American Mineralogist, Volume 92, pages 1112–1118, 2007

High-pressure phase relations and crystal chemistry of calcium ferrite-type solid solutions in the system $MgAl_2O_4$-Mg_2SiO_4

HIROSHI KOJITANI,* RYOSUKE HISATOMI, AND MASAKI AKAOGI

Department of Chemistry, Faculty of Science, Gakushuin University, 1-5-1 Mejiro, Toshima-ku, Tokyo 171-8588, Japan

ABSTRACT

To map the stability field of calcium ferrite-type $MgAl_2O_4$–Mg_2SiO_4 solid solutions, high-pressure phase relations in the system $MgAl_2O_4$-Mg_2SiO_4 were studied in the compositional range of 0 to 50 mol% Mg_2SiO_4. The calcium ferrite solid solutions are stable above 23 GPa at 1600 °C, and the maximum solubility of Mg_2SiO_4 component in $MgAl_2O_4$ calcium ferrite is 34 mol%. Lattice parameters and unit-cell volume of calcium ferrite-type $MgAl_2O_4$ (space group *Pbnm*) determined by Rietveld analysis are $a = 9.9498(6)$ Å, $b = 8.6468(6)$ Å, $c = 2.7901(2)$ Å, and $V = 240.02(2)$ Å^3. Lattice parameters for the $MgAl_2O_4$–Mg_2SiO_4 solid solutions with the compositions of 14, 24, and 34 mol% Mg_2SiO_4 indicated the following compositional dependency of lattice parameters: a (Å) = $9.9498 + 0.1947 \cdot X_{Mg_2SiO_4}$, b (Å) = $8.6468 - 0.1097 \cdot X_{Mg_2SiO_4}$, and c (Å) = $2.7901 + 0.0086 \cdot X_{Mg_2SiO_4}$, where $X_{Mg_2SiO_4}$ is the mole fraction of Mg_2SiO_4 component. A linear extrapolation of the composition-molar volume relationship gave an estimated volume of 36.49(2) cm^3/mol for the hypothetical calcium ferrite-type Mg_2SiO_4. This value is larger than that of the isochemical mixture of $MgSiO_3$ perovskite and MgO, 35.72(1) cm^3/mol. This implies that the mixture of $MgSiO_3$ perovskite and MgO is more stable than the hypothetical calcium ferrite-type Mg_2SiO_4 under the lower mantle conditions.

Keywords: $MgAl_2O_4$, Mg_2SiO_4, calcium ferrite, high pressure, phase relation, Rietveld refinement