Grain boundary diffusion and its relation to grain boundary segregation of multiple elements in Garnet

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Grain boundary diffusion and segregation play a significant role in many polycrystalline materials, including engineering fabrics as well as Earth materials. They may influence abundance patterns and isotope systematics of various elements in mantle rocks as well as applicability, purity, and life-time of engineering materials, such as laser ceramics. Here, the diffusion of various elements (Fe, Mg, La, Ti) along a well characterized grain boundary in yttrium aluminium garnet (YAG) has been studied by a combination of transmission electron microscopy (TEM) and using a bicrystal setup developed with a wafer bonding method [1]. We performed diffusion experiments in a gas mixing furnace at 1000°C and 1450°C at ambient conditions for various durations and mapped the element concentration distribution using energy dispersive X-ray spectroscopy in scanning (S)TEM mode. Measured concentration distributions were simulated by solving the diffusion equations in 2D according to Fisher's model [2, 3] but including the segregation factor, s. From the simulations we were able to estimate the grain boundary diffusion coefficients (D_{gb}) as well as the product of the effective grain boundary width, δ, and the segregation factor.

We find that D_{gb} for all observed incompatible elements at 1450°C is > 9×10^{-11} m^2/s, which is 8 orders of magnitude faster than the respective diffusion coefficient for the crystal lattice. Due to the relatively large ionic radius of La compared to Y, it segregates to the grain boundary. We find that at 1450°C δs of La is > 10 nm, whereas δs of Fe and Mg is 1.7 nm and 1.8 nm, respectively. However, in case of the presence of Ti grain boundary diffusion of La seems to be prevented.

Our experiments confirm that incompatible elements can diffuse extremely effective along grain boundaries and that they may significantly influence each other's diffusion rates.

[1] Plößl & Kräuter (1999) *Materials Science and Engineering R: Reports*, **25,** 1–88. [2] Fisher (1951) *Journal of Applied Physics*, **22** (1), 74-77. [3] Dohmen & Milke (2010) *Rev. Mineral. Geochemistry,* **72** (1) 921–970.