MR23B-1327 The geometry of random mixing: quantifying spatial distributions

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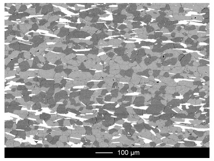
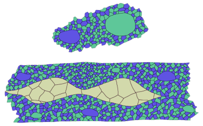
DEFORMATION MECHANISMS

Different deformation mechanisms may develop different phase distributions which may be use to identify or characterize the operating dominant mechanism. Phase distributions may also potentially be used to quantify deformation processes in cataclasites.

There are a number of deformation mechanisms that involve mixing of particles of different phases. For example, in cataclastic flow, particles are fragmented and displaced past each other, in diffusion creep, grains of one phase nucleate and grow between grains of other phases.



Example from a mylonite in the Truzzo granite (Swiss Alps), naturally deformed at ca. 500°C.



Schematic drawing of different phase distributions in diffusion and dislocation creep

diffusion creep

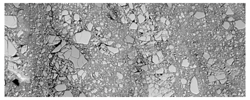
Grains of one phase nucleate and grow between grains of other phase(s).

Small grains derived from larger parent grains by nucleation usually form phase mixtures during diffusion creep while dynamically recrystallized grains during dislocation creep form clusters.

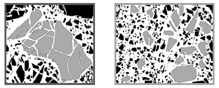
cataclastic flow

Particles are fragmented and displaced relative to each other during cataclastic flow.

Phase separation and mixing occurs during cataclastic flow. The degree of mixing may increase with progressively larger displacement but there is no data to quantify this process.



Cracked grains occur in low strain domains of an experimentally deformed granitoid sample. T = 300°C, confining P = 500 MPa, e = 10^{-4} sec^{-1}



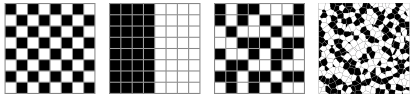
Displaced fragments occur in a mixed phase aggregate in large displacement cataclasite domains. Natural example from the Orobic Thrust (Italian Alps)

patterns

The resulting mixtures may form "random", "clustered" or "anticlustered" patterns. To derive the nature of the underlying process and to identify the active deformation mechanisms, it is necessary to find reliable descriptors by which random and non-random spatial distributions can be quantified and distinguished from one another.

MODELS FOR GEOMETRY

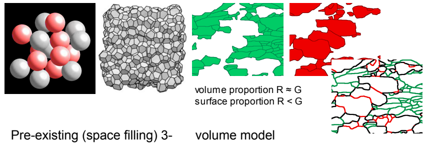
2-D chess / voronoi



Pre-existing 2-D chess board or Voronoi polygons. Phases (black or white) are assigned (ex post) via random numbering.

The probability for a field of the chess board or the Voronoi tesselation to be A or B can vary from 0 to 1.
pA + pB = 1

3-D volume / surface



Pre-existing (space filling) 3-D aggregates of polyhedra. Phases (black or white, A or B) are assigned (ex post) via random numbering.

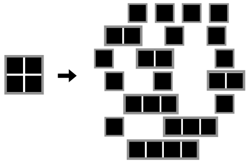
2-D sections are evaluated. The probability for a cross sectional area to be A or B can vary from 0 to 1.
pA + pB = 1

volume model
Constant grain size is assumed.
⇒ probability for a neighbour of phase A depends on volume proportion of A.

surface model
No assumption about grain size.
=> probability for a neighbour of phase A depends on surface proportion of A.

integer sums (= fragmenting clusters)

4 = 1 + 1 + 1 + 1
4 = 2 + 1 + 1
4 = 1 + 2 + 1
4 = 1 + 1 + 2
4 = 3 + 1
4 = 1 + 3
4 = 4



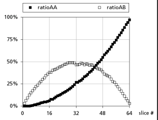
A pre-existing cluster of N grains is divided into 1 to N (sub-)clusters, consiting of N to 1 grains respectively. The probability for the number of clusters and their size distributions is calculated.

Only one phase (A) in matrix (B) considered.
A highly diluted situation is envisaged; clusters do not touch each other.

DERIVED MEASUREMENTS

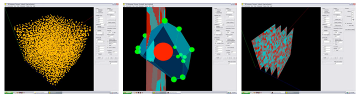
Binomial distribution

For all models, the phase boundaries AB (between A and B) and grain boundaries AA and BB are calculated.

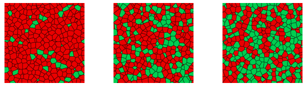


For the random chess boards, the binomial distribution is realized

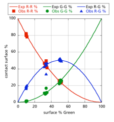
3-D - 2-D voronoi



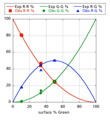
software by
Hugo Ledoux



area proportions = volume proportions:
10:90, 33:66, 50:50



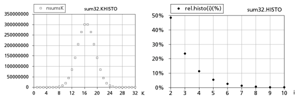
~380 grains



~1500 grains

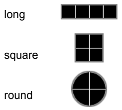
For the sections of the random 3-D Voronois, the relative amounts of grain contacts (AA, BB and AB) follow a binomial distribution.
Because of constant average grain size, the volume proportions and the surface proportions of both phases are identical.

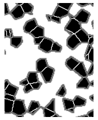
allsums



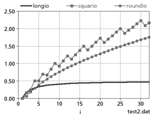
number of (sub-)clusters and size of (sub-)clusters for starting cluster size of 32

A more general model for random distribution considers only one phase (A) and two types of grain contacts (AA and AB, where B is the "matrix"). This model is based on fragmenting a cluster of phase a into smaller clusters. It predicts the most probable distribution of cluster sizes and the probability for contact types AA and AB.





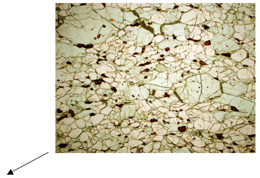
general shape

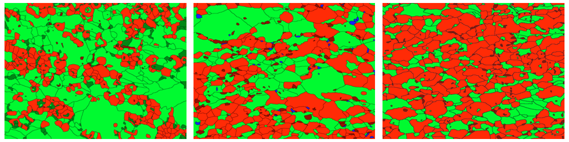


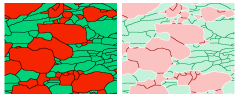
ratio of grain boundary to phase boundary for three types of clusters: long, square, round

EXAMPLE

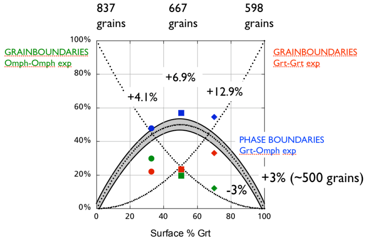
As an example of a non-random distribution of grains we studied the eclogites of the Troms Nappe (Caledonides, Norway). Previous studies indicate that the dominant deformation mechanism is diffusion creep, a process known to create anticlustered distributions of mineral grains. In the course of field observations we collected a large dataset of random and non-random 2-D geometries and compared it to results from 3-D numerical modelling.



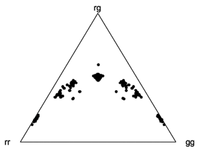




Grt = red
Omph = green
Phase boundary = white
Grt grain boundary = dark red
Omph grain boundaray = dark green



Because of the different grains sizes of omphacite and garnet, the eclogites were evaluated using the surface model. It can be shown that their microstructures deviate from spatial random distributions showing various degrees of anticlustering and in many cases, the degree of anticlustering depends on direction, being stronger in the direction of the stretching lineation than in direction of the foliation normal. From this we infer that diffusion creep occurred by solution-precipitation processes and heterogeneous nucleation.



Simplex plot of rr gg and rg bpoundaries obtained from 3-D numerical simulations

Since AA, BB and AB always add up to 100%, the error has to be calculated as in compositional data. This, however, is work in progress.