

Concentration dependence of trace element diffusion in minerals

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Trace element diffusion in minerals may control the closure of radiogenic isotopic systems, trace element thermometers, or element exchange between melt inclusions and host minerals. Preserved trace element zoning profiles in minerals can be also used for diffusion chronometry or speedometry. The knowledge of respective diffusion coefficients as a function of the relevant thermodynamic parameters is required to calculate closure temperatures and model diffusion profiles. However, in the recent past a complex behaviour was found in experiments on diffusion of trace elements that fundamentally differs from those of the major ions, e.g., for Li in olivine [1], Zr, Hf, Nb and Ta in rutile [2], Pb in perovskite [3], and also REE in olivine [4]. Diffusion rates of these trace elements depend strongly on their concentrations (up to four orders of magnitude) and may show complex diffusion profile shapes but for different or a combination of the following reasons: (i) the trace element is incorporated (heterovalent substitution) by two different species and hence the diffusive flux of these species is coupled by a homogeneous reaction within the crystal lattice [1]; (ii) the trace element reaches a concentration level (becomes a majority point defect) where other relevant point defects of the mineral are affected and hence diffusion is [2]; (iii) incorporation of the trace element creates a local strain that affects the diffusion process [3]. All these cases have in common that a threshold value exists for the concentration above which the complex diffusion behaviour appears but this value can depend on the chemical environment, e.g., oxygen fugacity [1,2]. The prediction of diffusion rates for the diverse applications is therefore difficult but possible if quantitative knowledge of the point defect chemistry of the mineral is available, as will be demonstrated with rutile and olivine for various cases. These studies allow us to explain some of the apparent inconsistencies between earlier published diffusion data for olivine and rutile.

[1] Dohmen et al. 2010, *Geochim Cosmochim Acta* 74: 274-292; [2] Dohmen et al. 2018, *Phys Chem Mineral*, <https://doi.org/10.1007/s00269-018-1005-7> [3] Beyer et al. 2019, *Am Mineral* 104: 557-568; [4] Chakraborty et al. 2018, *EMPG XVI Conf Abstr*