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LETTER

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

LUCA BINDI[1,2,*], EKATERINA SIROTKINA[3,4], ANDREY V. BOBROV[3,4], MICHAEL J. WALTER[5], DMITRY PUSHCHAROVSKY[3], AND TETSUO IRIFUNE[6,7]

[1]Dipartimento di Scienze della Terra, Università di Firenze, Via La Pira 4, I-50121 Firenze, Italy
[2]CNR–Istituto di Geoscienze e Georisorse, sezione di Firenze, Via La Pira 4, I-50121 Firenze, Italy
[3]Geological Faculty, Moscow State University, Leninskie Gory, 119234, Moscow, Russia
[4]Vernadsky Institute of Geochemistry and Analytical Chemistry of Russian Academy of Sciences, 119991Moscow, Russia
[5]School of Earth Sciences, University of Bristol, Bristol BS8 1RJ, U.K.
[6]Geodynamics Research Center, Ehime University, Matsuyama 790-8577, Japan
[7]Earth-Life Science Institute, Tokyo Institute of Technology, Tokyo 152-8550, Japan

ABSTRACT

A new Ti-bearing bridgmanite-like phase with a threefold commensurate superstructure of the ideal $MgSiO_3$-perovskite structure was observed in a $[Mg_{5/6}Al_{1/6}][Si_{1/2}Ti_{1/3}Al_{1/6}]O_3$ crystal synthesized in the model system $Mg_3Al_2Si_3O_{12}$–$MgTiO_3$ 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, $V = 494.4(2)$ Å^3, 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