Synthesis, structural features and isomorphism of oxide phases in the Ca-Al-O system

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The relative content of Al_2O_3 in the Earth's mantle ranges within 4.0–4.5 wt % [1]. It is generally believed that in the deep Earth Al is mostly incorporated in phases with the perovskite-type structure. However, according to data of atomistic modeling [2], only minor amounts of Ca and Al may be included in perovskite phases. Instead, Ca,Al(Fe)-oxides should be formed and absorb most of Al, especially for the MORB compositions [3].

Experiments on synthesis of the phases in the $CaO–Al_2O_3$ system with addition of Fe and Mg were carried out on a 1200-t multi-anvil Sumitomo press at P=15 and 24 GPa, T=1600°C at the Bayerisches Geoinstitut (Germany).

The phases $CaAl_2O_4$, $Ca_2Al_6O_{11}$ and $Ca(Al, Fe)_2O_4$ were synthesized. $Ca_2Al_6O_{11}$ was obtained for the first time. Orthorhombic phases $CaAl_2O_4$ and $Ca(Al, Fe)_2O_4$ crystallize in a space group *Pnma* and have the $CaFe_2O_4$-type structure. Two independent atoms Al1 and Al2 are in the octahedral sites, Ca cations are characterized by the eight-fold coordination (and are located in the tunnels formed by linked double chains). The tetragonal $Ca_2Al_6O_{11}$ phase crystallizes with a space group $P4_2/mnm$. There are two independent atoms Al1 and Al2 in the octahedral site. These AlO6-octahedra form two types of tunnels in the structure. Ca cations are in the eight-fold coordination and occupy one type of structure tunnel. The phase $Ca(Al,Fe)_2O_4$ studied in diamond anvils with synchrotron radiation up to a pressure of ~60GPa. There was no detected of phase transitions. Spin transition for iron was registered. Structures of the new phase $Ca_2Al_6O_{11}$ and phase $CaAl_2O_4$ were refined.

Our results suggest that both studied phases are stable in the transition zone and can be considered as potential aluminum concentrators in the Earth's deep geospheres.

Support: Russian Science Foundation, no. 17-17-01169.

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