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Microdynamics Simulation

With 185 Figures

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Preface

Paul Bons, Mark Jessell and Daniel Koehn

From the first observations of microstructures, geologists have tried to model and simulate their formation. Modelling and simulation are closely related terms, often used as synonyms. However, there is a difference. According to the Apple-Macintosh electronic dictionary, a *model* is *"a simplified description, especially a mathematical one, of a system or process, to assist calculations and predictions"*. The same dictionary defines *simulation* as the *"imitation of the appearance or character of [something]"*. As a special case it also lists *"product of a computer model"*. A *model* is therefore a theoretical abstraction, whereas the *simulation* is the actual application of the model to a specific case. For example, a rigid ellipsoid in a deforming homogeneous viscous matrix (Fig. 1b) can be a *model* for a porphyroblast or porphyroclast in a deforming rock (Fig. 1a) (Ghosh and Ramberg 1976). Applying and running the model for a specific case would be a *simulation* (Fig. 1c) (e.g. Bons et al. 1997, see also Ch. 4.7). We used the term *simulation* in the title of this book, because we are mainly concerned with the numerical implementation of models as a means to exploring their validity, not so much with the models themselves, which are amply dealt with in such works as Passchier and Trouw (2005).

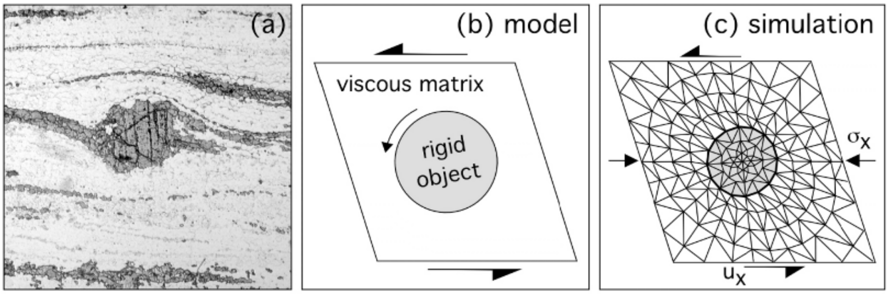

Fig. 1. (a) δ-shaped hornblende porphyroclast in a sinistral shear zone from Hidden Valley, South Australia. Width of view about 5 mm. **(b)** The model for the development of porphyroclast structures, such as the δ-clast, is that the porphyroclast rotates as a rigid object in a deforming ductile matrix. **(c)** To study the behaviour of porphyroclasts, the model can be implemented into, for example, a finite element program to run simulations

The purpose of this book is to provide an overview of the possibilities of using numerical techniques to study microstructures in rocks. Although wide-ranging, we cannot cover every technique that was ever applied to a microstructural problem. However we hope at least to demonstrate what is currently possible, and inspire users to investigate the field further if their particular interest is not currently met. In addition most of the numerical experiments we present may be repeated using the accompanying CD-ROM, so that the book can be used as a companion to an undergraduate or graduate level course on microstructures.

Chapter 1 gives a brief overview of the historical development of numerical simulation techniques as applied to grain scale phenomena in rocks, and discusses the principal constraints on applying numerical simulations to microstructural issues

There is no single way to simulate microstructural evolution. Some processes are best simulated using one method (e.g. Finite Elements), while other processes require other simulation methods, and many processes can in fact be adequately simulated by a whole range of techniques. Chapter 2 therefore gives an overview of the main numerical methods that are or can be used. This chapter is intended for those readers with no previous knowledge of numerical simulation methods, or only a subset of them.

A range of microstructural processes is presented in Chap. 3, which is process oriented. The theory of how each process may potentially affect a microstructure is briefly described followed by an overview of the way in which the process has been simulated numerically.

Based on Chap. 3, Chap. 4 gives some examples of the application of numerical simulation to particular problems. This chapter emphasises the need to combine different concurrent processes to simulate what happens in nature. Many highly sophisticated programs have been written to simulate single processes. However, these processes rarely operate in isolation in nature, and one therefore needs to be able to also simulate the interaction between different processes.

Many programs have been developed to simulate microdynamic processes. However, few of these are publicly available as these programs are usually developed for specific research purposes and remain with the authors. There is currently only one general package, called ***Elle***[1] that bundles a variety of simulation software for microdynamic modelling in earth sciences.

Elle is open source software that is developed by an informal consortium of earth scientists, many of whom have contributed to this book. The main advantage of *Elle* is that it is actually a growing collection of codes for individual processes, which allows the user to combine multiple processes in a single simulation. Where possible, *Elle* software is used for the examples presented in this book. " EXPERIMENT" at the end of a figure legend indicates that the figure can be replicated by running one of the example scripts on the CD-ROM (Appendix B). Thus, with the attached CD-ROM, the reader can run the examples exactly as they are shown in the book. As a next step, the reader can start to modify input parameters or data files to learn both how the simulation works and how particular processes act on a microstructure. The Appendices provide all the information needed to run *Elle*.

The open source *Elle* software is constantly being developed by researchers from all over the world. The software on the CD-ROM is represents the state of the code at the time of printing of this book. The latest version of *Elle* can be found on http://www.microstructure.info/elle. This web site also provides answers to frequently asked questions, fixes to the inevitable bugs and other information material.

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[1] The *Elle* project started in the Department of Earth and Planetary Sciences of Monash University (Melbourne, Australia) during a series of weekly coffee-with-cakes meetings in the early nineties. The (over) ambitious idea was to develop a "super model" that would be able to model everything (metamorphism, deformation, the lot!). The "super model" was quickly baptised "Elle" after a then famous Australian super model by the name of "Elle". We are indebted to Marlina Elburg to have come up with such a superb, easy to remember, but otherwise meaningless name for the project and software.

Contents

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The development of the code has been the work of the editors and most of the authors in this book, but in particular of Lynn Evans and Jens Becker, without whose technical expertise, and patience, we would not be where we are today.

Over the past 10 years we have held training courses and developer workshops on the numerical simulations of microstructures in Aachen, Hürtgenwald and Mainz (Germany), Leeds (UK), Estremoz (Portugal), Miglos and Toulouse (France), Pisa (Italy), Särghaua (Estonia), Orono, Maine (USA), and Cadaqués (Spain) where the participants of these workshops acted as willing guinea pigs for various versions of the code, and have stimulated its further development.

P. England, K. Stüwe, P. Molnar and other colleagues and students have provided assistance and motivation in the development of the *Basil* software package.

We would also like to thank the proof readers and software testers of this book, Lenka Baratoux, Marlina Elburg, Enrique Gómez-Rivas, Anne Peschler, and Kristjan Urtson, who have considerably reduced the number of internal inconsistencies, mistakes and bugs.

Finally we would like to acknowledge the use of several Open Source and Public Domain codes within the *Elle* platform:

wxWidgets	http://www.wxwidgets.org
Lesstif	http://www.lesstif.org
gnu scientific library	http://www.gnu.org/software/gsl
triangle	http://www.cs.cmu.edu/~quake/triangle.html
Generic Polygon Clipper	http://www.cs.man.ac.uk/~toby/alan/software/gpc.html
Graphics Gems	http://www.acm.org/tog/GraphicsGems/