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Complete substitution of Fe^{2+} by Mg in Fe_4O_5: The crystal structure of the $Mg_2Fe_2O_5$ end-member

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Abstract

The crystal structure of a novel $Mg_2Fe_2O_5$ oxide synthetized at 15 GPa and 1550 °C has been determined by means of single-crystal X-ray diffraction. This compound is isostructural with Fe_4O_5 and can be considered as the other end-member of a solid solution between these two oxides involving the substitution of Fe^{2+} for Mg. The resulting unit-cell lattice parameters $a = 2.8889(4)$, $b = 9.7282(4)$, and $c = 12.5523(7)$ Å are smaller than those of Fe_4O_5. Mg and Fe^{3+} cations are found to be disordered among the three crystallographic sites of the $Mg_2Fe_2O_5$ structure, although preference of Mg for the trigonal prism coordination (M3) is observed. Substitution of Mg into the Fe_4O_5 structure reduces the octahedral distortion of both the M1 and M2 sites. Like Mg, Cr has recently been found to substitute into Fe_4O_5, so that $Fe^{3+}/\sum Fe$ can vary from 0 to 1.0 in the Mg-Cr-Fe oxides system. Substitution of both Mg and Cr in Fe_4O_5 also makes this phase more relevant for bulk compositions expected in the Earth's transition zone and deep upper mantle. M_4O_5 phases having the $CaFe_3O_5$-type structure, therefore, need to be considered as a new addition to the phase relations of several simple oxide systems at pressure and temperature conditions at which the spinel-structured phases become unstable.

Keywords: $Mg_2Fe_2O_5$, Fe_4O_5, transition zone, high-pressure, crystal structure