Geophysical Research Abstracts,
Vol. 10, EGU2008-A-03602, 2008
SRef-ID: 1607-7962/gra/EGU2008-A-03602
EGU General Assembly 2008

IR Calibrations for Water in Olivine and SiO_2 Polymorphs

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Most frequently applied Infrared (IR) calibrations [1, 2] for quantitative water analyses in solids, primarily acquired on hydrous minerals and glasses with several wt% water, can not be adopted to nominally anhydrous minerals (NAMs) but mineral specific calibrations are needed [3]. The calibrations [1, 2] are based on a negative correlation between the absorption coefficient ε for water and the mean wavenumber of the corresponding OH pattern.

In the present work we provide ε-values for synthetic olivine and SiO_2 polymorphs. We were able to synthesize these minerals with specific isolated OH point defects, e.g., quartz with either B^{3+}+H^+=Si^{4+} or Al^{3+}+H^+=Si^{4+} substitutions. The IR spectra of e.g., Al- or B-doped quartz show separated OH bands at different wavenumbers and hence allow to study the frequency dependence of ε. Water contents of both natural samples and our run products were determined using independent techniques as proton-proton-scattering [4], confocal microRaman spectroscopy [5] and secondary ion mass spectrometry. Obtained data provided the basis to calculate new mineral specific IR absorption coefficients. Moreover, we present a routine to detect OH traces in isotropic and anisotropic minerals using Raman spectroscopy.

For olivine with the mean wavenumber of 3517 cm^{-1} an ε-value of 38,000 $\pm$ 4,000 $lmol_{H2O}^{-1}cm^{-2}$ was determined. But for another olivine (mean wavenumber 3550 cm^{-1}) we obtained an ε-value of 47,000 $\pm$ 5,000 $lmol_{H2O}^{-1}cm^{-2}$. Taking into account previous studies [6, 7] we will discuss here the frequency dependence of ε for olivine. In case of the SiO_2 system it turns out that the magnitude of ε for one structure is independent of the type of OH point defect and therewith the peak position, but varies as a function of structure. One single mean ε of 66,000 $\pm$ 8,000 $\mathrm{lmol}_{H2O}^{-1}\mathrm{cm}^{-2}$ was determined for a suite of quartz crystals with different OH point defects. For the high-pressure polymorph coesite a higher ε of 214,000 $\pm$ 14,000 $\mathrm{lmol}_{H2O}^{-1}\mathrm{cm}^{-2}$ was calculated, that is in good agreement with earlier established data [8]. For stishovite an even larger value of ε = 461,000 $\pm$ 68,000 $\mathrm{lmol}_{H2O}^{-1}\mathrm{cm}^{-2}$ was derived, similar to that determined by [9]. Evaluation of data from this study confirms that **not** using mineral specific IR calibrations for the OH quantification in NAMs leads to inaccurate estimations of OH concentrations, that constitute the basis for modelling the earth's deep water cycle.

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