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Sublattice disorder and Fe-Mg substitution in brucite: Implications for the subduction-zone water cycle

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Abstract

The vibrational properties of hydroxyl groups in pure and Fe-bearing brucite have been investigated under high-pressure and -temperature conditions relevant to subduction zones. Using externally heated diamond-anvil cell techniques combined with in situ Raman spectroscopy, we observed that the hydroxyl stretching modes in pure brucite change from blueshift to redshift at ~600 K and 1.2 GPa. This indicates a sublattice proton order-disorder transition associated with decreasing interlayer spacing in brucite. Moreover, the Fe-Mg substitution in brucite leads to a secondary hydroxyl stretching band at 3644.6 cm^{-1} for $Mg_{0.9}Fe_{0.1}(OH)_2$, while the primary Raman band is changed to 3636.7 cm^{-1}. This new Raman mode persists with increasing temperature at atmospheric pressure but disappears at about 3.0 GPa. The decomposition temperature of this Fe-bearing brucite sample is about 130 K lower compared to pure brucite under high oxygen fugacity conditions. These results suggest that the sublattice transition and Fe-Mg substitution may influence the stability of brucite, providing insight into the deep-water cycle at shallow subduction zones.

Keywords: Brucite, sublattice disorder, Fe-Mg substitution, subduction zone, oxygen fugacity