The numerical simulation of microstructure

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Abstract: This review discusses the attempts that have been made by geologists to numerically simulate the evolution of microstructures in rocks. The strengths and weaknesses of the differing techniques are compared and equivalent materials science results are included. In particular we focus on the application of techniques that have been used to predict texture development, grain boundary geometries, deformation in one and two-phase systems and crystal growth.
The role of deformation in modifying structures can be seen at all scales, from the formation and movement of dislocations in single grains to changes in the structure of the whole Earth (Hobbs et al. 1976; Poirier 1985; Passchier & Trouw 1996). Attempts to simulate the evolution of these structures at each scale have been undertaken, from molecular dynamics at the atomic scale (Schjøtz et al. 1998; Yamakov et al. 2001), through to simulations of mantle convection (Houseman 1988; Moresi & Solomatov 1995). At the grain scale an understanding of the coupling of deformation processes, mechanical properties and microstructural evolution underpins our ability to correctly interpret natural microstructures in terms of rock history and to develop relevant geodynamic models. The numerical simulation of microstructures in geological materials has progressed in parallel with techniques developed in the wider materials science community (see Raabe 1998 for a comprehensive bibliography). In recent years there has been an upsurge in interest in this field due to the easy access to powerful computers. Equally important has been the introduction of new measurement techniques such as Orientation Imaging Microscopy (OIM) and Electron Backscattered Diffraction (EBSD) (Lloyd and Freeman 1991; Panozzo-Heilbronner & Pauli 1993; Fueten 1997; Leiss et al. 2000). These techniques allow us to systematically characterize the grain boundary topologies and textures of rocks with relative ease and in much more detail (Trimby et al. 1998), thus provoking us to rethink what microstructural parameters we should use as indicators of specific processes.

It is beyond the scope of this review to describe in detail the numerous numerical techniques that have been developed to simulate microstructure evolution. Instead we will focus on their application to the simulation and prediction of some geologically important microstructures,
namely: texture (lattice preferred orientation) development; grain boundary geometries; deformation in two-phase systems and crystal growth.

**Numerical simulation of microstructures**

*Texture development*

The earliest microstructural numerical simulation studies in geology were focused on predicting the texture patterns or lattice preferred orientations found in naturally deformed rocks. This work was based on metallurgical models first developed by Taylor (Taylor 1938) which, with modifications, are still widely applied today (Tóth *et al.* 1997). Lister and co-workers used a standard Taylor-Bishop-Hill formulation to study the development of textures in quartz and calcite rocks, Fig.1 (Lister *et al.* 1978; Lister 1978; Lister & Paterson 1979; Lister & Hobbs 1980; Lister 1982). Other groups have since extended this work to a broader range of minerals and to allow refinements of the TBH scheme such as the relaxed-constraints (Ord 1988) and self-consistent approaches (Wenk *et al.* 1989a,b; Canova 1994; Takeshita *et al.* 1999). Their work was able to demonstrate that, even though many minerals do not fulfil the requirement for the strict application of the Taylor model (due to the limited number of slip systems available) many of the key features of natural textures could be accounted for.

An alternative approach recognizes that in some minerals, such as trigonal symmetry quartz at low temperatures, only one slip system may be readily activated. This necessitates incorporation of intra- and intergranular strain heterogeneity in models (Etchecopar 1977; Etchecopar & Vasseur 1987; Zhang *et al.* 1993, 1994a,b, 1996; Wilson & Zhang 1996; Wilson *et al.* 1996; Zhang & Wilson 1997). These models can reproduce some aspects of the behaviour of, for example, ice and low temperature quartz. The transition from a low
temperature (single slip) behaviour to a high temperature (multi-slip) response is beyond the scope of both the Taylor (uniform strain) and Etchecopar (uniform stress) models.

Grain boundary sliding was shown to enhance texture development in model materials which allowed sliding interfaces between grains deforming with one slip system (Zhang et al. 1994a,b). The model of Ribe (1989) has been extended to simulate texture development in quartz when grain boundary sliding is the dominant deformation mechanism (Casey & McGrew 1999).

Under a wide range of crustal conditions, rocks deforming by crystalline plasticity are also modifying their microstructure as a result of dynamic recrystallization processes (Urai et al. 1986; Hirth & Tullis 1992). Jessell drew upon experiments on cold worked copper (Kallend & Huang 1984) to support the assumption that the level of stored work is orientation dependent, and that the low crystal symmetry of the rock forming minerals would result in a larger anisotropy of stored work than is present in metals (Jessell 1988a,b; Jessell & Lister 1990). He developed a hybrid scheme that combined the Taylor code of Lister with a Monte Carlo simulation that simulated the evolution of textures in quartz polycrystals by iterating between small increments of lattice rotations and grain boundary migration and sub-grain formation (Figure 2). The recrystallization processes in these models were driven by a simple stored work term for each element in the Monte Carlo simulation, as well as the more normal boundary energy derived neighbour relations (Anderson et al. 1984; Weaire & Rivier 1984). These simulations showed a better correspondence with natural textures than that predicted by models with lattice rotations only, even though there was still no mechanical interaction between grains.
Comparable hybrid lattice rotation/recrystallization schemes have recently been developed that replace the Taylor-Bishop-Hill scheme entirely with finite element codes capable of heterogeneous intra-crystalline deformation (Radhakrishnan, et al. 1998; Raabe & Becker 2000; Bate 2001). Another approach to modelling the effects on texture of dynamic recrystallization in rocks has been to build in a grain size weighting to simulate the changes in grain size that may result from dynamic recrystallization driven by orientation dependent stored work terms (Takeshita et al. 1999) (Figure 1b).

Texture development is classically attributed to result from movement of dislocations (e.g. Wenk 1985). However, other deformation processes, such as dissolution-precipitation creep (Rutter 1976) may hypothetically also affect textures (Hippert 1994; Stallard & Shelley 1995; den Brok 1996). Recently, Bons & den Brok (2000) explored this possibility with a numerical model. They showed that reaction-controlled dissolution-precipitation creep, coupled with grain rotation can also lead to strong textures, similar to those described above. Their model used a constant stress approach, the opposite to the constant strain rate or Taylor approach, and which may over-estimate the strain rate heterogeneity and rotation rates of grains.

Many of the above mentioned models predict a texture in terms of a distribution of lattice orientations, without any predictions of the shape of grains and the locations of certain lattice orientations within a grain aggregate. This is a severe limitation, if textures are also affected by processes where the relation with neighbouring grains is important, such as in case of dynamic recrystallization, grain boundary sliding and dissolution-precipitation creep. The recently enhanced ability to actually map out lattice orientations (as in Sander's (1950) Achsenverteilungsanalyse or AVA) with techniques such as the aforementioned EBSD and
OIM (Leiss et al. 2000) also necessitates the development of models that include actual grain boundary topology and geometry.

**Grain boundary topology & geometry**

There have been a plethora of numerical simulation studies of grain boundary geometry in engineering materials, mostly focusing on grain growth, and recrystallization subsequent to deformation. The investigation of the grain growth phenomenon has in particular seen the application of a wide range of simulation techniques, in both 2D and 3D. These schemes can broadly be grouped into three classes:

a) Discrete schemes mapped onto regular grids, in which local changes in grain boundary position occur as a result of individual grid points switching their orientations, as a function of the local distribution of orientations. These include: Potts Models (Anderson et al. 1984; Kunaver & Kolar 1998) and Cellular Automata (Davies & Hong 1998).

b) Continuous schemes mapped onto regular grids, where the local change in orientation property is a function of the properties of the whole system, such as Phase Field techniques (Fan & Chen 1997; Le Bouar et al. 1998).

c) Discontinuous schemes mapped onto arbitrary networks. These schemes include Vertex Models (Soares et al. 1985; Cleri 2000); Front Tracking models (Wakai et al. 2000) and Finite Element techniques (Cocks & Gill 1996).

In comparison, there have been relatively few geological studies. Some of the studies mentioned in the previous section did make some predictions about grain geometries
(Etchecopar 1977; Etchecopar & Vasseur 1987; Jessell & Lister 1990), however the main focus of these studies was texture development. Bons and Urai applied a modified version of the Vertex model of Soares et al. (1985) to dynamic grain growth (Bons & Urai 1992), an approach also taken by Bate & Mackenzie (2001). This allowed them to study grain size and grain geometries for the case of normal grain growth in a system where homogeneous strain is combined with grain growth and demonstrate that the application of a bulk strain did not significantly alter the measured grain growth rates, but can slow down the development of a grain shape foliation (cf. Ree 1991) and play a role in the establishment of an oblique grain shape foliation (cf Berthé et al. 1979).

As yet, there has been very little work on the development of microstructures during chemically driven nucleation and growth of new phases in rocks, but this area has enormous potential for further study (Foster 1999).

**Deformation of one-phase systems**

Even with only a single phase present, the simulation of polycrystalline deformation is far from trivial. Hybrid techniques are often used since markedly different micro-processes need to be simulated, either concurrently or consecutively. These techniques combine two or more of the techniques outlined in the previous sections, so in general there needs to be a re-mapping of the underlying description of the microstructure geometry from one simulation scheme to the other. Examples of hybrid schemes are combined Taylor lattice rotation and Potts dynamic recrystallization models (Jessell & Lister 1990), combined Taylor and a dimensionless recrystallization algorithm (Takeshita et al. 1999), combined Finite Element deformation/lattice rotation and Potts primary recrystallization (Radhakrishnan et al. 1998;
Raabe & Becker 2000; Bate 2001) and a generalized hybrid scheme that attempts to combine a whole range of simulation techniques (Jessell et al. 2001).

The hybrid simulation of Jessell et al. (2001), named "ELLE", consists of an open system of individual modules each of which represents a specific grain-scale deformation process, including a Finite Element description of deformation, a Front Tracking model for grain boundary migration driven by surface and defect energy terms. Microstructure evolution is achieved by passing a data file (which describes the topology and geometry of the polycrystal) through each module in turn (Fig. 3). This system has been applied to the problem of grain growth to investigate the role of surface energy anisotropy in modifying textures and grain boundary geometries (Bons et al. 2000). Piazolo et al. have applied this same simulation system to a systematic study of grain boundary geometries in deformed coarse and fine grain rocks (Piazolo et al. 2002, this volume). At present the mechanical modelling in this scheme cannot represent full elastic-plastic behaviour, however this is not an intrinsic limitation of the system.

Deformation of two-phase systems

While much of the work in geology has sensibly concentrated on single-phase systems, in reality most rocks consist of a mixture of two or more minerals. Several studies have looked at the specific case of a single rigid grain surrounded by a matrix of a weaker mineral. This case is important because it has been extensively used as an indicator of the kinematics and mechanics of deformation in natural settings. Apart from a number of kinematic models based on analytical solutions for viscous flow around objects (Bjørnerud 1989; Passchier et al. 1993; Beam 1996), finite-element formulations have been used to study the flow field around
the rigid object (Bjørnerud & Zhang 1994, 1995; Bons et al. 1997; Kenkmann & Dresen 1998; Pennacchioni et al. 2000; Treagus & Lan 2000; Biermeier et al. 2001), and the pressure state around the rigid grain (Tenczer et al. 2001).

In terms of more general polyphase deformation, Finite Element codes have been used to develop models predicting the flow properties of materials in terms of the end-member behaviour of its constituent components (Tullis et al. 1991; Tóth et al. 1993; Bons & Cox 1994; Treagus & Treagus 2001; Treagus 2002). Compared to disciplines such as composite materials engineering, the geological modelling of polyphase rocks is still in its infancy.

Crystal growth

In a geological context, crystal growth at free surfaces plays a role in microstructure development in two main environments: during crystallization from igneous melts, and during precipitation from fluids. An originally two-dimensional model has been developed into a three-dimensional simulation of crystallization from a melt where an arbitrary number of seeds with different crystallographies may be specified (Amenta 2001). Schemes based on Potts or Ising models have been used by Mizuseki et al. (2000) to simulate crystal growth on planar surfaces and by Baker & Freda (1999) to simulate texture development in cooling silicate melts.

Microstructures of veins and pressure fringes potentially store much information of tectonic conditions during their formation (Durney & Ramsay 1973; Ramsay & Huber 1983; Bons 2000) and several numerical models have been developed to simulate their development (Etchecopar & Malavieille 1987; Kanagawa 1996; McKenzie & Holness 2000; Bons 2001).
Bons (2001) uses a front-tracking approach in which linked nodes that describe the surfaces of vein crystals can move into space that is produced by a gradually opening crack, essentially simulating the crack-seal mechanism of Ramsay (1980). This model formed the base for several studies in which the numerical simulations beautifully reproduced the vein and fringe structures under investigation (Koehn et al. 2000, 2001a,b; Hilgers et al. 2001) (Fig. 4). A similar approach has been taken by Paritosh et al. (1999) to investigate thin film diamond crystal growth. The investigation of growth kinetics when coupled with fluid flow has recently been tackled by Miller & Schröder (2001) using a Lattice Boltzmann approach. As with many other areas of microstructure simulation, the simulations listed here ignore the implications of the mechanical contrasts between different elements.

**Discussion and conclusions**

The distribution of the publication dates in the references section of this review shows that the numerical simulation of microstructures is a blossoming field in the Earth sciences. Many of the techniques that have been applied have direct parallels in the materials science literature, however the complexity of geological systems has meant that in many geological studies the problems involve poly-phase materials and multi-process behaviour, areas that are relatively unexplored in the wider materials science literature. The modelling scheme ELLE (Jessell et al. 2001) is currently the only attempt in geology to fundamentally address this problem, as its open structure puts no limits on the number and types of processes that are modelled. *The in principle* boundless opportunities this provides has one serious draw-back: the more processes that are involved, the harder it will be to check and test the validity of a model.
The solution of these problems will ultimately involve not simply the numerical simulation work, but an integrated approach that draws upon theory, field observations, classical mechanical experiments, and transmitted light experiments. The latter class of experiments are particularly useful, because they can be used as constraints, not just on the final microstructure, but also on the evolutionary path that that sample has undergone (Fig. 5).

Some geological processes are fundamentally difficult if not impossible to simulate experimentally in a laboratory. These are processes or combinations thereof that span large differences in scale, in both time and/or space, or those processes that involve different and conflicting scaling between experiment and nature. An example of the first could be deformation by occasional fracturing (strongly localized, occurring in seconds) punctuating slow ongoing ductile deformation (pervasive, time scales up to millions of years). An example of the second could be deformation during lower greenschist facies metamorphism of a pelite: to make an experiment possible in a reasonable time frame, deformation experiments need to be carried out at enhanced strain rate and temperature well above that for greenschist facies metamorphism. Here lie both a great challenge and opportunity for numerical modelling.

The application of new numerical models should always include a discussion about the verification and testing of these models. Models based on single processes can often draw upon analytical solutions as tests, however when several processes interact, these solutions are not often available. Finally the inputs to these models are the fundamental properties of geological materials at geologically relevant conditions. While some parameters, such as the elastic tensor, are quite well known, others, such as the surface energy properties of minerals under a range of conditions, are difficult to determine. Perhaps the greatest hope for the
determination of these fundamental properties is the field of molecular dynamics, where they may be calculated via numerical experimentation. Alternatively, numerical modelling may actually help to constrain possible values for such parameters.

Although many of the simulation techniques are specifically applied to deforming rocks, most simulations discussed here are kinetic models (e.g. Bons 2001) and fail to consider the full dynamic or mechanical aspects of the deformation. Finally we have to recognize that most of the simulation schemes that have been developed so far are two-dimensional, and there can be real limitations to two-dimensional schemes, especially when it comes to fluid flow and diffusional transport of materials. While some schemes are easily extended into three dimensions, such as particle codes and Potts Models (Fig. 6), there are real computational challenges in similarly extending others, including Front Tracking codes.

There is little doubt that the field of numerical simulation of microstructures will expand rapidly over the next five years, drawing upon techniques developed in the realm of materials science, and that the goal of a “virtual rock” may become a reality.

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References


Figure Captions

**Fig. 1.** Simulation of c-axis texture development in model quartzites. (a) Classical Taylor calculation for simple shear up to a shear strain of 3 (Lister 1981). (b) Texture development caused by both intracrystalline slip and dynamic recrystallization (i.e. nucleation and growth). Steps 30, 32 and 34 are shown (at shear strains of 0.75, 0.8 and 0.85 respectively), recrystallization starts after step 30, the texture illustrated in step 34 does not change appreciably with further straining. Equal-area projection. The symbol + indicates old grains and the symbol × grains that have nucleated at least once; the size of the symbols is proportional to the grain volume (Takeshita *et al.* 1999).

**Fig. 2.** The simulation of microstructure development in quartz deformed in simple shear. The technique combines a Taylor analysis that predicts new lattice orientations and stored work, with a Potts model which uses the stored work term to drive grain boundary migration and sub-grain formation. (a) Initial grain geometry, grey colours reflect c-axis orientations. (b) Microstructure after a shear strain of 3.0. (Jessell & Lister, 1990)

**Fig. 3.** Simulation of dynamic and meta-dynamic recrystallisation in quartz, modelled with ELLE. (a) Starting grain boundary geometry. Shading reflects internal energy of grains and subgrains (darker equals higher). (b) After dextral shear strain of 0.65, modelled in 13 steps. (c-f) Post deformation recovery and grain growth in intervals of 26 steps. (g,h,i) Same microstructure as in a, b, and f, respectively, but with shading reflecting the lattice orientations. Notice that although the grain shapes are restored to a foam texture, the lattice orientations are preserved.
Fig. 4. Fibrous crystal growth around a rigid mineral as it rotates clockwise during progressive dextral simple shear. (a) Example from Lourdes (France) of a quartz+calcite+chlorite fringe system that developed around a pyrite grain. Width of image is 8mm. (b) Numerical simulation of fringe growth around an object of the same shape, shading is used to distinguish different fibres. (Koehn et al. 2001a).

Fig. 5. Comparison between a transmitted light microscopy thin-film grain growth experiment in the polycrystalline organic compound octachloropropane (grey scale images) (Park, Ree & Means 1995, unpublished), and a numerical experiment with ELLE that used the same starting grain boundary geometry (white lines) (Jessell et al. 2001). Although the simulated isotropic growth successfully follows the development of some grains (arrow), it fails at other places, probably because growth in octachloropropane is not isotropic (Bons et al. 2000).

Fig. 6. Simple 3D Potts simulation of normal grain growth. (a) Starting configuration, with 6 possible lattice orientations randomly distributed through 50x50x50 site sample. (b) After 100 time steps, with 125,000 trials per time step (Jessell 2001, unpublished).
Figure 1
Figure 2
Figure 5
Figure 6