

LETTER

Bridgmanite-like crystal structure in the novel Ti-rich phase synthesized at transition zone condition

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ABSTRACT

A new Ti-bearing bridgmanite-like phase with a threefold commensurate superstructure of the ideal MgSiO_3 -perovskite structure was observed in a $[\text{Mg}_{5/6}\text{Al}_{1/6}][\text{Si}_{1/2}\text{Ti}_{1/3}\text{Al}_{1/6}]\text{O}_3$ crystal synthesized in the model system $\text{Mg}_3\text{Al}_2\text{Si}_3\text{O}_{12}$ – MgTiO_3 at 20 GPa and 1600 °C. The compound was found to be orthorhombic, space group *Pnma*, with lattice parameters $a = 14.767(3)$, $b = 6.958(1)$, $c = 4.812(1)$ Å, $V = 494.4(2)$ Å³, which represents a $3\mathbf{a} \times \mathbf{b} \times \mathbf{c}$ superstructure of the typical *Pnma* perovskite structure. The structure was refined to $R = 0.024$ using 846 independent reflections. The superstructure mainly arises from the ordering of titanium in one of the octahedral positions. Crystal-chemical details of the different polyhedra in the superstructure are discussed in comparison to pure MgSiO_3 . This is the first documented superstructure of a bridgmanite phase, and Ti-rich bridgmanite in the lower mantle arising from local Ti-enrichments may exhibit different physical properties and elemental partitioning behavior from Ti-poor, peridotitic bridgmanite. The study also shows that large amounts of Ti can stabilize bridgmanite-like compounds at considerably lower pressure than lower mantle conditions.

Keywords: Bridgmanite, titanium, lower mantle, crystal structure, microprobe analysis, synthesis