The Fast Grain Boundary diffusion model: an updated tool for recovering thermal histories from zoned minerals

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We present an updated and expanded version of the Fast Grain Boundary (FGB) program, originally developed by [1]. In its current form, FGB forward models the oxygen-isotope compositional evolution of a rock resulting from diffusive oxygen isotope exchange. FGB is a tool for 1) constraining thermal histories (cooling rates and durations) from measured intragrain oxygen isotope zoning profiles, and 2) predicting oxygen isotope zoning that results from coupled volume and grain boundary diffusion. The FGB model is mass-balance constrained through exchange with a finite, grain-boundary reservoir and does not require a Dodson-like infinite reservoir assumption. The new FGB program code is written in Python and includes a graphical user interface.

The inverse modeling capabilities for FGB are currently under development. We present preliminary results for thermal history inversion from a test case using oxygen-isotope diffusion zoning data from titanite. Both the gradient descent and the Levenberg-Marquardt (LM) algorithms are applied to the FGB model in search of cooling histories that maximize agreement between the model output and recorded data. Various schemes of regularization are employed to ensure meaningful realizations of cooling histories. Additionally, to prevent local extrema entrapment, the results of these algorithms are compared to long-run brute force methods that have been implemented through Amazon's cloud computing services.

The observed zoning profiles in the example titanite dataset can be forward modeled with several arbitrary (and potentially biased) cooling histories. The preliminary results of inverse modeling reduce initial bias and suggest an episodic cooling history that may include an isothermal period or even a reheating event. These results demonstrate both the potential for oxygen-isotope zoning to preserve prevailing thermal events and the potential of the FGB model for recovering these events.

[1] Eiler, Baumgartner & Valley (1994), *Computers & Geoscience* 20, 1415-1434.