

Al, Fe and H incorporation in natural rutile

B. JOACHIM-MROSKO^{1*}, J. KONZETT¹, T. LUDWIG² AND R. STALDER¹

¹Institute of Mineralogie and Petrography, Univ. of Innsbruck, 6020 Innsbruck, Austria

(*correspondence:bastian.joachim@uibk.ac.at)

²Institute of Earth Sciences, Heidelberg Univ., 69120 Heidelberg, Germany

Rutile is one of the most common accessory minerals in igneous and metamorphic rocks and their high- and ultrahigh-pressure counterparts. Though nominally anhydrous, rutile may store trace amounts of water and thus has the potential to transport volatiles to depths beyond sub-arc magmatism and even down to the lower mantle.

We investigated experimentally the incorporation of Al, Fe and hydrogen in natural rutile embedded in a granitic host rock at fixed $\mu(\text{Al}_2\text{O}_3)$, at $\Delta f\text{O}_2$ between QFM-1 and QFM-2, in the P-T range 2-7 GPa, and at temperatures between 1173-1373 K.

SIMS shows in all experiments diffusion profiles of H_2O that are significantly shorter compared to diffusion profiles of Al_2O_3 and FeO. Microprobe analyses further reveal a complex distribution of oxygen defects at the scale of the diffusion profiles. FTIR-analyses point toward the incorporation of hydrogen dominantly as Fe-H and Ti-H related defects [1].

Based on these results, we suggest a complex combination of mechanisms that explains the incorporation of Al, Fe and hydrogen in rutile at our experimental conditions. These are amongst others:

- The incorporation of Al on octahedral Ti-sites and, at high pressures, on interstitial sites in combination with the formation of oxygen vacancies [1].
- Incorporation of Fe^{3+} on a Ti-site charge balanced by the incorporation of H^+ [1]
- Formation of vacancies on Ti-sites accompanied by incorporation of oxygen [3] and hydrogen.

Calculated diffusion profiles further reveal a sudden increase in maximum H_2O , Al_2O_3 and FeO-solubilities between 6 and 7 GPa that may be explained by the transition from a CaCl_2 type to an $\alpha\text{-TiO}_2$ type polymorph [2].

[1] Bromiley & Hilairet (2005) *MinMag*, **69**, 345-358.

[2] Escudero *et al.* (2011) *J. Phys. Chem.* **115**, 12196-12201.

[3] Dohmen *et al.* (efirst) *Phys. Chem. Mineral.*

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