

A shallow origin of so-called ultrahigh-pressure chromitites, based on single-crystal X-ray structure analysis of the high-pressure $\text{Mg}_2\text{Cr}_2\text{O}_5$ phase, with modified ludwigite-type structure

**TAKAYUKI ISHII^{1,*}, NORIYOSHI TSUJINO², HIDEKAZU ARII^{1,†}, KIYOSHI FUJINO³,
NOBUYOSHI MIYAJIMA⁴, HIROSHI KOJITANI¹, TAKEHIRO KUNIMOTO³, AND MASAKI AKAOGI¹**

¹Department of Chemistry, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171-8588, Japan

²Institute for Study of the Earth's Interior, Okayama University, Misasa, Tottori 682-0193, Japan

³Geodynamics Research Center, Ehime University, Matsuyama, Ehime 790-8577, Japan

⁴Bayerisches Geoinstitut, University of Bayreuth, 95440 Bayreuth, Germany

ABSTRACT

The crystal structure of the high-pressure $\text{Mg}_2\text{Cr}_2\text{O}_5$ phase was studied by single-crystal X-ray diffraction (XRD) analysis for the recovered samples. The 61 parameters including anisotropic displacement parameters of each atom and site occupancies of Mg and Cr in cation sites were refined with $R_1 = 1.26\%$, $wR_2 = 4.33\%$, and $S_{\text{fit}} = 1.265$ for 470 unique reflections. The results show that the structure of the recovered $\text{Mg}_2\text{Cr}_2\text{O}_5$ phase is the same as modified ludwigite (mLd)-type $\text{Mg}_2\text{Al}_2\text{O}_5$ [space group: *Pbam* (no. 55)], and the lattice parameters are $a = 9.6091(2)$, $b = 12.4324(2)$, $c = 2.8498(1)$ Å ($Z = 4$). The refined structure of the $\text{Mg}_2\text{Cr}_2\text{O}_5$ phase has four (Mg,Cr) O_6 octahedral sites and a MgO_6 trigonal prism site, and is similar to but distinct from that of CaFe_3O_5 -type $\text{Mg}_2\text{Fe}_2\text{O}_5$ phase, which has two octahedral sites and a bicapped trigonal prism site with two longer cation-oxygen bonds. The isotropic atomic displacement parameter of the trigonal prism site cation in mLd-type $\text{Mg}_2\text{Cr}_2\text{O}_5$ is relatively small compared with that of CaFe_3O_5 -type $\text{Mg}_2\text{Fe}_2\text{O}_5$, suggesting that the trigonal prism site is less flexible for cation substitution than that of CaFe_3O_5 -type structure. To stabilize mLd-type $A_2^{2+}B_2^{3+}\text{O}_5$ phase, it would be an important factor for the B^{3+} cation to have high octahedral-site preference, resulting in only A^{2+} cation being accommodated in the tight trigonal prism site. Our study also suggests that mLd-type phase with $(\text{Mg,Fe}^{2+})_2\text{Cr}_2\text{O}_5$ composition would crystallize as one of decomposed phases of chromitites, when the chromitites were possibly subducted into the mantle transition zone.

Keywords: Single-crystal structure analysis, high pressure, modified ludwigite structure, chromite, $\text{Mg}_2\text{Cr}_2\text{O}_5$