Geophysical Research Abstracts, Vol. 9, 00274, 2007
SRef-ID: 1607-7962/gra/EGU2007-A-00274

Diffusion couple Experiments in Garnets: Effect of grain boundary Diffusion owing to 2D numerical Modeling

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Induced compositional profiles in diffusion couple experiments may contain different irregularities (plateau-like segments, "shoulders" and flexures). Reasons of the irregularities are not well understood and thus corresponding profiles are always considered as inappropriate for retrieving diffusion coefficients out of experimental runs. We simulated numerically diffusion between two garnets of dissimilar composition in order to reproduce experimentally induced profiles containing the irregularities and thus understand their origin and possible applications. Different fracture patterns (narrow zones with fast diffusion penetration) have been tested in one of the modeled garnets. The diffusion problem was solved using finite element method in FEMLAB© environment, which allows one to study the influence of pressure, temperature, grain shape and fractures orientation on the zoning pattern. The modeling reveals that plateau-like segments of the profiles normal to the interface (NTI) are set along the NTI fracture. Similar profiles near the fractures contain "shoulders". Therefore both “shoulders” and plateau-like segments are resulted from fast migration of elements along the fractures. Leakage of components along the inclined fractures causes flexures on the profiles (always measured NTI). In general, the flux along the crack strongly modifies shape of the microprobe profile at both sides of the interface. The more fracture inclined from NTI direction, the less its contribution to the measured diffusion profile. Accordingly, an isolated fracture which is located parallel to the interface does not affect the interdiffusion profile.

The modeled profiles reproduce experimentally induced profiles when the grain boundary (fracture) diffusion coefficient (D^{GB}) to the volume diffusion coefficient (D^{V}) ratio for Fe-Mg interdiffusion $lg(D^{GB}/D^{V}) \geq 4$. Enhanced migration of components along fractures or grain boundaries deserves further study because this is a clue for deciphering rates of yet unknown grain boundary diffusion coefficients in garnet.