Crystal structure of 143 Zintl phase thermoelectric compound

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Zintl phase compounds are one of the most famous systems of thermoelectric materials. In particular, Sb-based 122-Zintl compounds AM_2Sb_2 (*A*: alkaline-earth metal, *M*: transition metal) have been intensively explored and found to exhibit high thermoelectric performance in various compositions. Some of them show the value of the dimensionless figure-of-merit (*Z*T) to be over 1. On the other hand, we have found that As-based Zintl compounds also exhibit high thermoelectric performance [1-3]. Although lighter atomic mass of As than Sb is a disadvantage in terms of the lattice thermal conductivity, those exhibit low thermal conductivity. Recently, we have found that As-based 143-Zintl compounds (AM_4As_3) of $NaZn_4As_3$ exhibit extremely low lattice thermal conductivity [4]. The crystal structure of 143-Zintl compounds resembles $CaAl_2Si_2$-type 122-Zintl compounds. It can be obtained by removing A ion layer in every two *MX* (X : pnictogen) layers. Because it consists of double conduction layers, higher carrier mobility than 122 compounds could be expected. Thus, high *Z*T value can be expected in 143-Zintl compounds.

In this experiment, we conducted powder diffraction measurements of $RbZn_4As_3$ at temperatures from 100K to 670K using HERMES diffractometer. The wavelength of incident neutron was 1.34 Å. Powder samples were installed in a vanadium cell with size of 6 mm in diameter.

Figure 1 shows a typical neutron diffraction pattern of $RbZn_4As_3$ at T = 278 K. A green line depicts calculated values of the Rietveld method using RIETAN-FP. The solid line at the bottom indicates the difference between observations and calculations.

Atomic parameters of $RbZn_4As_3$ were determined by the Rietveld analysis in the temperature range of 100 < T < 670 K. The value of isotropic atomic displacement parameters of Rb atom was approximately twice comparing with other atoms though it has heavier atomic mass. The result suggests large vibration of Rb atom, which can be anharmonic.

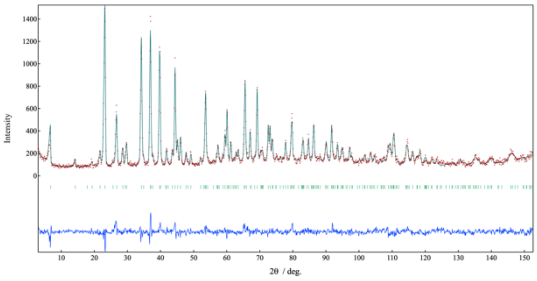

Fig. 1. Neutron diffraction patterns of $RbZn_4As_3$ at T = 278 K with the result of the Rietveld analysis. Vertical bars show the calculated positions of the diffraction peaks.

[1] K. Kihou, et al., Inorg. Chem. 56, 3709 (2017).

[2] H. Kunioka et al., Dalton Trans. 47, 16205 (2018).

[3] H. Kunioka et al., Inorg. Chem. 59, 5828 (2020).

[4] A. Yamashita et al., J. Solid State Chem. 291, 121588 (2020).