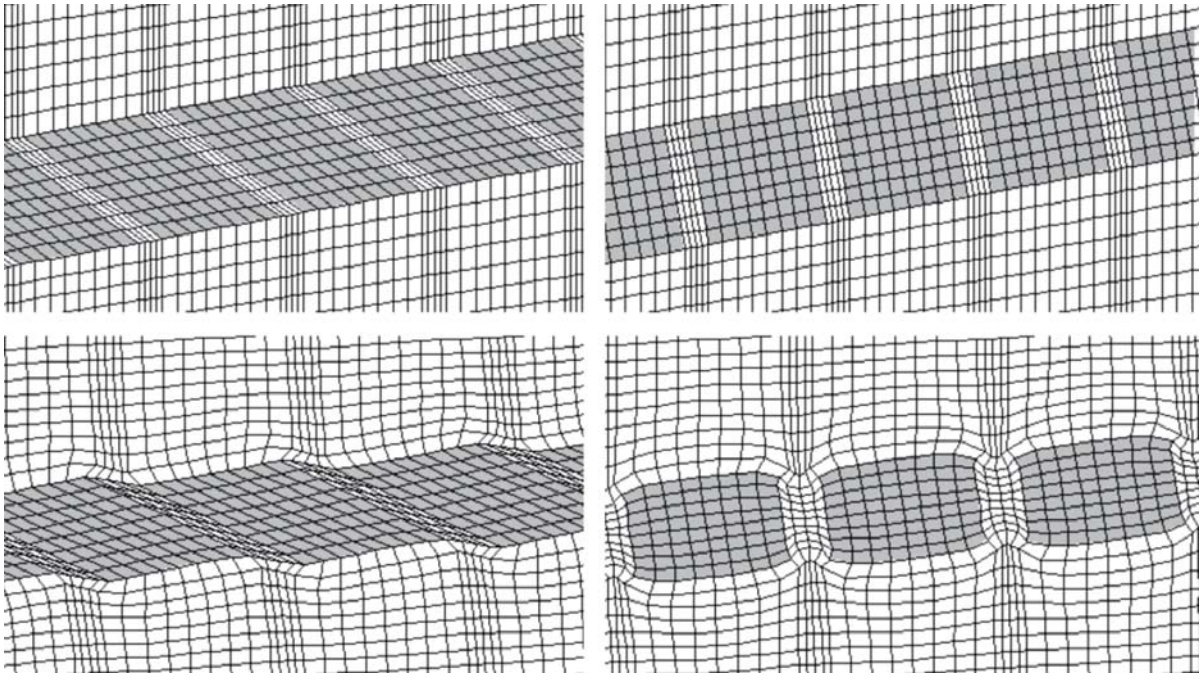


Fig. 11.9. Example of a deformation experiment using a finite difference code to model boudinage. At the *top*, two initial geometries are shown of a grid with two rheologies; a low viscosity (*light grey*) and high viscosity (*dark grey*). The bottom row shows the same grid after a deformation of $R = 2$ by pure shear vertical compression. The experiment shows how the initial orientation of a gap between boudins influences the final shape. (After Passchier and Druguet 2002)

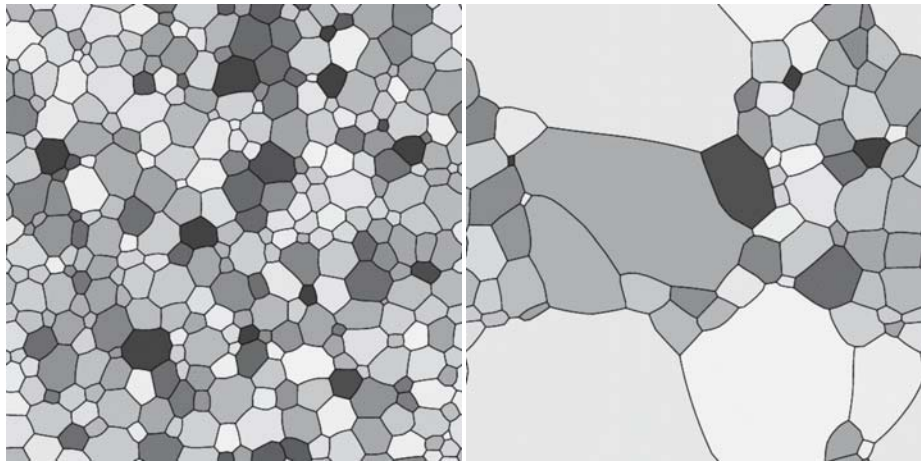


Fig. 11.10.
Example of the initial and final stages of an experiment carried out with ELLE. The grain aggregate at left is allowed to grow without deformation by a decrease in grain boundary energy but grain growth is dominated by high surface energy anisotropy, which prevents most boundaries from moving. Grains with boundaries that can still move eventually dominate the microstructure. Even though the starting microstructure is a foam texture, many of the triple junctions that develop deviate from 120°, which would be the equilibrium angle if there was no surface energy anisotropy. See also ◴Video 11.10e. (Courtesy Mark Jessell)



Fig. 11.11. Result of an experiment carried out with ELLE, modelling the development of fractures. The model used is an elastic spring model where grains consist of a number of circular elements that are connected with each other via linear elastic springs. Springs can break if they are stretched beyond a limit value, which leads to the development of larger scale fractures or faults in the model. The material is first loaded uniaxially and then vertically shortened and horizontally extended in pure shear deformation. Different *grey tones* indicate different differential stress (see ◴Video 11.11b for colour). The developing fractures are hybrid shear fractures at a small angle to the compression direction. During later stages the shear fractures open so that in principal material could precipitate and veins could form. (Courtesy Daniel Köhn)

11.5.3 Full Microstructural Modelling

The most useful and complete type of modelling available at present for work on microstructures is a supermodel known as ELLE (Jessell et al. 2001). ELLE is an open-source computer environment specifically meant for numerical modelling of the development of microstructures (Figs. 11.10, 11.11; Videos 11.10a–f, 11.11a–c; Jessell et al. 2001; Jessell and Bons 2002). It is based on a graphical program in which microstructures can be represented by a large number of nodes, which delimit grain and subgrain boundaries. Any original geometry of a microstructure can be set up from a simple digital drawing or photograph. Different parts of the microstructure can be given specific properties including crystallographic orientation and composition. This file is than passed through a number of modules, each of which represents a process such as grain growth, deformation, diffusion etc. A desired number of processes can be switched on for a certain study. Deformation is realised through a finite element deformation program called BASIL (Video 11.10a; Barr and Houseman 1996). The structure is then passed through each process in turn with very short time intervals, before a second step repeats the sequence. Time steps are chosen sufficiently small that the end result is almost similar to simultaneous occurrence. ELLE presently only operates in 2D, and can be set up on most computer platforms. The modules of the ELLE environment are part of an open system and new modules can be added in coordination with the developers. As a result, ELLE is expanded to a more powerful environment all the time and promises to become a major tool in microstructural analysis. The environment has been used to study grain growth and grain boundary anisotropy (Video 11.10a–e; Bons et al. 2001; Piazolo et al. 2002), grain growth in the presence of a fluid (Video 11.10f; Becker et al. 2003) and can even be used to model brittle deformation (Fig. 11.11; Video 11.10a–c).