Diffusion of water through quartz

the use of synthetic fluid inclusions

Ronald J. Bakker

Mineralogy and Petrololgy

University of Leoben

Austria

Diffusion of H_2O in nominally anhydrous minerals (quartz)

Definition:

Matter is transported from one part of a system (higher concentration) to another (lower concentration) as a result of „random“ molecular motions.

- H_2O is part of a <u>solid solution</u> in the SiO_2-H_2O system
- SiO_2 lattice is a <u>membrane</u> through which H_2O can freely move

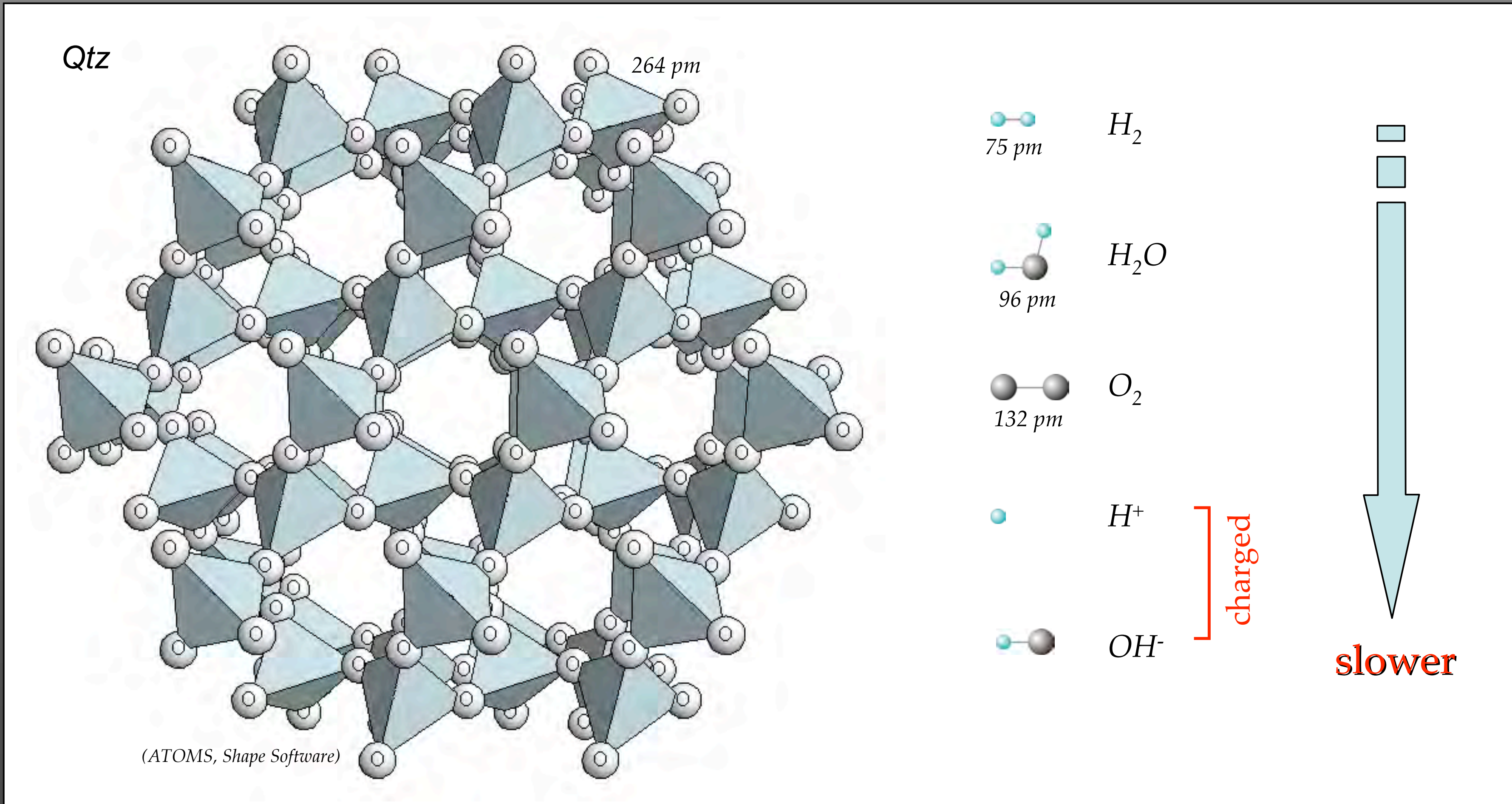
H_2O is not a part of the solid solution

simplified research objective:

How fast can H_2O move in/through the quartz crystal?

Theory H_2O in Quartz

1. substitutional impurity
2. interstitial impurity
3. fluid inclusions



H_2O diffusion: evidence from experimental work?

What was measured: Isotopic variation of quartz (oxygen isotopes)

Tracer particles in quartz

Deformation Phenomena (hydrolitic weakening)

Detection method: Infrared Spectroscopy → H_2O and OH^-

Mass Spectroscopy (secondary ions) → ^{18}O and ^{16}O

What was modelled: Concentration Profile of isotopic composition of quartz

One-dimensional diffusion model

H_2O diffusion: evidence from experimental work?

Deformation experiments

1. Diffusion of H_2O is too slow within the limits of experimentation

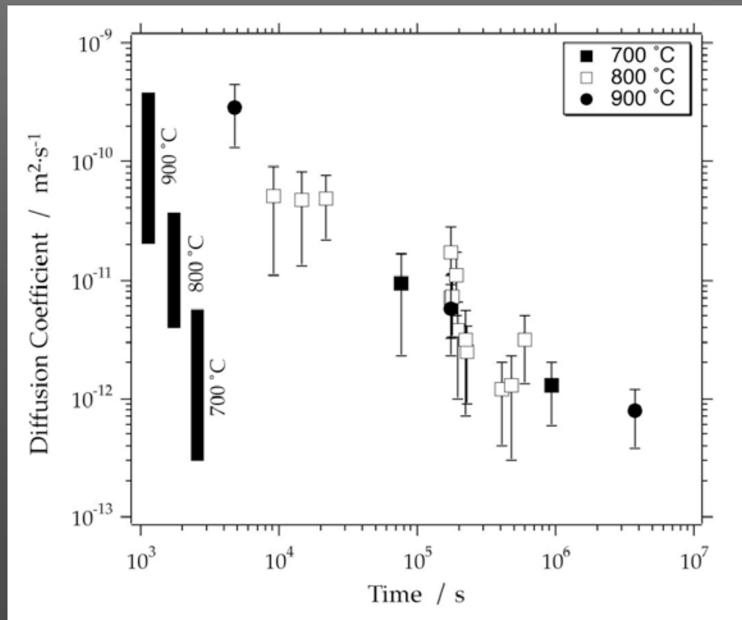
Ref. Kronenberg et al. (1986)
Gerretsen et al. (1989)

2. Synthetic quartz behaves completely different

→ grown-in water defects during synthesis

Diffusion coefficients

1. Temperature dependence?
2. Pressure dependence?
3. 1D diffusion?



re-evaluated data Kronenberg et al. (1986)

Mathematical Diffusion Models

One Dimensional

1D diffusion in a semi-infinite body with constant surface concentration

$$c_i^{qtz}(x,t) = \tfrac{1}{2}\left(c_i^{\max} - c_i^{0}\right) \cdot erfc\left(\frac{x}{2\sqrt{D_i t}}\right) + c_i^{0}$$

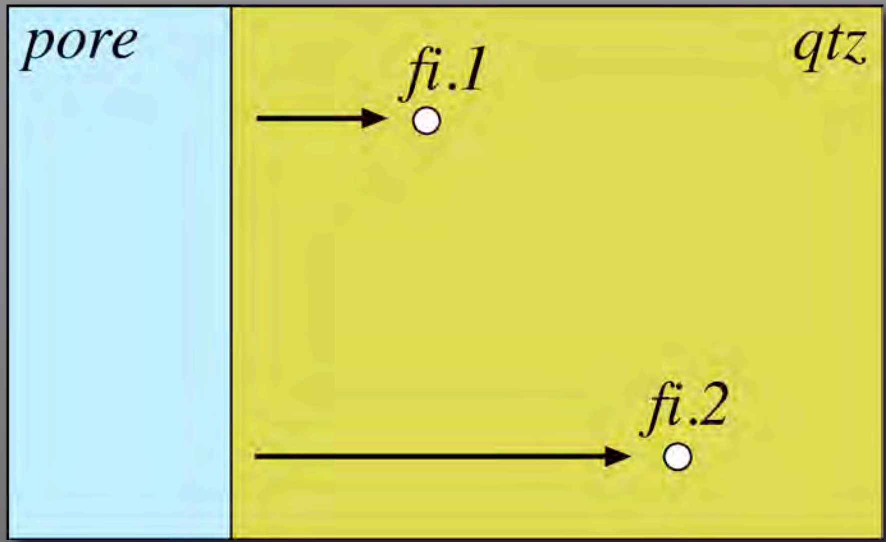
e.g. Farver & Yund (1991)
Brady (1995)

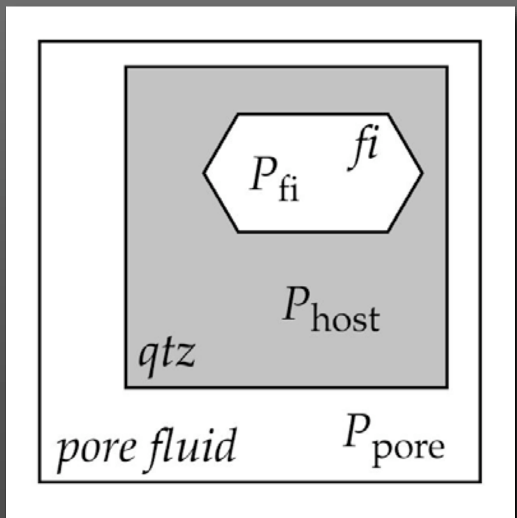
1D diffusion into a plane sheet of thickness *l*
uniform initial distribution, equal surface concentrations

$$c_i^{qtz}(x,t) = \left(c_i^{\max} - c_i^{0}\right) \cdot \left[\sum_{n=0}^{\infty} (-1)^n \, erfc \, \frac{(2n+1)\cdot l - x}{2\sqrt{Dt}} + \sum_{n=0}^{\infty} (-1)^n \, erfc \, \frac{(2n+1)\cdot l + x}{2\sqrt{Dt}} + \right] + c_i^{0}$$

small times approximation, n=1   Kronenberg et al. (1986)

New experimental set-up for diffusion models



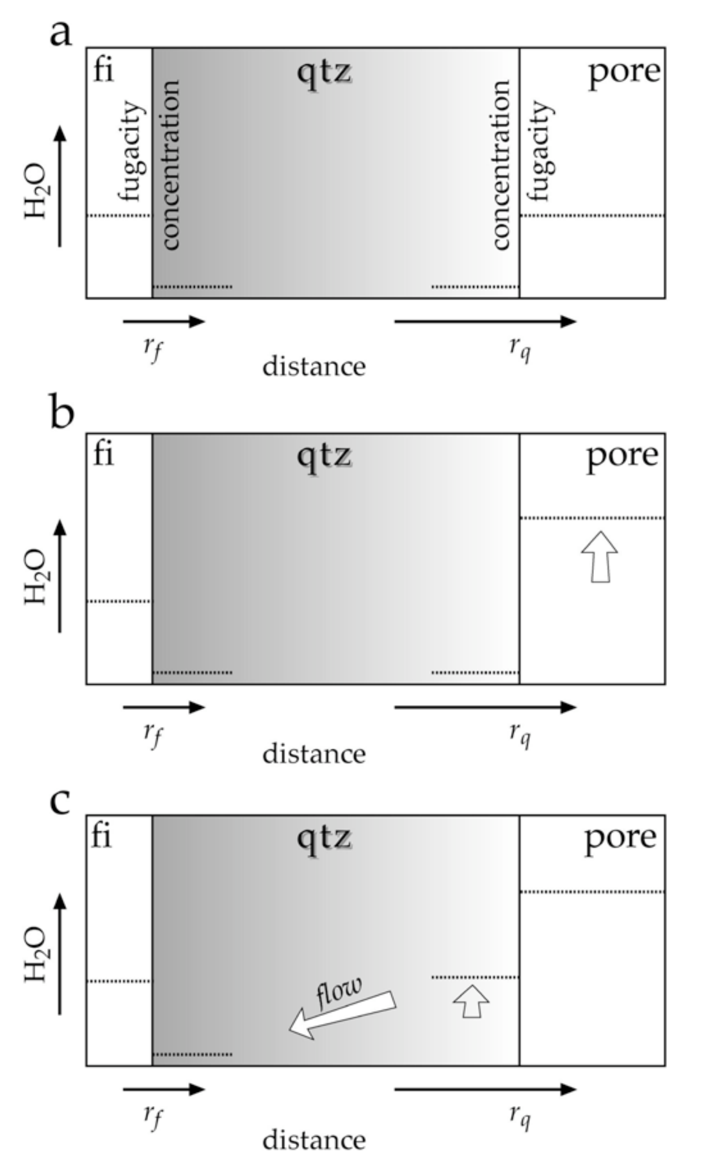


chemical potential gradient (concentration)

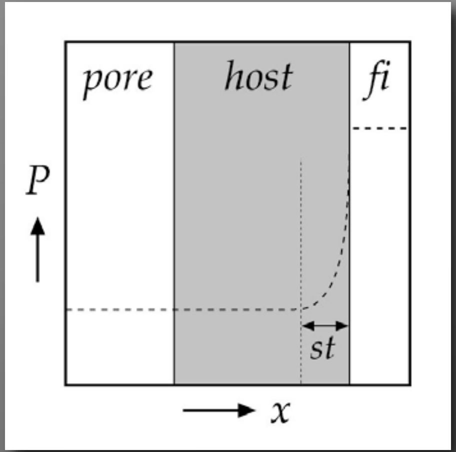
pressure gradient

Gradients

Fugacity



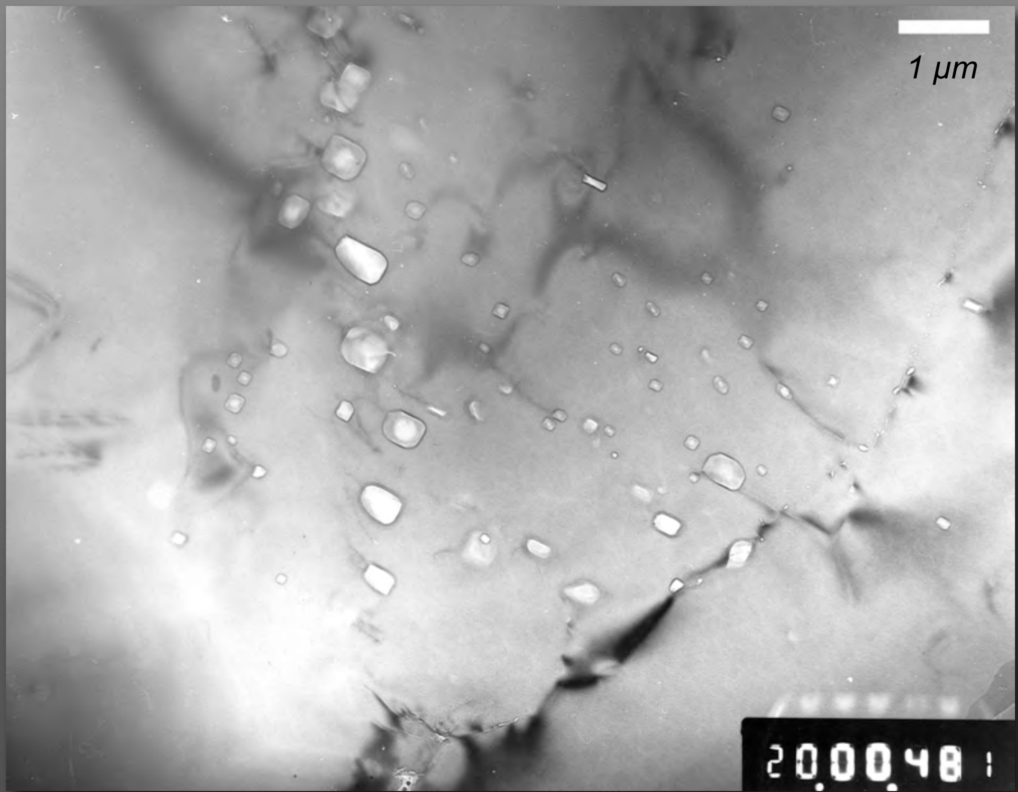
Pressure



Fluid Inclusions

isolated pocket of fluid in crystal

large sized crystal-defect



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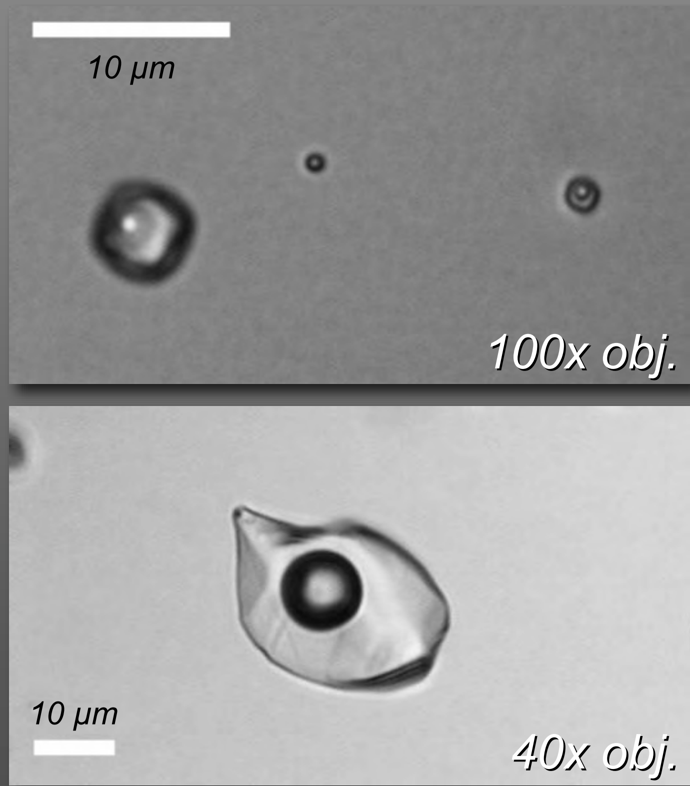
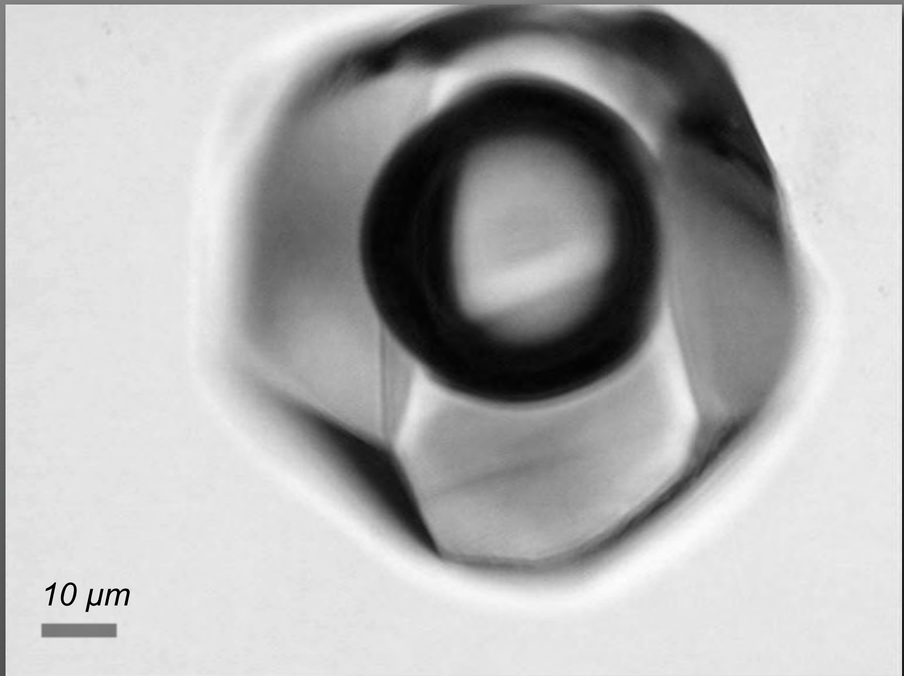


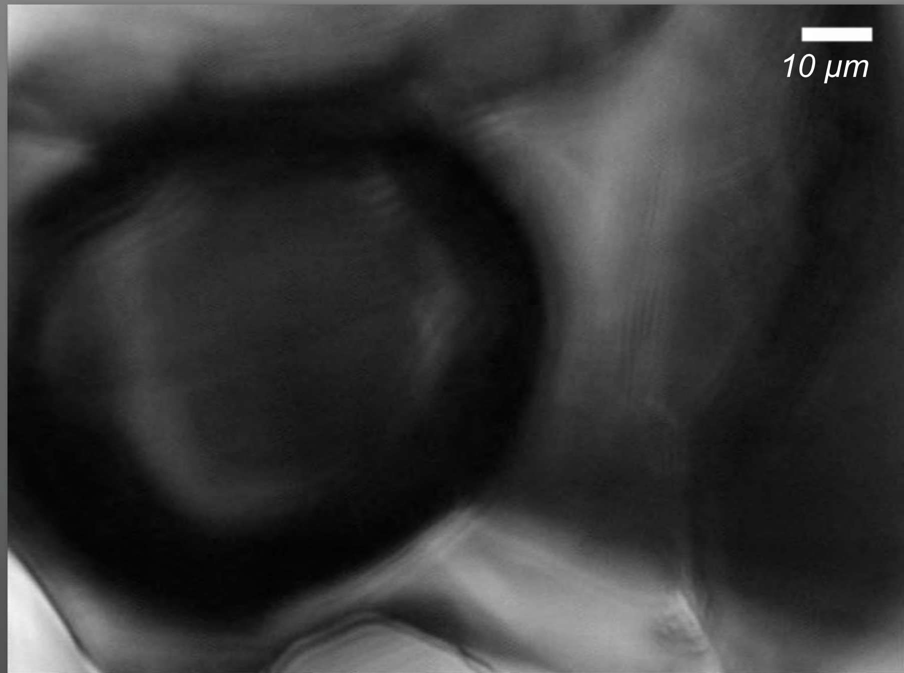
opt. microscopy

Fluid Inclusions

isolated pocket of fluid in crystal

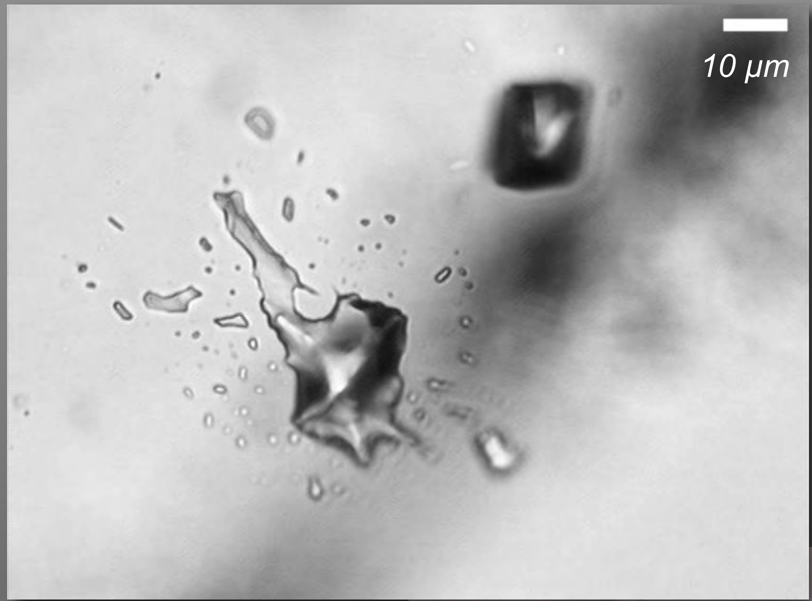
large sized crystal-defect





opt. microscopy

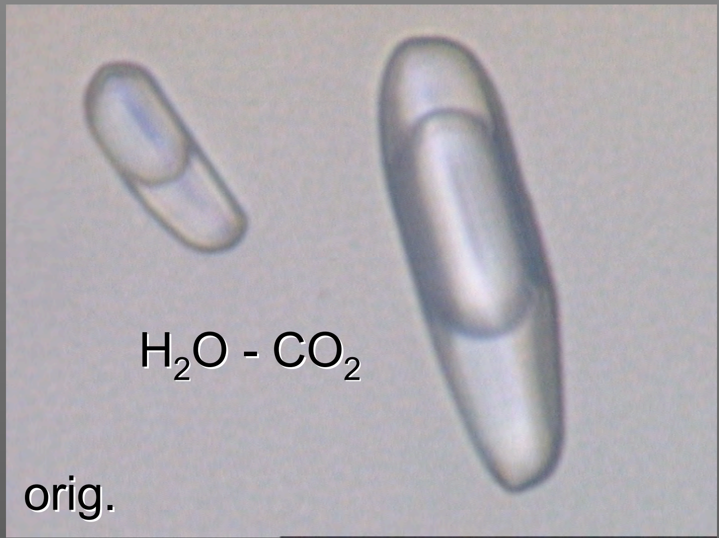
Can fluid inclusions change their density and composition?

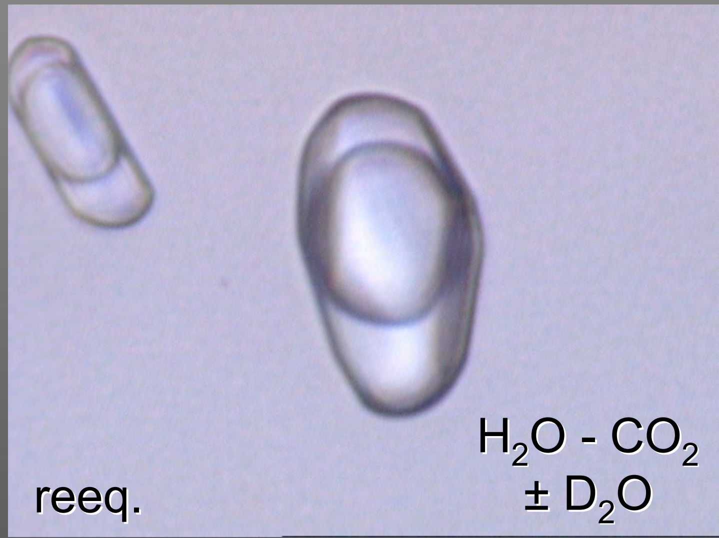


Re-equilibration experiments with fluid inclusions

Properties of fluid inclusions (alterations in composition and density)

600 ˚C
500 MPa

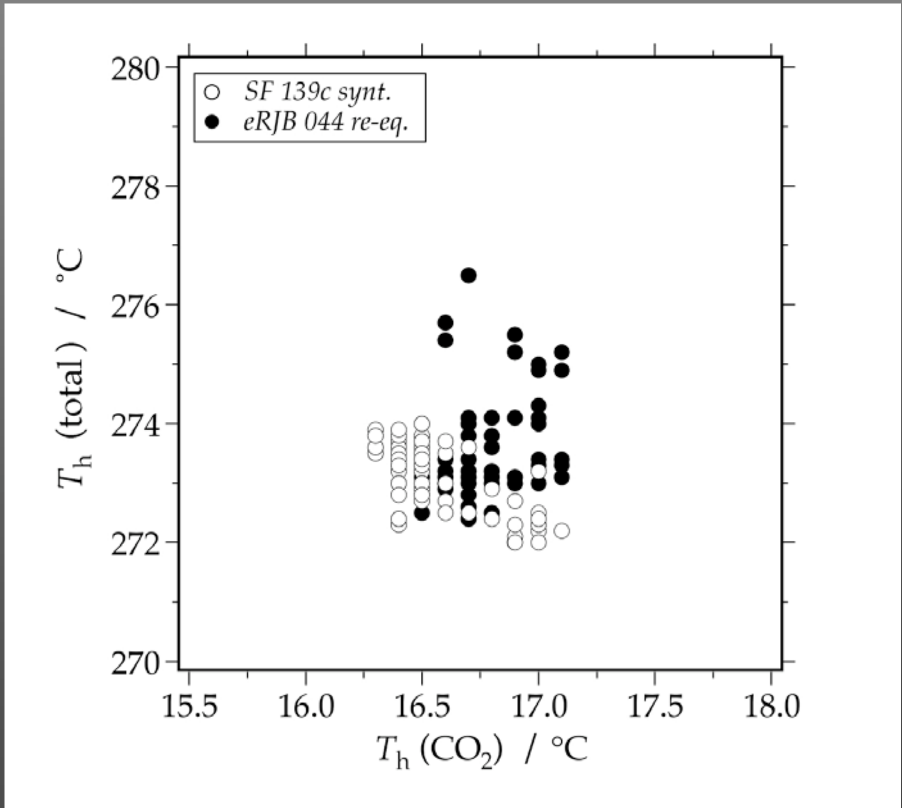


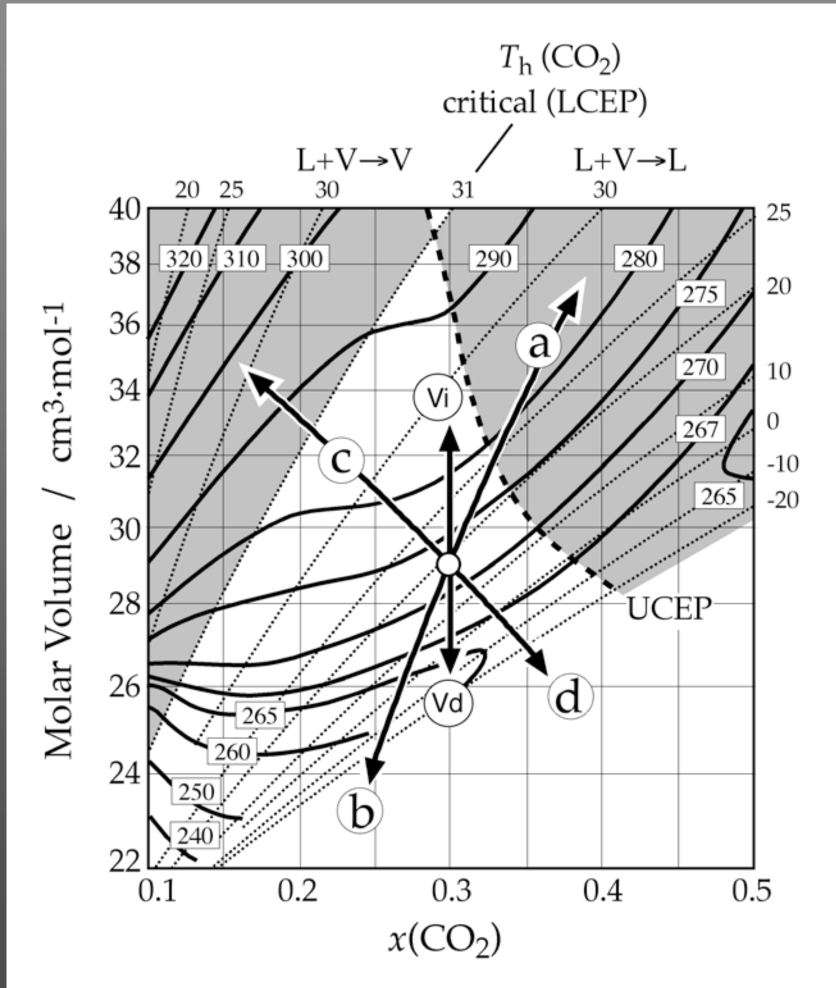


Microthermometry
Raman spectroscopy

Microthermometry

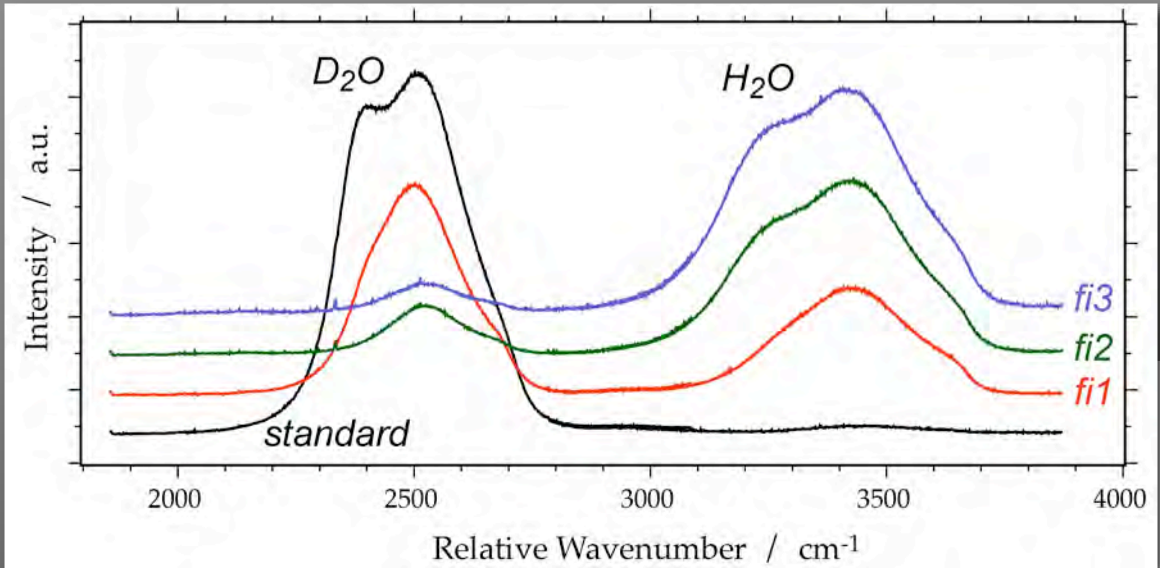
diffusion → change in density → change in homogenisaton temperature

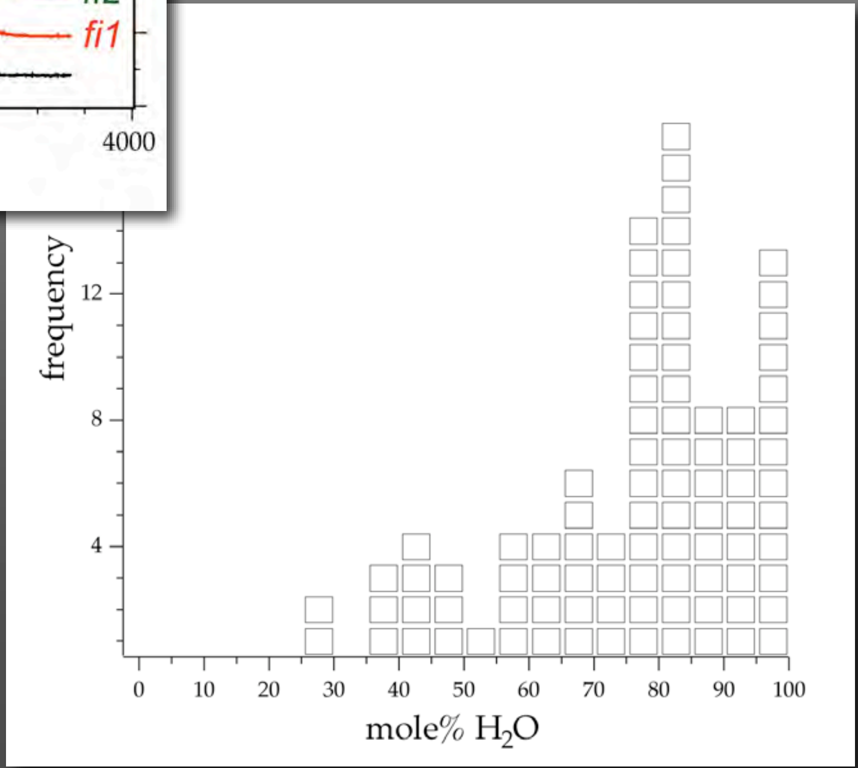




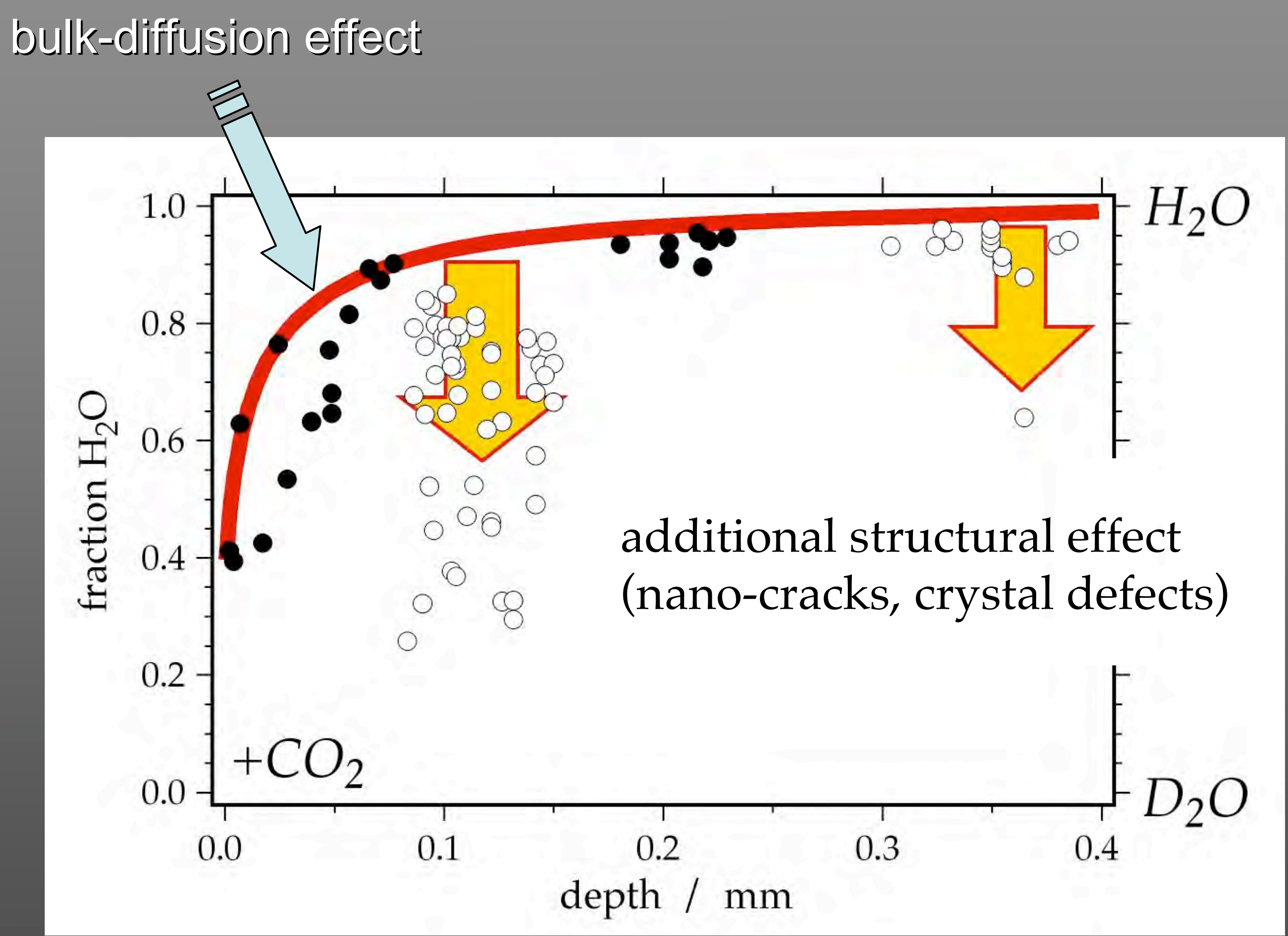
Raman Spectroscopy

diffusion → change in composition → change in spectra



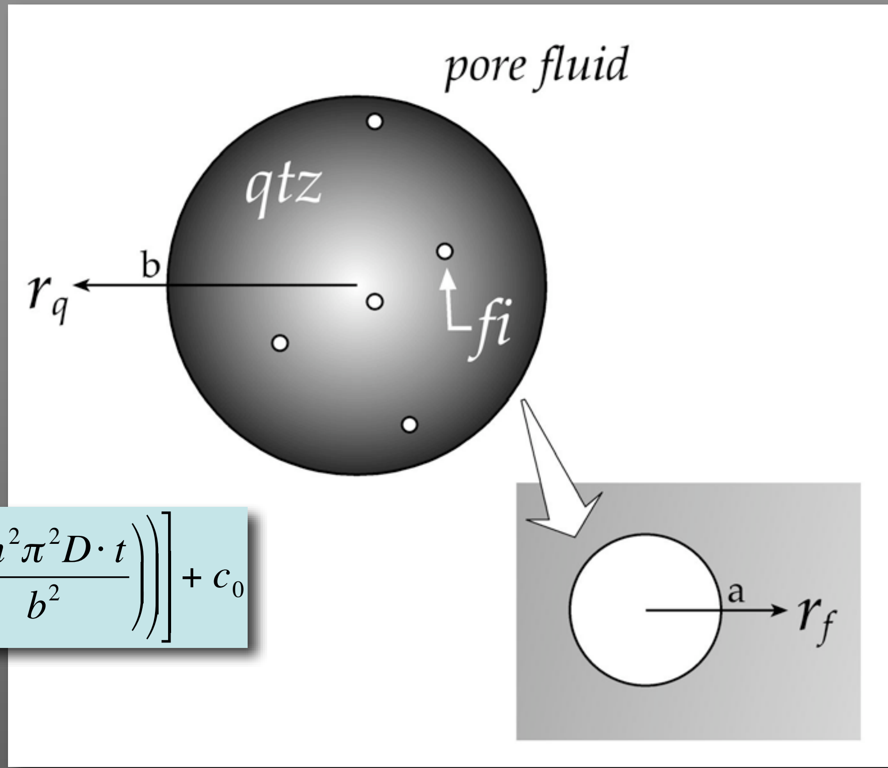


Fluid Inclusions properties: distance to surface



New mathematical diffusion models

For example: 3D diffusion



1. diffusion pores → quartz

infinite external source

$$c = (c_1 - c_0)\cdot\left[1 + \frac{2b}{\pi\cdot r_q}\sum_{n=1}^{\infty}\left(\frac{(-1)^n}{n}\sin\left(\frac{n\cdot\pi\cdot r_q}{b}\right)\exp\left(\frac{-n^2\pi^2 D\cdot t}{b^2}\right)\right)\right] + c_0$$

2. diffusion quartz → inclusions

instantaneous point source

$$c = c_0 + \frac{(c_1 - c_0)}{2}\cdot\left[erf\left(\frac{a + r_f}{2\sqrt{D\cdot t}}\right) + erf\left(\frac{a - r_f}{2\sqrt{D\cdot t}}\right)\right] - \frac{(c_1 - c_0)}{2}\sqrt{\frac{D\cdot t}{\pi}}\cdot\left(\exp\left(\frac{-(a - r_f)^2}{4\cdot D\cdot t}\right) - \exp\left(\frac{-(a + r_f)^2}{4\cdot D\cdot t}\right)\right)$$

Conclusions

Fluid inclusions are suitable to characterize diffusion through quartz

new diffusion coefficients
new diffusion model

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