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LETTER

Crystal chemistry of hydration in aluminous orthopyroxene

JOSEPH R. SMYTH,[1,*] KATRIN MIERDEL,[2] HANS KEPPLER,[3] FALKO LANGENHORST,[4] LEONID DUBROVINSKY,[3] AND FABRIZIO NESTOLA[5]

[1]Department of Geological Sciences, University of Colorado, Boulder, Colorado 80309 U.S.A.
[2]Institut für Geowissenschaften, Universität Tübingen, D-72074 Tübingen, Germany
[3]Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany
[4]Institut für Geowissenschaften, Friedrich-Schiller-Universität Jena, Burgweg 11, D-07749 Jena, Germany
[5]Dipartimento di Geoscienze, Università di Padova, Corso Garibaldi 37, I-35137 Padova, Italy

ABSTRACT

Hydrogen incorporation in aluminous orthopyroxene may control the generation of melt and dominate the seismic properties at the base of the Earth's lithosphere. To clarify the substitution mechanism of H, we have synthesized, characterized, and refined the crystal structure of this potentially significant variant of orthopyroxene. The experimentally produced crystals are small needles up to approximately $20 \times 20 \times 100$ μm in size. Electron microprobe chemical analysis indicates about 11.7 wt% Al_2O_3. FTIR spectra indicate 7500 ppmw H_2O with absorbance features qualitatively similar to natural mantle orthopyroxenes. TEM imagery indicates that the phase is pure orthopyroxene with low concentrations of defects and inclusions. Cell-parameter refinement from single-crystal X-ray diffraction gives a = 18.1876(7) Å; b = 8.7352(7) Å; c = 5.1789 (5) Å, V = 822.79(11) Å^3, which is 1.2% smaller than pure Mg anhydrous orthoenstatite. The crystal structure has been refined from single-crystal X-ray intensity data measured using a rotating anode X-ray generator, micro-focused X-ray beam, and CCD detector system. The refined structure indicates about 5% vacancy in M2 and significant Al occupancy in both M1 and T2, consistent with its composition, $(Mg_{0.95,0.05})^{M2}$, $(Mg_{0.79}Al_{0.21})^{M1}$, $(Al_{0.25}Si_{0.75})^{T2}$ Si^{T1} O_6. The existence of hydrous orthopyroxene in the mantle could absorb water released from olivine on decompression to delay the onset of melting in the spinel stability region in mantle peridotite compositions.

Keywords: Orthopyroxene, crystal synthesis, high-pressure studies, X-ray data, crystal structure