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Pressure-induced *Pbca-P*$2_1/c$ phase transition of natural orthoenstatite: Compositional effect and its geophysical implications

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Abstract

Raman spectroscopy has been employed to investigate possible compositional effects on the high-pressure phase transition of Mg-rich orthoenstatite to a newly discovered $P2_1/c$ phase. Three natural orthoenstatite (OEN) samples were used in this study: near end-member Mg orthoenstatite (Zabargad Island, Egypt), Al-free, Fe-bearing orthoenstatite (Morogoro, Tanzania) and Al-rich, Fe,Ca-bearing orthoenstatite (Kilbourne Hole, New Mexico). Experiments were carried out at room temperature. For all samples, the high-pressure phase transition is characterized by a splitting of the 660–680 cm^{-1} doublet in the Raman spectrum into a triplet, with a corresponding change of peak intensities. These spectral changes are caused by the lowered symmetry of the high-pressure phase, as indicated by structural refinement from single-crystal X-ray diffraction results. The high-pressure phase of all samples appears to have space group $P2_1/c$. No evidence for a $C2/c$ phase was observed. Our results indicate that upon compression, the presence of 10 mol% Fe decreases the onset pressure of formation of the high-pressure $P2_1/c$ phase by about 1 GPa. Results for the Kilbourne Hole OEN show that upon compression, a combined enrichment of Al and Ca contents increases the onset pressure of formation of high-pressure clinoesntatite (HPCEN2) by over 3 GPa relative to Tanzania OEN. Upon decompression, all samples revert to single crystals of the orthoenstatite starting phase. Our measurements suggest that orthoenstatite is the prevalent phase of Mg-rich pyroxene throughout the uppermost mantle, whereas the newly discovered $P2_1/c$ phase might be present near the bottom of uppermost mantle, slightly shallower than the top of the transition zone.

Keywords: Orthoenstatite, high-pressure clinoenstatite, high-pressure phase transition, upper mantle, Raman spectroscopy