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Structural change of hauyne with increasing temperature

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Hauyne, $Na_3CaSi_3Al_3O_{12}SO_4$, belongs to the sodalite group. Most of nature hauynes have modulated structure. Previous researchers (e.g. Saalfeld, 1961; Tsuchiya and Takeuchi, 1985) studied the modulated structure of hauynes from some localities by X-ray and electron diffraction methods. The results from heating experiments showed there is a discontinuity of thermal expansion between 550 ℃ and 700 ℃, and the themal expansion coefficient of hauyne changed to small value above 700 ℃ (e.g. Taylor, 1968). Disappearance of satellite reflections, which indicated the phase transition, was observed between 390 ℃ and 407 ℃ by high temperature in situ synchrotron X-ray powder diffraction experiment (Hassan *et al*., 2004). The relationship between the structural change and the discontinuity of thermal expansion is unclear. High temperature in situ single crystal X-ray diffraction experiments was conducted to investigate relationship between structural charge and discontinuity of thermal expansion.

Hauyne from eifel, German was used to our experiments. The backscattered electron images showed the chemical composition of the crystal was homogenerous, and its chemical formula was determined as $Na_{2.83}Ca_{0.95}K_{0.21}Si_{3.06}Al_{2.93}O_{12}(SO_4)_{0.95}Cl_{0.03}$ by using an energy dispersive X-ray spectrometer (JEOL, JSM-7001F). High temperature in situ single crystal X-ray diffraction experiments were examined by using an imaging plate type X-ray diffractmeter (Rigaku, R-AXIS IV++) with a horseshoe-shaped Pt heater (Huber). Observation of the satellite peaks and determination of cell parameter were performed at eight points between 20 ℃ and 700 ℃. Crystal Clear-SM 1.4.0 (Rigaku) was used for data analysis.

The lattice parameter of the modulated structure of the sample was approximately eight times long as the basic structure. Satellite reflections were disappeared around 700 ℃ although they were observed until 600 ℃, therefore, structural change was indicated in the temperature range. Also, the axial length of a-axis increased monotonously with increasing temperature, and the thermal expansion coefficient between 600 ℃ and 700 ℃ have smaller value. The results suggested structural change of hauyne would affect the discontinuity of thermal expansion.

Keywords: hauyne, modulated structure, single-crystal X-ray diffraction, high temperature, in situ observation