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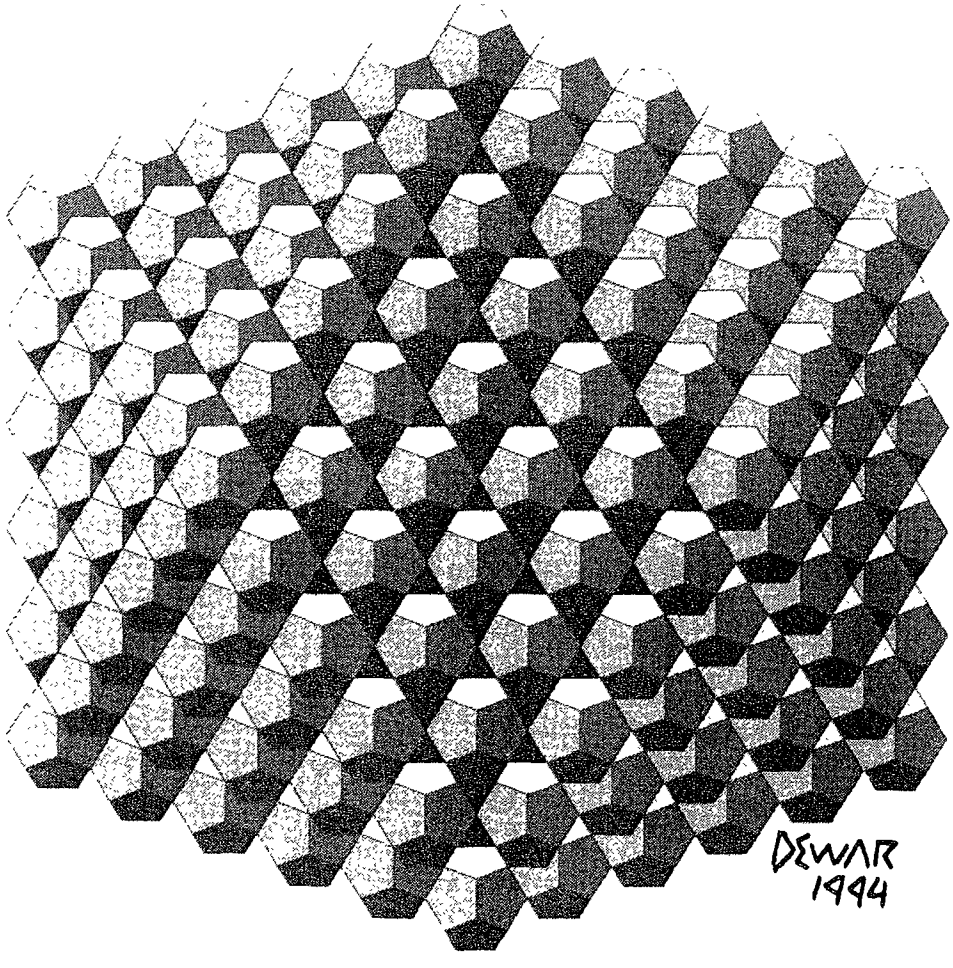

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SUTURED GRAIN BOUNDARIES: THEIR FRACTAL SHAPE, FORMATION AND BEAUTY

Jörn H. Kruhl

Geologisch-Paläontologisches Institut, JW Goethe-Universität, D-60054 Frankfurt/M., Germany

Under special circumstances, crystals of the same composition and structure develop complex interfingering along their common boundaries. These sutures are formed because atoms or groups of atoms migrate across the boundaries In this way a dynamic equilibrium arises which is related to different parameters. Probably, temperature is the most important one. Already on the atomic scale, boundaries may form steps which are controlled by the relative distortion of the neighbouring crystal structures (Fig.1). These steps also occur on a larger scale and build up a strong interfingering of the crystals. The number, size and shape of the fingers (sutures) are related to the temperature. This relationship together with the beauty of grain boundary sutures and their use for material studies shall be demonstrated with the mineral quartz as an example.

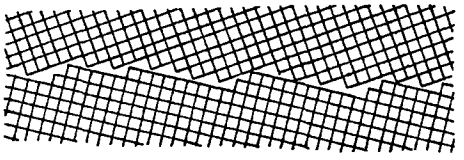

Fig.1:
Simplified 2-D model of a grain boundary along which two neighbouring crystal structures form steps against each other. The intersection points of the grids represent atoms or specific groups of atoms.

At "low" temperatures (300-350°C for quartz) only very short straight grain-boundary segments are developed, which add up to strongly sutured boundaries (Fig.2A). At "higher" temperatures (e.g. 500-550°C) the length of the straight segments increases. Consequently, the shapes of the boundaries appear angular (Fig.2B). Finally, at "high" temperatures (e g 600-700°C), the shapes of the boundaries are dominated by a few long and straight segments (Fig.2C).

It can be shown that these sutured grain boundaries are self-similar over several orders of magnitude, i e. show the same appearance at different scales (Kruhl et al. 1995). As a consequence, the boundaries can be replaced by polygons of different step-length, which follow the power law $L = r^{1-D}$, where L is the total length of the polygon, r the step length and D the fractal dimension of the grain boundary (Fig.3). D represents a measure of the strength of

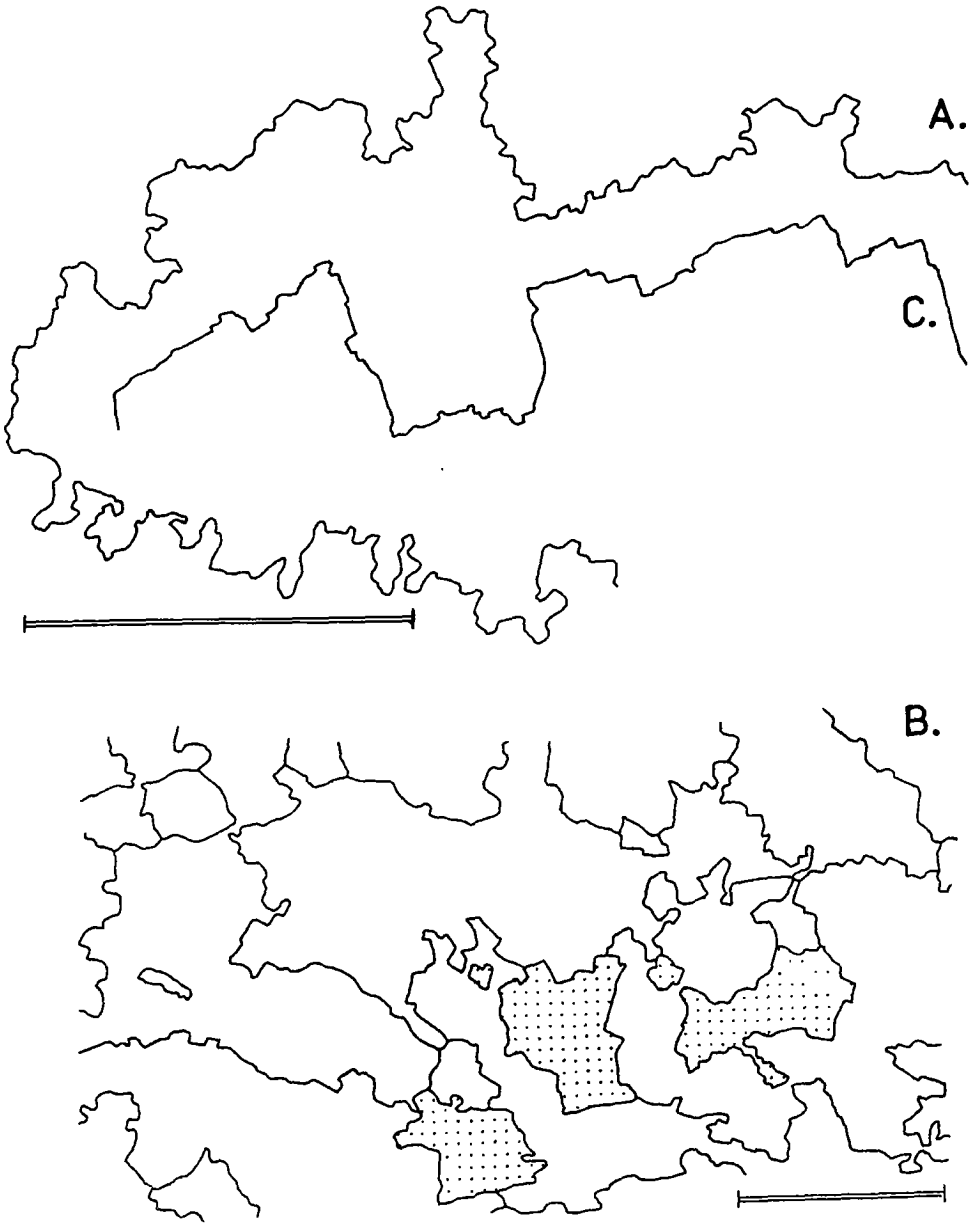

Fig.2: 2-D boundary patterns of quartz grains, which have been formed at various temperatures The length of the double bars is approx. 0.5 mm **A.** approx. 350°C; **B.** 500-550°C, **C.** 600-700°C. The dotted areas in sketch B represent one grain, different large sutures of which are cut by the drawing plane.

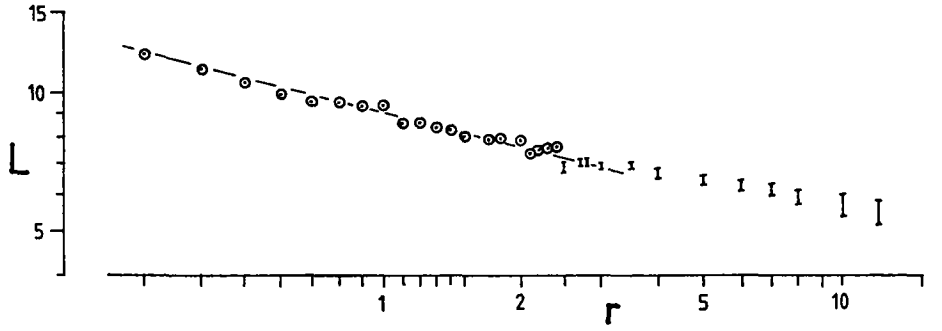

Fig.3: Polygon representation of the quartz grain boundary from Fig. 2A. In a double logarithmic diagram the total length L of each polygon is plotted versus the step length r. At high r-values the range of L-values point to the statistical uncertainty of the data. The fractal dimension D of the grain boundary is 1 minus the slope of the linear L/r relationship. D = 1.25 The "steps" within the linear relationship reflect different suture sizes of the boundary.

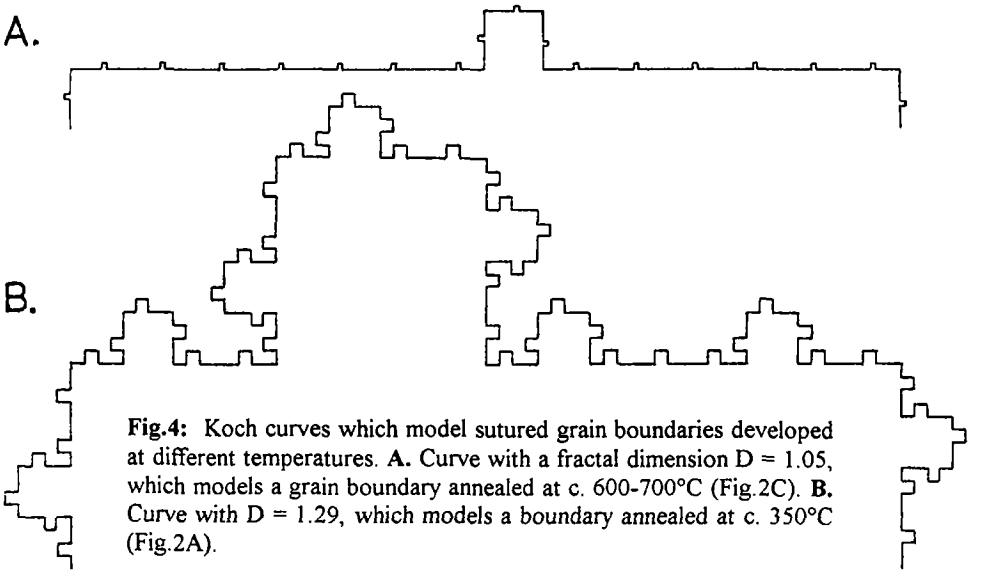

Fig.4: Koch curves which model sutured grain boundaries developed at different temperatures. **A.** Curve with a fractal dimension D = 1.05, which models a grain boundary annealed at c. 600-700°C (Fig.2C). **B.** Curve with D = 1.29, which models a boundary annealed at c. 350°C (Fig.2A).

interfingering. From a mathematical viewpoint, the sutured boundaries are Koch curves (Mandelbrot 1983) varied by a random process. Each sutured boundary with a specific fractal dimension D has a Koch-curve pendant with the same D-value (Fig.4). These Koch curves show that a high D-value is related to a strong and a low D-value to a weak interfingering. A weak interfingering means: Relatively few long boundary sutures are combined with relatively many short sutures. Consequently, the D-value is near 1, the Euclidian dimension of a line.

From a physical viewpoint, boundaries with a low D-value consist of long segments parallel to a low-index crystallographic plane, i e. a plane with a relatively dense packing of atoms and with strong binding forces At high temperatures the motion of the atoms in the crystal structure is strong and it is relatively easier to hold atoms in low-index crystallographic planes of strong binding forces than in high-index crystallographic planes of weak binding forces Therefore, long straight segments parallel to low-index planes are preferentially developed. In quartz, annealed at high temperatures, long straight boundary segments parallel to the rhombohedral planes are most common.

The development of sutured grain boundaries can be simulated in a quite simple way by allowing pixels on a screen to "jump" from one side of a boundary to the other side. The jumps are initiated by a controlled random process. Such simulations may help to understand the influence of temperature, but also of other parameters, on the development of grain boundaries First results of simulations show that a purely random-driven diffusion of atoms across a boundary destabilizes this boundary and leads to sutures of various complexity The interfingering of the boundary does not only create patterns of complex symmetry and esthetic charm but may also change the physical behaviour of the material. E.g. stronger interfingering leads to a higher strength of the material. On the other hand, complex boundary sutures hinder the migration of fluids. In general, a better understanding of the development of grain-boundary interfingering might also increase the possibilities to influence the physical properties of a material.

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