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Simulating crystalline microstructures – an aid in quantifying the spatial distribution of phases in two-phase crystalline rocks

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A convenient way of quantifying the spatial distribution of major rock constituents in 2-D sections compares observed grain and phase boundary fractions with those expected if the grains of each phase were randomly distributed in the given volume (Kretz, 1969). In a two-phase mixture the expected values are calculated from the volume fractions of phases A and B (a and b, respectively) by $a^2 + 2ab + b^2 = 1$, where a^2 gives the proportion of A-A grain boundaries, 2ab the proportion of A-B phase boundaries and b^2 the proportion of B-B grain boundaries. A significant difference between observed and expected values indicates a departure from randomness toward either a clustered (higher proportion of grain boundaries) or anticlustered (higher proportion of phase boundaries) distribution of phases.

As part of a study of deformation microstructures and mechanisms in eclogites and amphibolites we performed a number of phase distribution analyses on naturally deformed two-phase rock samples. The outcome of these analyses suggests that the distribution of phases in our samples is not random but anticlustered, i.e. there appears to be a higher proportion of phase boundaries than expected for a random distribution. Anticlustered distributions may be typical products of diffusion creep deformation. The observed differences from the expected percentage of phase boundaries in our samples (with volume per cent ratios of 32:68, 50:50 and 70:30) range from +1 to +8 %. Do these values constitute a *significant* departure from randomness?

In this contribution we attempt to answer this question by analysing sections through computer-generated 3-D crystalline microstructures in which two phases with varying volume fractions are randomly distributed. The microstructures are composed of 5000 Voronoi polyhedra with anticlustered centre points in order to obtain a narrow grain

size distribution. A number of three-dimensional simulations have been carried out for three different volume and grain surface area ratios (10:90, 33:66 and 50:50) of the two phases. Four parallel sections (each containing c. 380 grains) through each 3-D simulation have been analysed both individually and combined (so as to give a larger, c. 1520-grain sample).

The first results of our analyses confirm that: (i) The observed boundary fractions for random distributions lie on or very close to the theoretical values given by the terms a^2, $b^2$and 2ab. (ii) Departures from the theoretical values depend on the sample size. For 380-grain analyses these deviations range between 2 and 3 %; for 1520-grain analyses the differences are $< 1\%$. We tentatively conclude therefore that differences greater than these values constitute significant departures from randomness towards either clustering or anticlustering.

Reference

Kretz, R., 1969. On the distribution of crystals in rocks, Lithos, 2, 39-66