

## Al, Fe and H incorporation in natural rutile

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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  $\text{H}_2\text{O}$  that are significantly shorter compared to diffusion profiles of  $\text{Al}_2\text{O}_3$  and  $\text{FeO}$ . 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  $\text{Fe}^{3+}$  on a Ti-site charge balanced by the incorporation of  $\text{H}^+$  [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  $\text{H}_2\text{O}$ ,  $\text{Al}_2\text{O}_3$  and  $\text{FeO}$ -solubilities between 6 and 7 GPa that may be explained by the transition from a  $\text{CaCl}_2$  type to an  $\alpha\text{-TiO}_2$  type polymorph [2].

[1] Bromiley & Hilair (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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