FINDIF and AutoDiff – 2-D and 1-D diffusion processing from BSE images with uncertainty constraint

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This contribution presents a pair of processing tools for the modelling of diffusion profiles in crystals. FINDIF is a finite-difference model coded in C^{++} that allows for diffusion anisotropy (within the limitations of a square grid), composition dependence tied to diffusing species, varying mineral phases, dynamic temperature-dependent partitioning and variable conditions of temperature. In this regard it provides an open-ended tool for the modelling of complex diffusion geometries in natural samples. AutoDiff uses a database of profiles generated in FINDIF to enable rapid matching of profiles measured in natural samples with those in the database. This provides a quick method to determine timescales from natural crystals that does not involve lengthy iteration of finite difference methods. This also provides a constraint on whether the profile is likely to be diffusion-generated or could represent crystal growth processes, as deviations from ideal profiles indicate a difference in process from that assumed; i.e., a simple square-wave initial geometry.

Finally, a method for propagating uncertainties in diffusional geochronometers is presented, that incorporates several key parameters in measured data that can influence the accuracy of the end result. This can be presented as a full statistical treatment (via Monte Carlo methods) or as a near-equivalent method that can estimate uncertainties with good precision with less computational overhead, suitable for rapid investigation.