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Synchrotron powder X-ray diffraction study of the structural thermal properties on hydrogrossular

KATO, Masato[1*] ; KYONO, Atsushi[2]

[1]Graduate School of Life and Environmental Science, [2]Graduate School of Life and Environmental Science

Synchrotron powder X-ray diffraction study on synthetic Si-free hydrogrossular, katoite $Ca_3Al_2(O_4H_4)_3$, were performed at temperature range from 300 to 10 K. The temperature dependence of structure parameters was refined by Rietveld analysis. Since structural contraction with decreasing temperature would directly cause a phase transition on the hydrogrossular structure, three candidates for space group: *Ia*-3*d* (katoite at ambient), *I*-43*d* (katoite at high pressure), and $I4_1/acd$ (majorite), were applied to the X-ray diffraction profile fitting collected at 10 K. The final Rw with the *Ia*-3*d* space group consequently results in the smallest value, which suggests that the katoite structure remains unchanged up to the lowest temperature of 10 K. However, the temperature dependence of the unit cell volume shows two different expansion coefficients at temperatures above and below 100 K. It can be accounted for by the effect of the repulsion between atoms of the same species. Whereas the unit cell of katoite is monotonously contracted with decreasing temperature, the O_4H_4 tetrahedron and AlO_6 octahedron are alternatively expanded and contracted. Compared with the phase transition in katoite under high pressure, moreover, the unit cell volume contraction up to 5 GPa is about eight times larger than that under low temperature. The structural characteristics could therefore explain the reason why no phase transition occurs in katoite at low temperature condition.

Keywords: katoite, synchrotron pwder X-ray diffraction, Rietveld analysis, O4H4 tetrahedron