

Structural study of the coherent dehydration of wadsleyite

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ABSTRACT

The coherent dehydration of pure-Mg wadsleyite has been investigated by single-crystal X-ray diffraction at high temperature and room pressure. Hydrous wadsleyite with 2.8 wt% H₂O has monoclinic unit-cell parameters of $a = 5.6693(4)$, $b = 11.571(1)$, $c = 8.2407(5)$ Å, $\beta = 90.209(3)^\circ$, and $V = 540.59(7)$ Å³. Dehydration begins at 635 K with an abrupt increase in the a -axis and decrease in b . After dehydration is complete, the dehydrated sample is orthorhombic with $a = 5.6995(3)$, $b = 11.4589(8)$, $c = 8.2556(5)$ Å, and $V = 539.17(6)$ Å³ at ambient conditions. Atom position and displacement parameters have been refined for both hydrous and dehydrated wadsleyite samples from intensity measurements conducted at high temperatures. The most significant changes during dehydration are systematic decreases in M2–O1 and M3–O1 bond lengths. After dehydration, M2–O1 and M3–O1 bonds decrease by 3% and 2.5%, respectively. While the length changes of the other M–O bonds are no more than 1%, consistent with the hydration mechanism being protonation of O1. For the monoclinic structure, the average thermal expansion coefficient is $38.4(3) \times 10^{-6} \text{ K}^{-1}$ before dehydration and $28.1(8) \times 10^{-6} \text{ K}^{-1}$ for the dehydrated sample. The volumetric thermal expansion coefficients for MgO₆ octahedra in the hydrous sample, $\alpha_0(V)$, are 36(4), 41(4), 49(5), and 35(4) (10^{-6} K^{-1}) for M1, M2, M3A, and M3B, respectively. In the dehydrated sample, they are 35(5), 34(4), and 36(2) (10^{-6} K^{-1}) for M1, M2, and M3, respectively. No significant thermal expansion is observed for SiO₄ tetrahedra of either the hydrous or dehydrated sample.

Keywords: Hydrous, dehydrated, wadsleyite, thermal expansion