Appendix B

Values used for simulations

In simulations a certain set of parameters were kept constant. These values were chosen in accordance to values provided from the literature. If no such values existed values where chosen to fit the general proposed relationship between different values. Values were primarily chosen to fit dynamic recrystallization at low to medium grade conditions (T = 450°, P = 3 kbar) and deformation of wet quartz (*Fluid_Factor* = 1). At the same time, the calculation time for one individual experiment had to be reasonable (below 5 days). Used values are given in Tab. B2.

The modelled type of deformation with BASIL was deformation with pistons at the upper and lower limit of the unit cell and plane strain, dextral simple shear (W_n = 1) with a displacement Δs in the x direction of 0.025 per time step (Fig. B1). This results in a strain increment $\Delta \gamma$ of 0.05. This value was chosen to ensure a balance between process discretization and computational calculation time. Perfect bonding between polygons, hence no slip along grains is assumed. To assure reasonable results the accuracy of output of the deformation program basil was regularly checked using the value display program SYBIL. The general flow behaviour of the simulated material was chosen to be Newtonian viscous. The commonly cited non-linear viscous behaviour of rocks (e.g. Carter, 1976; Schmid, 1976; Urai, 1983; Stöckert et al., 1999) is to some extent already modelled separately within the crystallographic lattice rotation routine (section A3.2). In this routine, the increase of the dislocation density with stress is already taken into account. It is therefore reasonable to allocate an n value of 1 for the general deformation of the material used in the viscous deformation routine BASIL.
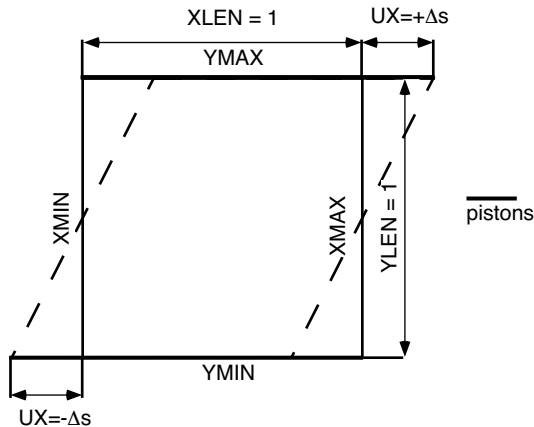

Figure B1 *Illustration of simple shear deformation and the parameters specified in BASIL.*

Values for *SwitchDistance* (=0.00625), *MinNodeSep* (=0.00625), *MaxNodeSep* (=0.03175), *MinAngle* (=9˚) (Tab. B2) which affect the resolution of the mesh were chosen to result in a balance of a resolution as high as possible while keeping computational calculation sufficiently short.

To scale the values of the model to real world values several scaling factors had to be specified. The time scaling factor (t_{scale} = 3.1536e^{10} s) and the chosen strain per time step ($\Delta \gamma$ = 0.05; see above) result in a strain rate of 1.6 • 10^{-12} s^{-1}. This is in accordance to strain rates of 10^{-10} s^{-1} and 10^{-15} s^{-1} which are suggested for midcrustal rocks (e.g. Pfiffner and Ramsay, 1982; Carter and Tsenn, 1987; Prior et al., 1990; Stöckert et al., 1999). The stress scaling factor was chosen to assure a reasonable viscosity range for the simulated rock (quartzite) which is between 3.15 • 10^{18} Pa s and 6.3 • 10^{18} Pa s. This value corresponds to the range of proposed

kinematic viscosity values for mid-crustal rocks 10^{16} Pa s to 10^{21} Pa s (Kirby, 1983; Carter and Tsenn, 1987; Evans and Kohlstedt, 1995; Clark and Royden, 2000). The length scaling factor l_{scale} is 10^{-3} and ensured the representation of fabric in the dimensions of a normal thin section (1 cm by 1 cm). The dislocation density factor ρ_{scale} (=10^{12}) is chosen to result in a modelled dislocation density ranges between $1 \bullet 10^{10}$ m^{-2} and $1 \bullet 10^{13}$ m^{-2} corresponding to dislocation densities observed in undeformed and deformed rocks and metals (e.g. Hacker and Kirby, 1993; Gottstein and Shvindlermann, 1999; Stöckert et al., 1999). The lowest dislocation density value is corresponds to $\rho'_{nucl} = 0.01$.

The used critical resolved stress values (CRSS) which are used in ELLE_TBH are given for each slip system in Tab. B1. These values correspond to data for greenschist to lower amphibolite facies conditions provided by Hobbs (1985) and Jessell and Lister (1990). Constants a and b (Eq. A3) are 0.4 and 0.7, respectively.

The value for energy of dislocations ρ_{energy} ($7 \infty 10^{-9}$ J/m^2) was chosen according to the range given by Hacker and Kirby (1993) and Gottstein and Shvindlermann (1999) (used in ELLE_SPLIT, ELLE_NUCLXX, ELLE_GBM).

Table 1 *Critical Resolved Shear Strass*

Slip number	Slip system	CRSS
1	BASAL a	5.00
2	PRISM c	11.00
3	PRISM a	6.00
4	PRISM c+a	$1e^{10}$
5	PRISM -c-a	$1e^{10}$
6	(2-1-1- 1) c+a2	9.50
7	(2-1-1- 1) c+a3	9.50
8	(2-1-1- 1) -c-a2	9.50
9	(2-1-1- 1) -c-a2	9.50
10	RHOMB a	15.00
11	RHOMB —a	15.00
12	RHOMB c+a	$1e^{10}$
13	RHOMB -c-a	$1e^{10}$

The orientation vector O of the subgrain boundaries (used in ELLE_SPLIT) was chosen to be crystallographically determined. It is chosen in such a way that "Splitting" occurs preferably parallel or perpendicular to the c-axis. This corresponds to observations of Lloyd et al. (1992) and Stöckert et al. (1999). The energy thershold value above which a grain has a probability to split Th_{split} is $2.4 \bullet 10^5$ J/m^2. The area of newly created subgrains was between $3.12 \bullet 10^{-4}$ mm^2 (*MinArea*) and $1.25 \bullet 10^{-3}$ mm^2 (*MaxArea*) which is in the range of observed recrystallization grain sizes for quartz (e.g. Twiss, 1977; White, 1979a; Christie et al., 1980; Kronenberg and Tullis, 1984).

Constants c used in ELLE_NUCLXX (Eq. A7) is 1000.

The *MisorientAngle* used in ELLE_ROTXX, SHOWELLE; ELLE_STATS was set to be 10° according to values given for quartz (e.g. White, 1977; Lloyd et al., 1992; Trimby et al., 1998).

The threshold value for recrystallization by nucleation (RX_{nucl}) is $4.8 \cdot 10^5$ Jm^{-2}. This value was chosen to be in the general range of the proposed driving force magnitude for nucleation of new grains of Gottstein and Svindlerman (1999; p. 343).

In ELLE_GBM the fraction *d* of *SwitchDistance* used to calculated D_{trial} is 0.01. The chosen value for surface energy Γ is $7 \cdot 10^{-2}$ J/m^2. This value is in accordance to the value range proposed ($0.01 - 1$ J/m^2) for surface energy in rocks and metals (Urai et al. 1986 and references therein; Hacker and Kirby, 1993; Gottstein and Shvindlermann, 1999; Stoeckert & Dyster, 2000). The influence of the crystallographic c-axis misorientation angle $\prod$ between adjacent grain or subgrains is chosen so that the crystallographic factor (*xx_factor*) is 0 at a c-axis misorientation angle of 0°, 0.1 at a misorientation of 10° and 0.99 at 20°, which corresponds to the general relationships observed in metals (Fig. A13). A_α is always 1; hence the surface energy is assumed to be isotropic with respect to the orientation of the boundary relative to the lattices of the crystals. The mobility is assumed to be isotropic, i.e. is it is not lattice orientation controlled. An isotropic nature of the grain boundary mobility is justified if the mobility is controlled by the transport rate across the boundary layer. In wet mineral aggregates this seems to be the case (Tullis and Yund, 1982; Bons et al., in press) and therefore this assumption is in accordance to the wet quartz model (*Fluid_Factor* = 1) in simulations. The grain boundary mobility (*GBMob*) is $1 \cdot 10^{-12}$ m^{2}s^{-1}J^{-1}; this value was chosen so that the resultant grain boundary migration rates are in the same order of magnitude range as those derived by Prior et al. (1990) for dynamic recrystallization of a quartz band in a low to medium grade pelite; given values are $1.2 \cdot 10^{-9}$ µms^{-1} and $1.2 \cdot 10^{-11}$ µms^{-1}. Constant *d* (Eq. A10) is 0.01 so that no computational and geometric problems arise.

Constants *e* and *f* used in ELLE_RECOVERY (Eq. A28) are 0.97 and 1000, respectively. RF_{base} is 0.95.

The base viscosity η_{base} used in ELLE_VISCOSITY is 1.

At the beginning of experiments the following Elle attribute values were pre-defined for all polygons: dislocation density = 0, viscosity = 1 and random Euler angles.

One parameter was varied in simulations this is the initial fabric (R_Φ): a coarse grained and fine grained monomineralic microstructure. A initially "coarse grained" microstructure has a mean ratio of initial grain size to numerical mean subgrain grain size R_Φ of 48 and the initially "fine grained" microstructure a R_Φ of 2.2.

Tab. 2 *Values used*

description and symbol	value	unit	literature
temperature T	450	°C	-
pressure P	3	kbar	-
Fluid_Factor	1	-	-
type of deformation W_n	1		-
flow behavior of material	Newtonian viscous		
displacement per time step Δs	0.025	-	-
strain per time step $\Delta\gamma$	0.05	-	-
strain rate	$1.6 \cdot 10^{-12}$	s^{-1}	Prior et al, 1990; Pfiffner & Ramsay, 1982
finite strain γ	2	-	-
sense of shear	dextral	-	-
SwitchDistance	$0.00625 \cdot 10^{-3}$	m^2	-
MinNodeSep	$0.00625 \cdot 10^{-3}$	m^2	-
MaxNodeSep	$0.03175 \cdot 10^{-3}$	m^2	-
MinAngle	9	°	
time scaling factor t_{scale}	$3.1536e^{10}$ (1000a)	s	-
length scaling factor l_{scale}	10^{-3}	m	-
dislocation density scaling factor ρ_{scale}	10^{13}	m^{-2}	Gottstein & Shvindlermann, 1999; Hacker & Kirby, 1993
stress scaling factor t_{scale}	10^8	Pa	-
dislocation density of new recrystallized grain ρ'_{nucl}	0.001	m^{-2}	
constant *a*	0.7	-	-
constant *b*	0.4	-	-
dislocation energy ρ_{energy}	$7 \cdot 10^{-9}$	Jm^{-2}	Hacker & Kirby, 1993
given vector for splitting direction *O*	parallel & perpendicular to c-axis	mm^2	Lloyd et al., 1992; Stöckert et al., 1999
SplitThreshold Th_{split}	$2.4 \cdot 10^5$	J/m^2	Gottstein & Shvindlermann, 1999
MinArea	$3.12 \cdot 10^{-4}$	mm^2	Twiss, 1977
MaxArea	$1.25 \cdot 10^{-3}$	mm^2	Twiss, 1977
constant *c*	1000	-	-
MisorientAngle	10	°	White, 1977; Lloyd et al. 1992; Stöckert et al., 1999
surface energy Γ	$7 \cdot 10^{-2}$	Jm^{-2}	Gottstein & Shvindlermann, 1999; Urai et al., 1986; Dyster & Stöckert, 2000
constant *d*	0.01	-	-
Boltzmann constant B	$1.3806503e10^{-23}$	JK^{-1}	-
activation energy H	$1.3806503e10^{-23}$	JK^{-1}	-
grain boundary activation energy QGBM	$1.3806503e10^{-23}$	$Jmol^{-}$	-
Recovery_factor RF_{base}	0.95	-	
constant *e*	0.97	-	-
constant *f*	1000	-	-
Base_viscosity η_{base}	$3.15 \cdot 10^{18}$	Pa s	Clark and Royden, 2000