

# High-pressure decomposition phases of SrSiO<sub>3</sub>

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CaSiO<sub>3</sub> is one of the major components of the Earth's materials. Therefore, high-pressure phase transformations of CaSiO<sub>3</sub> has been investigated by a lot of researchers. For better understanding it by the method of crystal chemistry, it is needed to compare the high-pressure and high-temperature behavior with analogous materials to CaSiO<sub>3</sub>. SrSiO<sub>3</sub> is mentioned as such an analogous material. It has reported that SrSiO<sub>3</sub> transforms from pseudo-wollastonite type SrSiO<sub>3</sub> at ambient pressure to SrSiO<sub>3</sub>-2 and then to SrSiO<sub>3</sub>-3 with increasing pressure. The phase transition of SrSiO<sub>3</sub>-3 to another phase was observed at about 1000 C and beyond 10 GPa in this study. The composition analysis of a recovered sample by using SEM-EDS showed that SrSiO<sub>3</sub>-3 decomposed to two phases which had compositions of Sr<sub>2</sub>SiO<sub>4</sub> and SrSi<sub>2</sub>O<sub>5</sub>. This high-pressure decomposition reaction for SrSiO<sub>3</sub>-3 is very similar to that of CaSiO<sub>3</sub> walstromite to Ca<sub>2</sub>SiO<sub>4</sub> larnite + CaSi<sub>2</sub>O<sub>5</sub> titanite. Therefore it is expected that Sr<sub>2</sub>SiO<sub>4</sub> and SrSi<sub>2</sub>O<sub>5</sub> phases might have Ca<sub>2</sub>SiO<sub>4</sub> larnite and CaSi<sub>2</sub>O<sub>5</sub> titanite type structures, respectively. In this study, the Sr<sub>2</sub>SiO<sub>4</sub> and SrSi<sub>2</sub>O<sub>5</sub> phases were synthesized separately, and we tried determining the crystal structures of them.

The larnite type Sr<sub>2</sub>SiO<sub>4</sub> was synthesized by heating the mixture of SrCO<sub>3</sub> and SiO<sub>2</sub> silicic acid (2:1 in mole ratio) at 1250 C, 1 atm for 12 hours. High-pressure and high-temperature synthesis of SrSi<sub>2</sub>O<sub>5</sub> phase was made by using a Kawai-type multi-anvil apparatus at Gakushuin University. WC anvils with the truncated edge length of 5 mm were used. A pressure medium, a thermal insulator and a heater were MgO, LaCrO<sub>3</sub> and Pt, respectively. Temperature was observed by the Pt/Pt-13%Rh thermocouple at the center of the heater. A starting material was the mixture of pseudo-wollastonite type SrSiO<sub>3</sub> and SiO<sub>2</sub> quartz (1:1 in mole ratio). The starting material was heated at 16 GPa, 900 C for one hour. A powder X-ray diffractometer (Cr Kalpha, 45 kV, 250 mA) at Gakushuin University was used for measuring XRD patterns of the synthesized samples. The XRD measurement was performed with the 2theta range of 20-140 degree using the step scanning method.

As the XRD pattern of the synthesized larnite type Sr<sub>2</sub>SiO<sub>4</sub> shows very good agreement with part of XRD peaks for the high-pressure recovered sample of the decomposition phases, the high-pressure Sr<sub>2</sub>SiO<sub>4</sub> phase was identified as larnite type. On the other hand, a XRD pattern of the synthesized SrSi<sub>2</sub>O<sub>5</sub> phase is completely different from that of CaSi<sub>2</sub>O<sub>5</sub> titanite. It was found that the XRD pattern was very similar to that of BaGe<sub>2</sub>O<sub>5</sub>-3(orthorhombic, space group: Cmca) which has been reported as one of the high-pressure polymorphs of BaGe<sub>2</sub>O<sub>5</sub>. Since all of observed diffraction peaks for the SrSi<sub>2</sub>O<sub>5</sub> could be assigned by using the corresponding peaks for BaGe<sub>2</sub>O<sub>5</sub>-3, it is suggested that high-pressure SrSi<sub>2</sub>O<sub>5</sub> phase may have the same crystal structure as BaGe<sub>2</sub>O<sub>5</sub>-3. Therefore, we determined lattice parameters for SrSi<sub>2</sub>O<sub>5</sub> phase by using the crystal structure of BaGe<sub>2</sub>O<sub>5</sub>-3 as a model. The lattice parameters for the BaGe<sub>2</sub>O<sub>5</sub>-3 type SrSi<sub>2</sub>O<sub>5</sub> were obtained to be a = 5.2376(2) Å, b = 9.2751(3) Å and c = 13.4352(3) Å.