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Ordering of hydroxyl defects in hydrous wadsleyite (β-Mg_2SiO_4)

S.C. KOHN,[1,*] R.A. BROOKER,[1] D.J. FROST,[2] A.E. SLESINGER,[1] AND B.J. WOOD[1]

[1]Department of Earth Sciences, University of Bristol, Bristol, BS8 1RJ, U.K.
[2]Bayerisches Geoinstitut, Universität Bayreuth, D-95447, Germany

ABSTRACT

Samples of wadsleyite (β-Mg_2SiO_4) containing a range of dissolved water concentrations up to 1.5 wt% were synthesized at 1300 °C and 15 GPa. The samples were studied using ^{1}H MAS NMR and FTIR spectroscopy to determine the ordering of OH within the structure. As the ^{1}H NMR chemical shift and O-H···O stretching frequency are both known to be correlated with the O-H···O distances in silicate and other materials, the spectroscopic data were compared with O···O distances calculated from the published crystal structure of hydrous wadsleyite.

Using this approach we show that the hydroxyl ions in wadsleyite containing 0.8–1.5 wt% H_2O are highly disordered, occupying at least 14 of the 17 possible O-H···O environments, including some with strong hydrogen bonding. In contrast, for low water concentrations (<0.4 wt%) the hydroxyl ions are less disordered, with four environments being much more abundant than the others are. Three of these environments appear to involve protonation of O1, in agreement with most previous suggestions, and the fourth is probably O2-H···O2.

It is probable that the degree of disorder will increase with increasing temperature, so it should be taken into account when predicting phase equilibria involving hydrous wadsleyite and when extrapolating data on density and elastic properties from room temperature measurements.