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## Crystal growth of Na-Si clathrates by the flux method

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**Introduction:** Si clathrate compounds have been widely studied due to their unique open-framework structures of Si polyhedrons. Two types of Si clathrates encapsulating Na atoms have been known: type I ( $\text{Na}_8\text{Si}_{46}$ ) and type II ( $\text{Na}_x\text{Si}_{136}$ ,  $0 < x \leq 24$ ). These Na-Si clathrates have been generally synthesized by thermal decomposition of a Na-Si binary compound,  $\text{Na}_4\text{Si}_4$ , at 673–823 K under high-vacuum conditions ( $< 10^{-2}$  Pa), and the obtained samples were in the form of powder with a particle size in the micrometer range.

**Purpose:** The purpose of this study is the crystal growth of the type I and type II Na-Si clathrates by using a Na-Sn flux.

**Experiment:** The starting material of a mixture of Na,  $\text{Na}_4\text{Si}_4$ , and  $\text{Na}_{15}\text{Sn}_4$  was prepared by heating Na, Si, and Sn (molar ratio, Na/Si/Sn = 6:2:1) at 1173 K in Ar atmosphere. The mixture was heated at 673–873 K for 6–24 hours in the container with a temperature gradient. After heating, air-sensitive compounds in the samples, such as Na-Sn compounds, were reacted with ethanol, and the water-soluble reactants were removed by washing with water. Sn present in the products or formed by the ethanol treatment was removed by dissolution in a dilute nitric acid aqueous solution.

**Results:** The single crystals of type I clathrate were crystallized due to the evaporation of Na from the Na-Sn-Si solution at 673–773 K. Most of the single crystals had sizes of several hundred micrometers to 1 mm, and the maximum size reached to about 3 mm. Heating the starting mixture at 823–873 K resulted in the crystal growth of the type II clathrate. The single crystals having {111} habit planes grew up to about 2 mm in size.

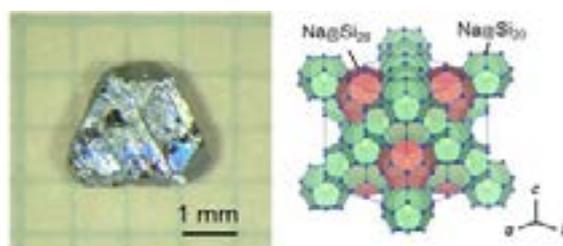


Figure 1: Single crystal (left) and the crystal structure (right) of type II Na-Si clathrate.

## Biography

Haruhiko Morito has his expertise in Material Science and Engineering. The main objective of his research is to develop an emerging material which has a new function and new physical properties. In particular, he has developed new functional ceramics containing alkali metals. He has also developed a new crystal growth process based on the binary phase diagram of sodium and silicon. He has synthesized various silicon-based materials by the sodium flux method.

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