Model Uncertainties in Diffusion Geospeedometry

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Minerals often occur in the form of solid solutions, i.e. solid phases of varying chemical composition. Due to the changes in their physico-chemical environment, minerals tend to develop concentration gradients during their growth[1,2]. These gradients drive solid-state diffusion which may lead to the homogenization of the chemical composition in minerals.

Due to the high sensitivity of solid-state diffusion on temperature, the inverse modeling of composition profiles in chemically zoned crystals is commonly used to infer cooling rates and timescales of geologic processes (Fig. 1). This approach is commonly known as “Geospeedometry”[3] and it is used in a broad range of applications. However, the actual parameters which are needed in order to model the forward diffusion problem are largely extrapolated to conditions that are beyond the experimental calibration.

In this work, the doctoral candidate is expected to develop a numerical framework for dealing with the propagation of uncertainties in diffusion problems. In this framework the candidate will construct algorithms that can (i) enhance the signal of the primary data by deconvolution methods, using a detailed model of the measurement process, and (ii) assess the uncertainty of the forward-model predictions combining all available information on data uncertainties.

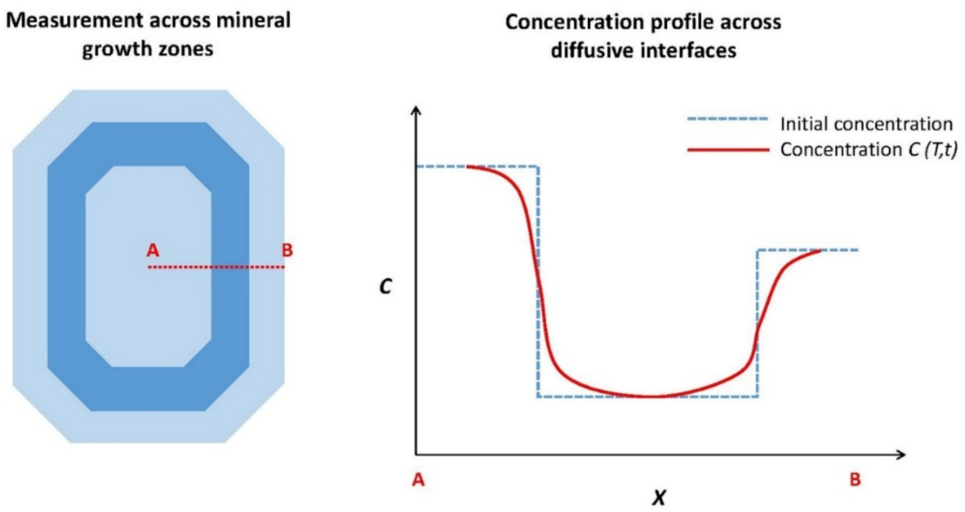

Figure 1. Basic principles of geospeedometry (source: Wikipedia). The original chemical composition (C) is measured on a polished crystal surface (left). Knowledge of the initial concentration profile may be used in order to deduce the time for which the crystal experienced high-temperature conditions (right).

References

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2. Spear, F. S. *Metamorphic Phase Equilibria and Pressure-Temperature-Time Paths*. (Mineralogical Society of America, 1993).

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