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LETTER

Chromium solubility in perovskite at high pressure: The structure of $(Mg_{1-x}Cr_x)(Si_{1-x}Cr_x)O_3$ (with $x = 0.07$) synthesized at 23 GPa and 1600 °C

LUCA BINDI[1,2,*], EKATERINA A. SIROTKINA[3], ANDREY V. BOBROV[3] AND TETSUO IRIFUNE[4,5]

[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]Department of Petrology, Geological Faculty, Moscow State University, Leninskie Gory, 119234, Moscow, Russia
[4]Geodynamics Research Center, Ehime University, Matsuyama 790-8577, Japan
[5]Earth-Life Science Institute, Tokyo Institute of Technology, Tokyo 152-8550, Japan

ABSTRACT

The crystal structure and chemical composition of a crystal of $(Mg_{1-x}Cr_x)(Si_{1-x}Cr_x)O_3$ perovskite (with $x = 0.07$) synthesized in the model system $Mg_3Cr_2Si_3O_{12}$–$Mg_4Si_4O_{12}$ at 23 GPa and 1600 °C have been investigated. The compound was found to be orthorhombic, space group *Pbnm*, with lattice parameters $a = 4.8213(5)$, $b = 4.9368(6)$, $c = 6.9132(8)$ Å, $V = 164.55(3)$ Å^3. The structure was refined to $R = 0.046$ using 473 independent reflections. Chromium was found to substitute for both Mg at the dodecahedral X site (with a mean bond distance of 2.187 Å) and Si at the octahedral Y site (mean: 1.814 Å), according to the reaction $Mg^{2+} + Si^{4+} = 2Cr^{3+}$. Such substitutions cause a shortening of the <X-O> and a lengthening of the <Y-O> distances with respect to the values typically observed for pure $MgSiO_3$ perovskite. Although high Cr-contents are not considered in the pyrolite model, Cr-bearing perovskite may be an important host for chromium in the lower mantle. The successful synthesis of perovskite with high-Cr content and its structural characterization are of key importance because the study of its thermodynamic constants combined with the data on phase relations in the lower-mantle systems can provide new constraints on thermobarometry of perovskite-bearing assemblages.

Keywords: Perovskite, chromium, lower mantle, crystal structure, microprobe analysis, synthesis