Animations of dynamic recrystallization with the numerical modelling system Elle

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Abstract: The visualization of the development of microstructures during progressive deformation is a powerful tool both in geological education and in the advancement of understanding of processes. In this contribution a numerical modelling system is briefly explained. The use of this program is illustrated by two sets of numerical animations simulating the effect of dynamic recrystallization on the microstructural development of a quartzite are shown. The movies depict the changes in grain shape, grain size, dislocation density and crystallographic orientation of grains during progressive deformation. Such simulations can help to gain a better understanding of the interaction of concurrent processes on the microstructural development of a rock and vice versa. With this better understanding, microstructures observed in rocks may now be interpreted in a more quantitative way.

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Introduction

Dynamic recrystallization is an important process during deformation of many rock forming minerals and occurs under a wide range of metamorphic conditions (Urai *et al.*, 1986; Drury and Urai, 1990). In general, it leads to the formation of new grains at the expense of old ones. Therefore, dynamic recrystallization significantly influences the microstructure as well as the mechanical properties of a rock (Hirth and Tullis, 1992, Rutter, 1998). Resultant microstructures are used to derive processes active during deformation (*e.g.,* Guillopé and Poirier, 1979; Urai *et al.*, 1986; Drury and Urai, 1990; Hirth and Tullis, 1992) and delineate the conditions during which the rock was formed and/or deformed (*e.g.,* Hobbs *et al.* 1976; Hirth and Tullis, 1992; Twiss and Moores, 1992). Two main mechanisms active during dynamic recrystallization are rotational recrystallization and grain boundary migration recrystallization (*e.g.,* Poirier and Nicolas, 1975; Guillopé and Poirier, 1979; Urai *et al.* 1986 and references therein).

To be able to interpret microstructures that developed due to dynamic recrystallization, it is vital to know how they form. Questions to be answered involve the way and extent to which specific processes, combination of processes and parameters such as grain boundary mobility affect the microstructure and the rheology of a rock during progressive deformation. Additionally, we still have insufficient knowledge of how and to what extent the initial fabric of rock influences the microstructural development and flow properties of rock during subsequent deformation.

Movies showing the evolution of a microstructure through time and progressive deformation can improve our understanding of how processes change a microstructure. In such movies the formation of microstructural features can be observed and analysed. When interpreting the movies and extrapolating the findings to rocks the observer should always be aware of the limitations of numerical or analogue models. Nevertheless, watching a microstructure development may stimulate our imagination, give rise to new questions, may verify, challenge or change our current understanding of modelled processes and their interaction. In the last two decades movies showing the microstructural development of samples deformed and/or heated in in-situ experiments with organic and salt analogue materials have provided invaluable insight in microstructural development (*e.g.,* Means, 1983, 1989; Means and Ree, 1988; Bons and Urai, 1994; Herwegh and Handy 1998; Bons and Jessell, 1999). Numerical simulations using modelling systems like Elle, which visually represent a microstructure in specific time steps, can also be used to generate movies depicting the development of microstructures. In addition, in such numerical models movies depicting different attributes such as grains and subgrains, dislocation density, crystallographic orientation can be generated. Furthermore, such movies are very useful for teaching.

In this study, two sets of simulations showing the microstructural change due to dynamic recrystallization during progressive deformation are shown. The only difference between the two sets of simulations is the initial fabric. These simulations show that simulations which model the evolution of a microstructure with time may be a powerful tool to improve our understanding of interacting processes and their effect on microstructure through time. This contribution is primarily aimed to illustrate the potential of such numerical models for teaching purposes, scientific investigations of the interaction of concurrent processes active at the grain scale and determination of values such as temperature and grain boundary mobility, which may be characteristic for a specific observed microstructure.

The numerical modeling system Elle - general description

Elle (Jessell *et al.* 2001; see title Microdynamics Simulation Bons et al., 2008) is a modelling system with which it is possible to simulate a variety of concurrent microstructural processes that are active at the grain scale during continuous deformation. Individual grains are defined by polygons constituted of nodes and straight boundary segments and form the highest level in the hierarchical polygonal grain boundary structure. Each grain in turn is made up by a number of second-order polygons (subgrains). The lowest level discretization of the microstructure is a Delaunay triangulation (Shewchuk, 1996) of each polygon. A data file stores a complete description of the microstructure at a specific time interval and contains information about geometry, viscosity, strain, stress, dislocation density and age of each individual grain, node and boundary segment. A shell program iteratively combines an ordered set of individual micro-processes which are each described as a distinct code to simulate the effect of a single grain-scale process over a small time increment. The shell program passes the data file from one process to the other. The data file is changed according to the operation of one micro-process.

Editor's note: the original Elle website is no longer accessible - the above is provided as a more recent reference].

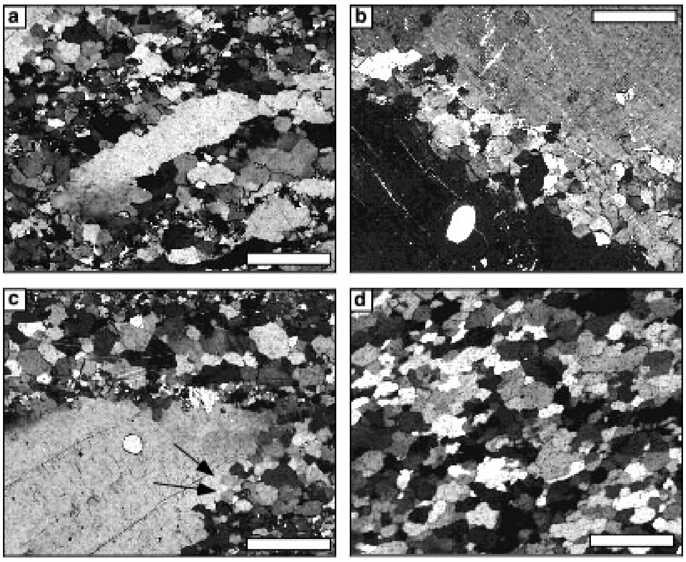
Specific model used

In our model we simulate dynamic recrystallization involving viscous simple shear plane strain deformation, crystal lattice rotation, formation of subgrains, rotational recrystallization, recrystallization by nucleation, grain boundary migration and recovery. Driving forces used in our model are dislocation density, grain boundary and surface energy. Theoretical considerations, detailed description and computational explanation of the different microstructural processes simulated are provided in the Appendix A: model description and Piazolo (2001, chapter 3). Simulations model the microstructural development of a quartzite at low grade conditions. Two initial fabrics are used; the fabric is either coarse grained (Movies 1A, 1B and 1C) or fine grained (Movies 2A, 2B and 2C). In both cases, the grain size distribution is unimodal. For specific values implemented in the model are given in Appendix B: values.

General features seen in movies

The simulated microstructures shown in Movies 1A-1C and Movies 2A-2C, closely correspond to microstructures that are commonly attributed to dynamic recrystallization (Figure 1; *e.g.,* Poirier and Nicolas, 1975; Guillopé and Poirier, 1979; Urai *et al.*, 1986; Jessell, 1987; Hirth and Tullis, 1992). During progressive deformation and recrystallization a bimodal grain size distribution develops from the initially coarse grained example (Movie 1A). This feature is commonly observed in dynamically recrystallized quartzites (Figure 1A, Hirth and Tullis, 1992). A few large, strongly elongated grains that are surrounded by small grains remain even at a strain of 2. Similar to natural examples (Figure 1B) small recrystallized grains develop predominately at the rim of large, old grains and trains of recrystallized grains are seen which crosscut old, large grains (Figure 1B; Movie 1B)). Additionally, domains of similarly oriented grains are observed (Figure 1C, (Movie 1C)). which compare well to grains that developed during dynamic recrystallization in natural examples (Figure 1C). Microstructures developing from an initially fine grained fabric exhibit a unimodal grain size distribution throughout the deformation experiment (Movie1A). Again, this is often observed in dynamically recrystallized rocks (Figure 1D, Hirth and Tullis, 1992).

Figure 1. Photomicrographs of typical microstructure seen in rocks that have undergone dynamic recrystallization

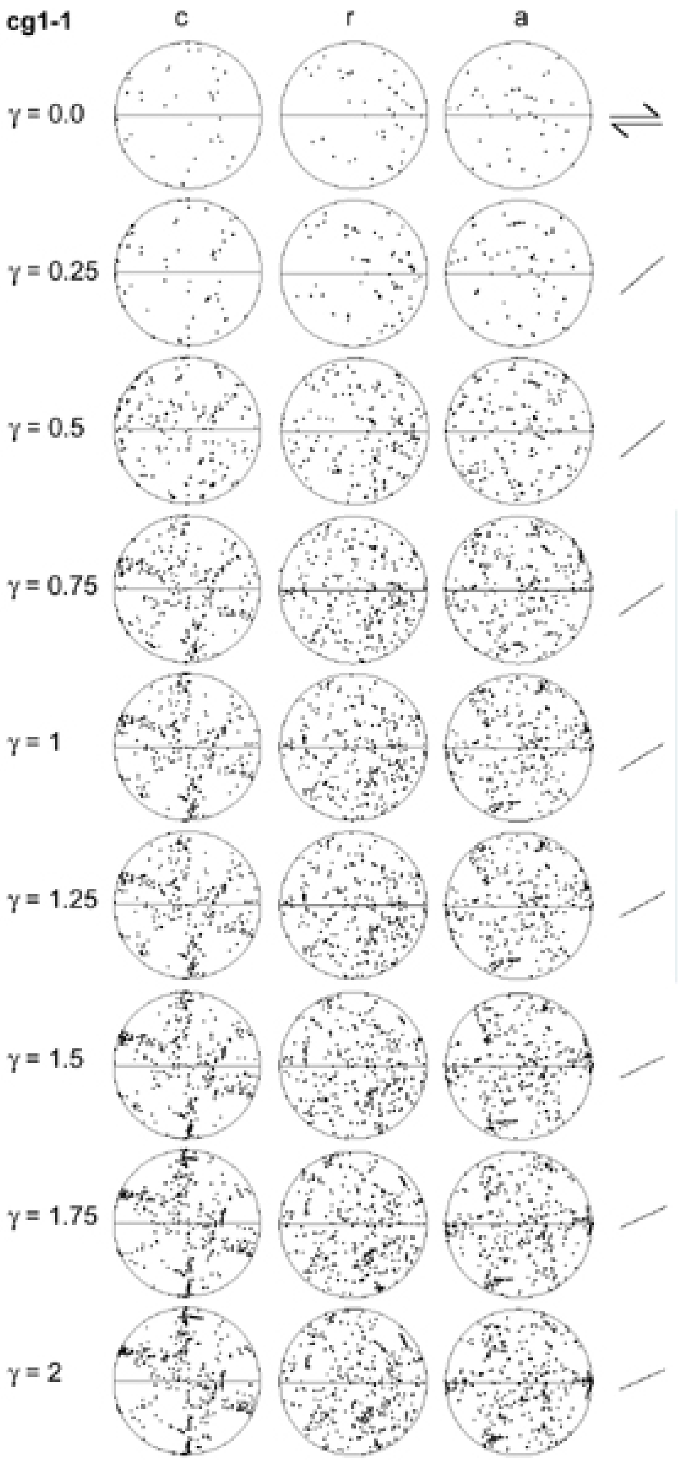


Photomicrographs of typical microstructure seen in rocks that have undergone dynamic recrystallization - scale bars = 0.5 mm; (a) Microstructure characterized by elongate grains with undulatory extinction and recrystallized grains surrounding the large, "old" grains, Qtz-Fsp mylonite, bimodal grain size distribution, Schirmacher Oasis, East Antarctica, crossed nicols. A similar microstructure is seen in Movies 1A-1C (b) Large grain cut by train of small recrystallized grains. Qtz-Fsp mylonite, Schirmacher Oasis, East Antarctica, crossed nicols. A similar feature is seen in (Movies 1A, 1B and 1C). (c) Tip of a large, elongate, "relict" grain. Recrystallized grains are present at the rim of the large, "old" grain. Grain size of recrystallized grains are in the range of subgrains (arrows). Qtz-Fsp mylonite, Schirmacher Oasis, East Antarctica, crossed nicols. A similar feature is seen in Movies 1A, 1B and 1C . (d) Completely recrystallized quartzite, unimodal grain size distribution, Conceição do Rio Verde, Minas Gerais, Brasil (courtesy of S. ten Grotenhuis), crossed nicols. A similar feature is seen in Movies 2A, 2B and 2C .

Completely recrystallized microstructures were not achieved in any of the experiments, where completely recrystallized means that all grains have gone through at least one stage of either recrystallization by nucleation or recrystallization by lattice rotation of adjacent grains.

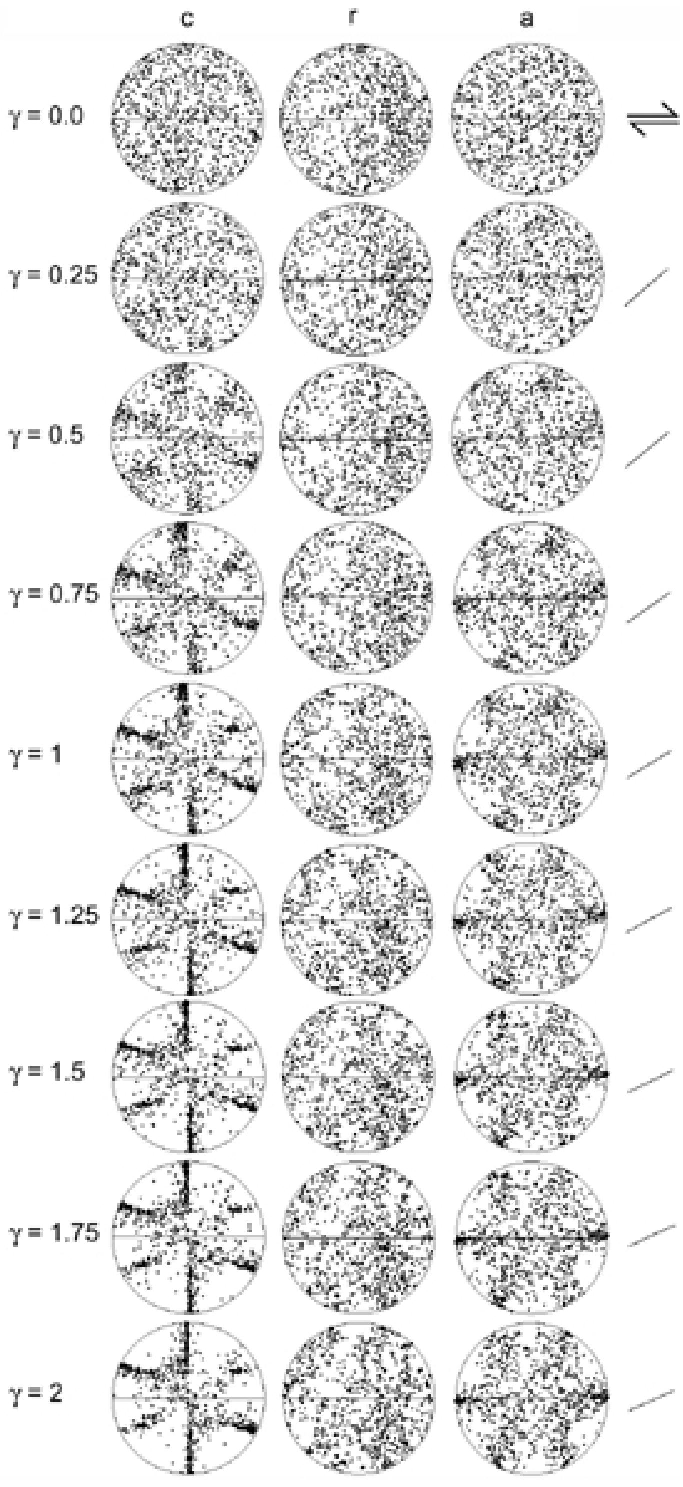
In none of the simulations a true steady state microstructure (Means, 1981) developed. This means that the characteristics of the microstructure such as the grain size, orientation of the long axes of grains, or subgrain size still change with ongoing deformation at least up to a finite strain of 2.

Figure 2A. Crystallographic orientation



Crystallographic orientation of the c-, r- and a-axes during progressive deformation of the microfabric that was initially coarse grained (cf Movie 1) The shear plane is oriented E-W. For each stage the orientation of the line of maximum finite elongation is shown as a tick mark next to the lower hemisphere equal area projections. With progressive deformation a preferred crystallographic orientation of c-axes with a crossed girdle develops. At high strain clusters of c-axes following a great circle are seen. These are rotated subgrains of large remaining grains. Projections of a-axes show the development of 6 weakly developed maxima that are oriented 60¡ to each other.

Figure 2B. Crystallographic orientation



Crystallographic orientation of the c-, r- and a-axes during progressive deformation of the microfabric that was initially fine grained (cf. Movies 2). The shear plane is horizontal. For each stage the orientation of the line of maximum finite elongation is shown as a tick mark next to the lower hemisphere equal area projections. With progressive deformation a preferred crystallographic orientation of c-axes with a crossed girdle develops. There are also 2 noticable maxima at an agble of 40-60¡ to the girdle maxima. Projections of a-axes show the development of 6 weakly developed maxima that are oriented 60¡ to eachother, whereby the two maxima on the horizontal are most pronounced.

Summary and Conclusions

Animations of dynamic recrystallization with the numerical modelling system Elle are useful to illustrate and understand the effect of dynamic recrystallization on the microstructural development of a rock during progressive deformation.

With such a numerical model it is now possible to simulate the evolution of a microfabric at know conditions and investigate the effect of different conditions on the microstructural development in a systematic manner. For example, in this model, processes can be turned on and off, conditions such as temperature, pressure and strain rates and parameters such as grain boundary mobility varied. Accordingly, the influence of specific processes and a large set of variables can be studied and results compared to rock samples. The existing structure of the model allows the addition of other process algorithms to the currently existing set. By implementing new algorithms for processes of interest, the underlying physical concepts of these algorithms can be tested and if necessary modified. Simulations with a specific set of parameter values and active processes may result in the recognition of indicative microstructural characteristics, which can then be used to interpret natural microstructures.

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A. Description of model

This appendix is presented as a PDF - to download click here

B. Values used

This appendix is presented as a PDF - to download click here

C. Reference list for Appendix A and B

This appendix is presented as a PDF - to download click here