

DYNAMIC GRAIN BOUNDARY MIGRATION
AND FABRIC DEVELOPMENT:
OBSERVATIONS, EXPERIMENTS AND SIMULATIONS

by

Mark Walter Jessell

A Dissertation

Submitted to the State University of New York at Albany

in Partial Fulfillment of
the Requirements for the Degree of
Doctor of Philosophy

College of Sciences and Mathematics
Department of Geological Sciences

1986

ABSTRACT

In-situ observations of a deforming aggregate of the hexagonal material octachloropropane have been analysed. Calculations of micro-strains and measurement of c-axis orientations have enabled the processes influencing fabric development to be distinguished, and the importance of dynamic grain boundary migration to be assessed. It was found that in this material, inter-grain strain contrasts could be significant, and that the effect of grain boundary migration was to modify the fabric in a measurable way. A simple model for the driving force for grain boundary migration based on dislocation density contrasts, as controlled by intra-grain strains and grain orientations, is proposed and tested and can account for the migration direction of most of the observed boundaries.

Several grain-scale microstructures are described that demonstrate the migration direction of once-mobile grain boundaries in a naturally deformed quartzite. I present an analysis of the sense of migration of the boundaries and the characteristics of the patterns of relative grain growth and shrinkage. Grain boundary migration can be correlated with the relative crystallographic orientations of neighbouring grains.

A new computer simulation of the development of grain shape and crystallographic preferred orientations is presented. This model combines homogeneous strains,

simplified versions of the lattice rotations predicted by Taylor-Bishop-Hill theory, mobile grain boundaries and the nucleation of new grains, and allows the progressive development of the fabrics to be followed. The model generates several commonly measured quartz c-axis fabrics, while at the same time predicting characteristic variations in average grain sizes and the intensity of grain shape fabrics that arise from differing recrystallization regimes and strain geometries.

ACKNOWLEDGEMENTS

The topic of this thesis was proposed by Win Means, many of the ideas contained herein first saw the light of day during discussions with him, and I am happy to acknowledge his continuous support during this project. During his stay in Albany, and since that time, Janos Urai has encouraged me in my studies and taught me much. Brian Bayly has had a friendly and provocative influence on my thoughts. I would like to thank Janos Urai, Brian Bayly, Jan Tullis, Chris Wilson, Rob Knipe, Steve Delong, Greg Harper and Falk Koenemann for taking the time to read part or all of this work and to suggest improvements to frequently tangled thoughts. I would also like to thank Jan Tullis for her permission to use previously unpublished experimental data. The idea for using orthogonal strain grids was first suggested to me by Peter Cobbold. Tom Ray collected the sample analysed in Chapter 3, and provided me with a detailed account of the regional characteristics of the Ottauquechee Quartzite. Mike Ramundo provided useful advice on the computer graphics used in this thesis. My time spent at the university has been enjoyably spent thanks to all of the members of the department, and especially Chris Steinhardt, Mauricio Roma, Thomas Will, Katherine Stone, Peter Hofmann, Matthias Ohr, Suzanne Baldwin and Antonio Teixell. Diane Paton helped ensure that my progress was smooth. Life in Albany would not have been the same without Patrice,

Hitomi, Chris, Maria, Sue, Ute, Foffi, Ricardo, Metta, Dave, Seth, Tom and Pam. This work was funded by a Presidential Fellowship from the State University of New York at Albany, and by National Science Foundation grants EAR820582001 and EAR8306166. Without the support of my parents and family I would never have got this far this happily. My final thanks go to Linda Bouzida, for everything.

TABLE OF CONTENTS

ABSTRACT

ACKNOWLEDGEMENTS

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1	INTRODUCTION	1
2	EXPERIMENTAL DEFORMATION OF OCTACHLOROPROPANE	4
2.1	INTRODUCTION	4
2.2	EXPERIMENTAL TECHNIQUE	5
2.3	ANALYSIS OF EXPERIMENTS	6
2.3.1	EXPERIMENT TO-47	6
2.3.2	EXPERIMENT TO-55	17
2.3.3	EXPERIMENT TO-58	20
2.3.4	EXPERIMENT TO-63	26
2.3.5	EXPERIMENTS TO-64 AND TO-65	50
2.3.5.1	OBERVATIONS AND ANALYSIS	50
2.3.5.2	GRAIN BOUNDARY KINEMATICS	61
2.3.5.3	MODEL TEST	68
2.3.6	EXPERIMENT TO-69	75
2.3.7	EXPERIMENT TO-77	78
2.4	DISCUSSION	86
2.5	CONCLUSIONS	90

3	GRAIN BOUNDARY MICROSTRUCTURES IN A NATURALLY DEFORMED QUARTZITE	91
3.1	INTRODUCTION	91
3.2	SAMPLE DESCRIPTION	92
3.3	GRAIN BOUNDARY MIGRATION MICROSTRUCTURES	97
3.4	ANALYSIS	112
3.5	DISCUSSION	120
3.6	CONCLUSIONS	122
4	A SIMULATION OF FABRIC DEVELOPMENT IN RECRYSTALLIZING AGGREGATES: DESCRIPTION OF THE MODEL	123
4.1	INTRODUCTION	123
4.2	DESCRIPTION OF THE MODEL	124
4.2.1	FABRIC INITIALIZATION	127
4.2.2	STRAIN INCREMENT	127
4.2.3	LATTICE REORIENTATIONS	136
4.2.4	RECRYSTALLIZATION	142
4.2.5	INTERACTION WITH MODEL	154
4.3	DISCUSSION	154
5	A SIMULATION OF FABRIC DEVELOPMENT IN RECRYSTALLIZING AGGREGATES: EXAMPLE MODEL RUNS	161
5.1	INTRODUCTION	161
5.2	EXAMPLE MODEL RUNS	161
5.2.1	RUN NUMBER 1	161

5.2.2	RUN NUMBER 2	171
5.2.3	RUN NUMBER 3	177
5.2.4	RUN NUMBER 4	185
5.2.5	RUN NUMBER 5	189
5.3	DISCUSSION	195
5.4	CONCLUSIONS	210
6	ASPECTS OF DYNAMIC GRAIN BOUNDARY MIGRATION	212
6.1	INTRODUCTION	212
6.2	DYNAMIC GRAIN BOUNDARY MIGRATION	212
6.3	ORIENTATION EFFECTS ON STORED ENERGY	214
6.3.1	MULTIPLICITY OF ACTIVE SLIP SYSTEMS	216
6.3.2	TOTAL SHEAR ON SLIP SYSTEMS	216
6.3.3	DIFFERENTIAL RECOVERY	218
6.3.4	REORIENTATION EFFECTS	218
6.3.5	STRESS RAISERS	219
6.4	THE EFFECT OF GRAIN SIZE ON FABRIC DEVELOPMENT	220
6.5	DISCUSSION	221
	REFERENCES	223
	APPENDIX A: THE CHEMICAL, PHYSICAL AND MECHANICAL PROPERTIES OF OCTACHLOROPROPANE	240
	APPENDIX B: DERIVATION OF STORED ENERGY FUNCTION	258

APPENDIX C: FORTRAN PROGRAM TO SIMULATE

FABRIC DEVELOPMENT IN SIMPLE SHEAR 262

LIST OF FIGURES

2.1	Hajeck apparatus	7
2.2	Geometry of deformation	8
2.3	Photographic record of experiment TO-47	12
2.4	Near single crystal fabric	15
2.5	Hypotheses to explain the widening of the high strain rate zone	16
2.6	Experiment TO-55	19
2.7	Information used to calculate local deformation matrices	21
2.8	Finite strain maps for experiment TO-58	25
2.9	Incremental strain maps for experiment TO-58	28
2.10	Photographic record of experiment TO-63	31
2.11	Frequency histogram of grain boundary orientations	36
2.12	c-axis reorientation trajectories	38
2.13	Comparison of OCP c-axis trajectories with predictions	41
2.14	c-axis fabric diagrams for each stage of the deformation	44
2.15	Theoretical c-axis fabric diagrams	48
2.16	Average grain size versus shear strain	49
2.17	Photographic record of experiment TO-64	52
2.18	Photographic record of experiment TO-65	54
2.19	Strain map for experiment TO-64	56
2.20	Strain maps for experiment TO-65	58

2.21	Model of grain boundary kinematics	64
2.22	Variation in copper of stored energy deformation with orientation	66
2.23	Grain boundary migration map for TO-64	69
2.24	Grain boundary migration map for TO-65	70
2.25	Comparison between predicted stored energy contrasts and grain boundary motions for TO-64 and TO-65	74
2.26	Photographic record of experiment TO-69	77
2.27	Photographic record of experiment TO-77	81
2.28	Strain map for experiment TO-77	83
2.29	Grain boundary migration map for TO-77	85
2.30	Comparison between predicted stored energy contrasts and grain boundary motions for TO-77	87
3.1	Photo-micrographs of quartzite	94
3.2	c-axes orientations of specimen as a whole	96
3.3	Pinning microstructure	100
3.4	Window microstructure	103
3.5	Dragging microstructure	106
3.6	Left over grains	108
3.7	Castellate microstructure	111
3.8	Zoning of calcium across olivine grain boundaries	113
3.9	Dislocation lines formed behind migrating olivine boundaries	114
3.10	c-axis orientations of growing and shrinking grains	116

3.11	The ratio $G/G+S$ for 36 equal orientation segments	119
4.1	Triangular arrangement of points in array	125
4.2	Flow chart of simulation	126
4.3	Results of strain algorithms	129
4.4	Principal of simple shearing strain algorithm	132
4.5	Principal of axisymmetric flattening strain algorithm	135
4.6	Lattice rotations used in model	139
4.5	Comparison of the c-axis fabrics that develop using Taylor-Bishop-Hill and this model with no recrystallization	141
4.7	The distributions of stored energy of deformation assumed in this model	145
4.9	Grain boundary migration algorithm	148
4.10	Nucleation algorithm	153
5.1	Grain boundary maps/c-axis projections for Run 1	164
5.2	Evolution of average grain areas with deformation	168
5.3	Grain boundary maps/c-axis projections for Run 2	173
5.4	Grain boundary maps/c-axis projections for Run 3	180
5.5	Histogram of grain elongation orientations for $\epsilon = 3.61$, Run 3	184
5.6	Grain boundary maps/c-axis projections for Run 4	187
5.7	Grain boundary maps/c-axis projections for Run 5	192
5.8	Natural example of double c-axis maximum	197
5.9	Natural example of Y maximum	198

LIST OF TABLES

2.1	Experimental conditions	9
2.2	Data derived from experiments TO-64 and TO-65	72
4.1	Range of variables used in simulations	155
5.1	Values of variables used in example runs	162

If you can look into the seeds
of time, and say which grain
will grow and which will not,
speak then to me.

Shakespeare

(Macbeth I iii)