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Crystal structure analysis of a new high-pressure strontium silicate

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$SrSiO_3$ is an analog material to $CaSiO_3$ which is an important component of the Earth's crust- and mantle-constituting minerals. High-pressure phase relation experiments in $SrSiO_3$ showed that δ'-$SrSiO_3$ is stable up to about 10 GPa and decomposes into $BaGe_2O_5$-III -type $SrSi_2O_5$ + larnite-type Sr_2SiO_4 between 14 and 20 GPa (Kojitani et al., 2005). Then, hexagonal perovskite-type $SrSiO_3$ becomes stable above about 20 GPa (Yusa et al., 2005). However, phases except for larnite-type Sr_2SiO_4 appearing in the pressure range between 10 and 14 GPa have been unclear. In this study, crystal structure and composition of one of the unknown phases were determined.

A sample for single-crystal structure analysis was synthesized by heating a mixture of pseudowollastonite-type $CaSiO_3$ and SiO_2 cristobalite (mole ratio of 1:1) with a little amount of water at 12 GPa and 1200 ℃ for 90 min using a Kawai-type multi-anvil high-pressure apparatus. A single-crystal sample with 120x80x60 μm was used for the single-crystal X-ray diffraction measurement. 953 reflection data were analyzed using the SHELX-97 software. Composition analysis of the high-pressure phase was performed using SEM-EDS.

The composition analysis showed that the new high-pressure phase had a composition of $Sr_4Si_9O_{22}$. The single-crystal structure analysis suggests the monoclinic crystal system with the space group of $C2/m$. Lattice parameters were determined to be a = 13.3765(4) $\AA$, b = 5.2321(2) $\AA$, c = 11.6193(6) $\AA$, β = 113.976(4)deg. R factor was 1.25%. The framework of the obtained crystal structure consists of two layers by corner-sharing single chains of edge-shared SiO_6 octahedra or SiO_5 rhombic pyramid polyhedra and by corner-shared SiO_4 tetrahedra and SiO_6 octahedra. It should be mentioned that this structure includes the SiO_5 rhombic pyramids which are very rare in silicates. Strontium ions in the structure are arranged between the two layers and are coordinated by seven oxygens. The structure of δ'-$SrSiO_3$ consists of four-membered rings of SiO_4 tetrahedra and strontium ions coordinated by seven oxygens. On the other hand, $BaGe_2O_5$-III type $SrSi_2O_5$ has a framework by corner-shared SiO_6 octahedra and SiO_4 octahedra and coordination number of Si^{2+} is 12. The crystal structure determined in this study is consistent with the fact that its density would be between those of the lower-pressure and higher-pressure phases.

Keywords: strontium silicate, high-pressure, single-crystal structure analysis, SiO5 polyhedron