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Statistical ensemble approach to measure the motion of crystal particles in viscous flow

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Magma often contains elongated crystals, which are embedded in its viscous flow. In solidified magma bodies, one of the principal features observed in the field is the coherent arrangement of crystals or a net polarization of their orientations in that segment. These arrangements are often observed as parallel to the dike or perpendicular to the sill or even at a very low angle to the edge of the inclined sheet. Such a structural arrangement is usually interpreted as the result of magma flow, which caused the crystals to rotate and align within direction of the flow. It was observed during experiments that while crystals rotate continually in a Couette-type shear flow, their major axis has a high probability and their minor axis has low probability to be aligned parallel to the flow direction.
In this study, we present a new method of numerically modelling crystal rotation in different flow regimes. Having a large number of small crystals in complex flows can make the problem very expensive or even impossible computationally. However, in general we are not interested in observing individual crystals, but instead we would like to know the distribution of crystal orientations as a function of time and three dimensional space. We therefore introduce the concept of a statistical ensemble and describe the crystal orientation by a probability density function P(θ) which varies in space and time. The evolution of P(θ) depends on the rotation rate of individual crystals. For elliptical crystals in a flow of constant viscosity, exact analytical solutions are known (Jeffery, 1922). For other shapes, we use numerical models of a single crystal in a pure shear flow to find the corresponding rotation rates.

Using our model we illustrate results with an “ideal” crystal (with infinite aspect ratio) and realistic crystal shapes. In a pure shear flow, we find that all elongate crystals eventually rotate into the same orientation, leading to a sharp peak in P(θ). In a Couette flow, we find that only the “ideal” crystals rotate into a direction parallel to the flow and remain in this orientation. All realistic crystals instead continue rotating indefinitely. However, the rotation is slower when the orientation is nearly flow-parallel, so that the crystals spend relatively more time in this orientation and the function P(θ) exhibits a corresponding diffuse peak. Interestingly, however, this peak in P(θ) is not permanent, but oscillates in time between a high amplitude peak and a perfectly flat P(θ). Additionally, we show results from other simple flow fields.