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Error propagation in garnet diffusion modelling

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An eclogite sample from the Grossglockner region of the Hohe Tauern, Austria, contains garnet with a pronounced compositional discontinuity between a Mn-rich core and an Fe-rich rim. This jump in composition was caused by a garnet-consuming reaction followed by growth of the garnet rim + omphacite and marks the prograde transition from epidote-amphibolite to eclogite facies metamorphism. Garnet growth ended at peak metamorphic conditions of 570 °C, 17 kbar, but intracrystalline diffusion continued until about 450°C, 4 kbar on the retro-

grade path. This garnet overgrowth texture represents a natural diffusion couple, and a time span of 1 Myr was calculated from the diffusion profile developing out of the original sharp compositional step yielding exhumation rates in the order of 4.6 – 7.4 cm/yr for vertical movement, which are one of the fastest ones reported (Dachs & Poyer, 2002).

During both analytical and numerical diffusion calculations it turned out that Fe- and Mn-profiles could not be modelled with the same time. In order to resolve

this discrepancy, we considered the errors associated with analytical diffusion modelling (effective binary diffusion coefficients, EBDCs). In a first step we refitted the experimental data of Chakraborty & Ganguly (1992) and Loomis et al. (1985) for Fe, Mg and Mn diffusion in garnet (including cited errors) to the logarithmic form of equation (1) by applying a least squares method:

$$D_i^*(P,T) = D_0 \exp [(-\Delta E - (P-1) \Delta V^+)/(RT)] \quad (1)$$

(where $D_i^*(P,T)$ is the tracer diffusion coefficient of element i, D_0 is the pre-exponential constant, ΔE is the activation energy, and ΔV^+ is the activation volume for diffusion).

The regressed values and their correlation coefficients (ρ) are:

Fe: $\ln(D_0) = -9.78 \pm 2.74 \text{ cm}^2/\text{s}$, $\Delta E = 59014 \pm 6968 \text{ cal/mol}$, $\Delta V^+ = 0.121 \pm 0.077 \text{ cm}^3/\text{mol}$,

$$\rho_{\ln(D_0)-\Delta E} = 0.96, \rho_{\ln(D_0)-\Delta V^+} = 0.53, \rho_{\Delta E-\Delta V^+} = 0.73,$$

Mg: $\ln(D_0) = -8.34 \pm 2.01 \text{ cm}^2/\text{s}$, $\Delta E = 63868 \pm 5107 \text{ cal/mol}$, $\Delta V^+ = 0.112 \pm 0.056 \text{ cm}^3/\text{mol}$,

$$\rho_{\ln(D_0)-\Delta E} = 0.97, \rho_{\ln(D_0)-\Delta V^+} = 0.54, \rho_{\Delta E-\Delta V^+} = 0.73,$$

Mn: $\ln(D_0) = -10.51 \pm 2.67 \text{ cm}^2/\text{s}$, $\Delta E = 52083 \pm 6805 \text{ cal/mol}$, $\Delta V^+ = 0.134 \pm 0.076 \text{ cm}^3/\text{mol}$,

$$\rho_{\ln(D_0)-\Delta E} = 0.96, \rho_{\ln(D_0)-\Delta V^+} = 0.52, \rho_{\Delta E-\Delta V^+} = 0.72.$$

Based on these values, the errors in the tracer diffusion coefficients $D_i^*(P,T)$ were estimated by performing error propagation to equation (1) including an assumed error of 50 °C for temperature and 1 kbar for pressure to account for the geothermobarometric uncertainty of our eclogite P-T estimate (570 °C, 17 kbar).

In a next step we propagated these D_i^* -errors through the calculation of interdiffusion coefficients, D_{ij} , which make up the composition dependent diffusion matrix \mathbf{D} (equation 2):

$$D_{ij} = D_i^* \delta_{ij} - \left(\frac{D_i^* z_i z_j C_i}{\sum_{k=1}^n z_k^2 C_k D_k^*} \right) (D_j^* - D_n^*) \quad (2)$$

(including an error of 0.01 in mole fractions of garnet endmembers; δ_{ij} is the Kronecker delta, z_i (z_j) is the charge on the i^{th} (j^{th}) component whose composition is C_i (C_j), and component n is the dependent component). The final errors in EBDCs were computed by propagating these D_{ij} -errors through equations of the type shown for Fe in the following equation (3) including an assumed error of 0.05 for the nonideal part of the EBDC:

$$D_{\text{Fe(EBDC)}} = D_{\text{FeFe}} + D_{\text{FeMg}} \partial C_{\text{Mg}} / \partial C_{\text{Fe}} + D_{\text{FeMn}} \partial C_{\text{Mn}} / \partial C_{\text{Fe}}$$

EBDC's used in analytical (one-dimensional) diffusion modelling via the equation

$$C_i(t,x) = C_i(0) + C_i^0 / 2 \{ 1 - \text{erf}(x / (\sqrt{4 D_i(\text{EBDC}) t})) \} \quad (4)$$

(where t = time, x = distance, $C_i(0)$ is the lower of the two initial values of C_i and C_i^0 is the initial concentration difference between the two sides of the couple), then have typical errors of 0.3-0.5 log-units. By varying the EBDC's of Fe and Mn within 2σ we found combinations of EBDCs that resulted in best matches of calculated and measured diffusion profiles for **single** time values (consistent for Fe and Mn), and we were able to derive a maximal time of diffusion possible within the error range of EBDCs.

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Die dynamische Entwicklung des Wiener Beckens: vom Miozän zur Gegenwart

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Die krustenmaßstäbliche Pull-Apart-Struktur des Wiener Beckens entwickelt sich während des Miozäns an einer sinistralen Transferstörung, die vom Mur-Mürztal über das Wiener Becken bis in die Westkarpaten Galiziens kartiert ist. Die Störung bildet die NW Begrenzung einer Fluchtscholle, die aus der Konvergenzzone der Ostalpen nach NE entkommt. Die Transferstörung ist mit NE-gerichteten Überschiebungen an der Front der Fluchtscholle in den äußeren Karpaten verbunden. Die Verbindung mit diesen Überschiebungen, die Subsidenzgeschichte des Pull-Apart-Beckens, die nur mit einem

Abscherungshorizont an der Basisüberschiebung der alpin-karpatischen Decken erklärbar ist, und die thermische Entwicklung des Beckens belegen eine "thin-skinned" Entwicklung des Beckens.

Die Lage von Erdbebenepizentren, GPS-Messungen, Rezentspannungen, geomorphologische Daten und detaillierte Kartierungen aktiver Störungen im Wiener Becken lassen darauf schließen, dass die rezenten tektonischen Prozesse gut mit den miozänen vergleichbar sind. Daten von seismisch und tektonisch aktiven Störungen aus dem Wiener Becken belegen, dass