## DIFFUSION MODELLING AS A TOOL FOR TRACKING TIMESCALES: POTENTIAL AND PROBLEMS

## CHAKRABORTY, S.

## Institut für Geologie, Mineralogie und Geophysik, Ruhr Universität Bochum, D-44780 Bochum, Germany e-mail: Sumit.Chakraborty@rub.de

Modelling frozen concentration gradients (or lack thereof) produced by diffusion is a powerful tool for understanding the rates and timescales of a wide range of geological processes. The method has a number of features that make it particularly attractive:

(i) it relies on a kinetic process that is governed by a well defined quantitative relation - the diffusion equation, (ii) it directly yields duration of processes rather than dates that must be combined to yield durations or rates, (iii) it relates timescales directly to the chemical reactions that are used to determine pressure, temperature and other intensive parameters (e.g.  $fO_2$ ), (iv) it accesses a wide range of timescales from hours to millions of years, (v) the temporal resolution of the method is independent of the age of the rocks, (vi) it depends on a process that is widespread, (vii) the tool can be applied on different minerals and elements on the same thin section, so that an internal consistency check is possible, and (viii) the tool can be applied to different specimens from the same sample or suit of rocks, so that it is possible to test the statistical significance of results with relatively modest investments of time and money

The last two features make the tool particularly versatile because it is possible to use the results of modelling some concentration gradients to predict the concentration distribution of other elements. The results can be used to falsify or vindicate the hypothesized model. A mismatch with observations immediately points to a flaw in some aspect of the model - in identifying the process (e.g. diffusion vs. dissolution precipitation), in setting up the initial and / or boundary conditions, or in the choice of parameters (e.g. diffusion coefficients). Modelling concentration distributions of elements that diffuse at very different rates can allow different segments of the thermal history of a rock to be characterized so that a combination yields a picture of the complete thermal evolution. Finally, accounting for diffusive coupling in multicomponent systems such as garnets provides additional constraints on the nature of the thermal history Nowadays easily available software tools provide convenient access to both - analytical models to study the general behavior of systems as well as numerical models to reproduce faithfully the details of individual systems.

In spite of the many positive aspects, there are obstacles that have prevented widespread application of the tool. The most significant among these is the unavailability of diffusion coefficients and uncertainties associated with their determination. Recent advances in experimental technology and theoretical developments in the area of ab initio calculations have alleviated some of the problems and hold great promise for the near future. The current status of some relevant diffusion data will be reviewed. Other difficulties arise from the very nature of the diffusion process for example, it is more challenging to retrieve thermal histories of rocks metamorphosed at 500 °C than of granulites. This aspect calls for care in the choice of rocks and problems to which diffusion modelling is applied.