Equation of state of NaCaAlF

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1. Introduction

In the high-pressure experiments above a few GPa, the generated pressure is usually estimated from the lattice parameters of a pressure marker compressed with sample, based on the known equation of state (EoS). To know it, the effect of the thermal expansion needs to be taken into account. In this study, we collected temperature dependence of lattice parameter of $Na_2Ca_3Al_2F_{14}$ in the temperature region from 10 to 300 K in order to determine EoS as functions of pressure and temperature by coupling with high-pressure data taken at the high-pressure beamline PLANET.

$Na_2Ca_3Al_2F_{14}$ is a cubic crystal with a lattice parameter of a=10.257 Å (Fig. 1). For its high symmetry and the large lattice constant, this material is often used to determine diffractometer parameters. The large lattice constant of this material is also considered to be effective in determining pressure in the experiments whose accessible Q-region is limited only to the large Q region, such as QENS and INS.

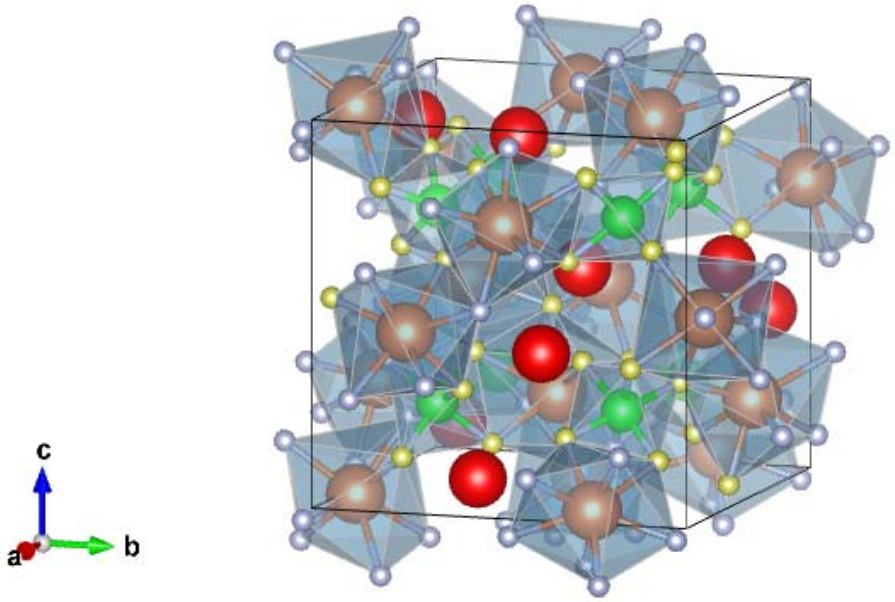

Fig. 1 Crystal structure of $Na_2Ca_3Al_2F_{14}$

2. Experiment

The experiment were conducted at BL08 using a standard cryostat. The sample was loaded in the ϕ3mm- vanadium can together with He gas. The diffraction patterns were collected at temperatures from 12K to 300K with the interval of 10 K in 10-200K and 20 K in 200-300K. The data were analyzed with the Z-code software, and the temperature dependence of the lattice parameters were finally obtained in the above temperature range.

3. Results

Figure 2 shows diffraction patterns obtained at various temperatures. High quality patterns were obtained in the whole temperature region of this study. The temperature dependence of the lattice

parameters are shown in Fig. 3. Now, we are trying to construct the EoS as functions of pressure and temperature by coupling with the data obtained at PLANET.

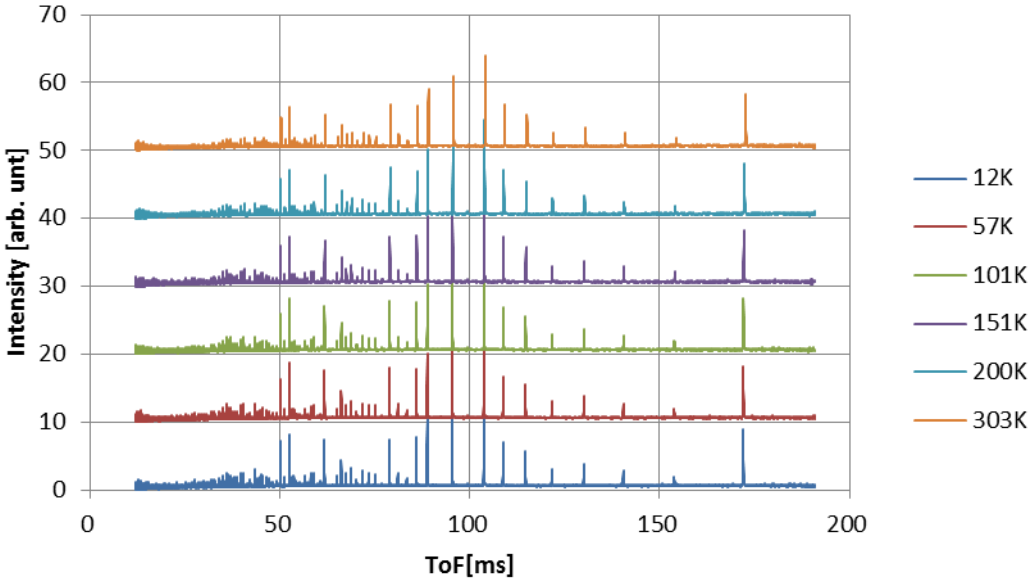

Fig. 2 Selected diffraction patterns taken at low temperatures.

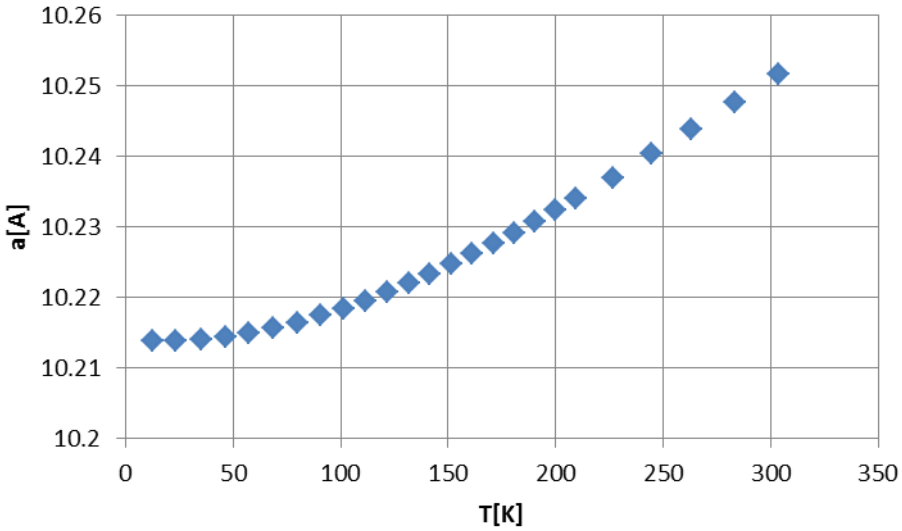

Fig. 3 Temperature dependence of the lattice parameter.

4. Conclusion

The temperature dependence of the lattice parameter of $Na_2Ca_3Al_2F_{14}$ was determined precisely by low-temperature neutron-diffraction experiments at BL08. By coupling with the pressure dependence, the EoS of $Na_2Ca_3Al_2F_{14}$ covering wide PT range is expected to be constructed. This will help us to determine the generated pressure at low temperatures in the QENS and INS experiments in which the accessible Q-region is limited only to high-Q region.