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Oxygen diffusion in rutile from 750 to 1000 °C and 0.1 to 1000 MPa

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ABSTRACT

Oxygen self-diffusion in rutile was studied in synthetic and natural samples over the temperature range 750 to 1000 °C and the pressure range 0.1 to 1000 MPa using an ^{18}O-enriched source. Most experiments investigated the dependence of *D* on temperature, water pressure, crystallographic direction, and experiment duration. A few experiments investigated the dependence of *D* on f_{O_2} and confining pressure. The uptake profiles of ^{18}O in experimental products were measured by nuclear reaction analysis using the reaction $^{18}O(p,\alpha)^{15}N$.

Two mechanisms are responsible for O diffusion in rutile, and one is faster than the other by about an order of magnitude. O that diffuses by the faster mechanism is described by the diffusion law:

$$D(\|c) = 4.7 \times 10^{-7} \exp(-258 \pm 22 \times 10^3/RT) \quad D_0 \text{ in m}^2/\text{s}; \quad E_A \text{ in J/mol}; \quad T \text{ in K}.$$

Diffusion by the slower mechanism is described by this law:

$$D(\|c) = 5.9 \times 10^{-5} \exp(-330 \pm 15 \times 10^3/RT) \quad D_0 \text{ in m}^2/\text{s}; \quad E_A \text{ in J/mol}; \quad T \text{ in K}.$$

Oxygen fugacity in itself does not affect *D* at fugacities between 1 atm and Ni-NiO. However, the presence or absence of water during reduction does affect the diffusion behavior. When water is absent during rutile growth and/or subsequent reduction, only the faster mechanism operates, and when water is present during growth or reduction, both mechanisms operate simultaneously, though the contribution from the slow mechanism dominates that of the fast mechanism. Because few geologic environments are truly dry, the slower law should generally be used for modeling O diffusion for rutile in nature. Comparison with other studies of rutile suggests that migration of O vacancies is the mechanism responsible for the faster diffusion law whereas migration of Ti interstitials is responsible for the slower diffusion law.

Oxygen diffusion in rutile is slower perpendicular to the *c* axis than parallel to that axis by about half an order of magnitude. There is no perceptible effect of confining pressure on *D* below 100 MPa, or between 600 and 1000 MPa. However, between 100 and 600 MPa, *D* decreases by nearly an order of magnitude.

Closure temperatures for O diffusion in rutile are high—650 °C for a crystal with a 100 μm radius and a 10 °C/Ma cooling rate. Rutile is retentive of its O isotopic composition. A crystal with a 100 μm radius will retain its initial core composition for just over 10 million years at 600 °C.