

Polarized Single-Crystal and High-pressure IR Study of Hydrogen in Coesite

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The incorporation of hydrogen into the coesite structure was investigated in multi-anvil experiments performed at 3.1 to 7.5 GPa and 700 to 1100 °C. Hydrogen enters the coesite structure at high pressure (> 5.0 GPa) and high temperature (1100 °C) only. The FTIR spectra show three relatively intense bands at 3575, 3516 and 3459 cm^{-1} (ν_1 to ν_3 , respectively) and two very weak bands at 3296 and 3210 cm^{-1} (ν_4 and ν_5 , respectively). The positions of the ν_1 - ν_4 bands agree very well with those previously reported by Li et al. (1997) and Mosenfelder (2000). The band at 3516 cm^{-1} is strongly asymmetric and can be resolved into two bands 3528 (ν_{2a}) and 3508 (ν_{2b}) with nearly identical areas. Polarized infrared absorption spectra of single-crystal slabs parallel to (010) and (100) reveal a strong pleochroism of the OH - vibrations. High-pressure FTIR spectra performed in DAC at pressures up to 8.0 GPa show that the peak positions of the ν_1 - ν_3 bands decrease linearly with pressure. The mode Grüneisen parameters for the ν_1 to ν_3 bands are -0.074, -0.144 and -0.398, respectively. There is a linear decrease of the pressure derivatives with band position which follows the trend proposed by Hofmeister *et al.* (1999). The FWHM's of the ν_1 to ν_3 bands increase from 35, 21 and 28 cm^{-1} in the spectra at ambient conditions to 71, 68 and 105 in the 8 GPa spectra. On the basis of these results a model for the incorporation of hydrogen in coesite has been developed: the OH-defects are introduced into the structure by the substitution $\text{Si}^{4+} + 4\text{O}^{2-} = \text{Al}^{3+} + 4\text{OH}^-$ which gives rise to the ν_1 to ν_3 vibrations - ν_4 and ν_5 are most probably coupled to Al substitution.

References:

- A.M. Hofmeister, H. Cynn, P.C. Burnley and S. Meade "Vibrational spectra of dense, hydrous silicates at high pressure: Importance of the hydrogen bond angle", *American Mineralogist*, **84**, 454 - 464, 1999.
- W. Li, R. Lu, H. Yang H., C.T. Prewitt and Y. Fei "Hydrogen in synthetic coesite crystals", *EOS*, **78**: 736, 1997.
- J. Mosenfelder "Pressure dependence of hydroxyl solubility in coesite". *Physics and chemistry of Minerals*, **27**, 610-617, 2000.