Re-equilibration studies of synthetic fluid inclusions in quartz

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Synthesised fluid inclusions in carefully selected inclusion-free Brazilian quartz crystals are used for re-equilibration experiments. Due to the possibility of post-entrapment changes of fluid inclusions, interpretations of fluid properties have to be done with particular attention. Therefore we perform re-equilibration experiments in cold seal pressure vessels under hydrothermal conditions (for applied experimental technique see Doppler et al., this abstract volume). The experiments are carried out at high experimental temperatures and pressures (max. 700 °C and 1 GPa). The experimental studies allow investigating the main factors that affect H₂O diffusion through nominally anhydrous minerals.

The present study illustrates the changes of primary synthesised H₂O-rich fluid inclusions which were exposed to D₂O during the re-equilibration process at high experimental temperatures and pressures.

The presence of D₂O in H₂O-rich fluid inclusions is detected with microthermometry and Raman spectroscopy. The melting temperatures of pure H₂O and pure D₂O are significant different, 0.0 °C and +3.8 °C, respectively. Intermediate melting temperatures can be directly reflected to relative amounts of H₂O and D₂O. Furthermore, the Raman spectrum of H₂O and D₂O are similar in shape, however, they occur in completely separated wavenumber intersections: 3000 – 3800 cm⁻¹ for H₂O and 2000 – 2800 cm⁻¹ for D₂O.

A variety of parameters that play an important role in diffusion experiments are examined: 1) concentration gradient (chemical potential) of H₂O (negative) and D₂O (positive); 2) distance of fluid inclusions to the quartz surface; 3) size of fluid inclusions; 4) experimentation time; (Fig. 1).

Fig. 1. Schematically illustrated quartz crystal with primary synthesised fluid inclusions with known composition at a. variable distances to the crystal surface and b. variable sizes. Re-equilibration experiments are performed with a different fluid phase at the same P-T conditions and different experimentation times.

The original synthesised inclusions have a large variety of shapes (Fig. 2, definitions according to Bakker & Diamond, 2006). After re-equilibration, the original equant and regularly shaped inclusions do not change their shape, whereas elongated and irregularly shaped inclusions tend to become equant and regularly shaped during re-equilibration (arrow in Fig. 2).

Fig. 2. Shape classification diagram (modified after Bakker & Diamond, 2006).
Analyses of re-equilibrated inclusions at variable distances to the crystal surface allow us to obtain concentration profiles in quartz. Concentration profiles of the D$_2$O content of fluid inclusions in quartz allow us to develop new three-dimensional diffusion models.

An example of a re-equilibration experiment is shown in Figure 3. The primary fluid inclusions have been synthesised with pure H$_2$O at 600 °C and 337 MPa, which corresponds to a molar volume of 25 cm$^3$ mol$^{-1}$. The experimental running time for the first synthesis was nineteen days. The primary synthetic fluid inclusions were re-equilibrated with pure D$_2$O at the same P-T conditions for one, five and nineteen days. An example of a concentration profile, as evidenced by the melting temperature of ice $T_m$(SV→LV), within a quartz crystal after five days is illustrated in Figure 3.

Potential changes of the ambient fluid inclusions during re-equilibration correlate with the size (total volume) of the fluid inclusion. Figure 5 demonstrates again three envelopes of the detected melting temperatures of re-equilibrated fluid inclusions.

These experiments have illustrated that H$_2$O and D$_2$O can diffuse relatively fast through quartz at 600 °C and 337 MPa. Variation in re-equilibration is controlled by distance to the quartz surface, size of the fluid inclusion and experimentation time.

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REFERENCES