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A shallow origin of so-called ultrahigh-pressure chromitites, based on single-crystal X-ray structure analysis of the high-pressure $Mg_2Cr_2O_5$ phase, with modified ludwigite-type structure

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ABSTRACT

The crystal structure of the high-pressure $Mg_2Cr_2O_5$ 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 $Mg_2Cr_2O_5$ phase is the same as modified ludwigite (mLd)-type $Mg_2Al_2O_5$ [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 $Mg_2Cr_2O_5$ 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 $Mg_2Fe_2O_5$ 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 $Mg_2Cr_2O_5$ is relatively small compared with that of $CaFe_3O_5$-type $Mg_2Fe_2O_5$, suggesting that the trigonal prism site is less flexible for cation substitution than that of $CaFe_3O_5$-type structure. To stabilize mLd-type $A_2^{2+}B_2^{3+}O_5$ 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 $(Mg,Fe^{2+})_2Cr_2O_5$ 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, $Mg_2Cr_2O_5$