Decoding the kinetic rulebook: H diffusion in quartz

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Hydrogen diffusion in quartz is presented as a potential tool for understanding very short (minutes to hours at 700-800 °C) timescales of eruption processes that involve changing water fugacity prior to quenching. The system also allows new insights into diffusive processes in general – H is a trace element but does not behave as a tracer diffusant, and has multiple sites even in the simple quartz structure.

Oriented cubes were cut from various optically perfect quartz crystals (Brazil, Tibet, Madagascar), all of which contained some structurally bound OH groups, but with different defect populations and water contents (2 to 90 wt. ppm H_2O). The crystals were then dehydroxylated (1 bar), or hydroxylated/deuteroxylated (1 kbar) at 400-900 °C.

Dehydroxylation was done in air, placing the crystals in Au containers, either alone or packed into a lithium disilicate-quartz powder (to induce Li^+-H^+ inter-diffusion). Experiments were conducted for minutes to weeks, then doubly polished and analysed using FTIR spectroscopy. Total OH versus distance from the crystal edge shows simple error function shapes, but resolved profiles show diffusion-induced OH band fractionation.

Following hydroxylation or deuteroxylation, profiles do not conform to the error function, rather they show two-step profiles (including plateaus) or linear concentration decreases, often with kinks. These shapes can be explained using a diffusion plus reaction model, were H diffuses along a pathway associated with one defect (e.g. associated with non-bridging O^{2-}) then hops into association with another defect (associated with Al^{3+}).

Despite clear differences between the different experimental series, the in-diffusion and out-diffusion (of H^+) can be approximately described by the same diffusion-reaction model. In the out-diffusion experiments the H^+ is already on its most stable site (Al^{3+} associated) so inter-site reaction is limited/negligible, and in the in-diffusion experiments the H^+ moves partially on a less favourable site, then hops into the more favourable Al-associated site.

Then, timescales of the last moments of silica-saturated volcanic eruptions can be unravelled, in the case where crystals do not experience considerable post-eruption heating. Diffusion is fast enough that easily measurable profiles (hundreds of μm) are formed in just minutes to hours at 700-800 °C.