Correlation between structural and thermoelectric properties in Zn13Sb10

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beta-Zn13Sb10 compound has been well known as a good thermoelectric material in the moderate temperature range because of its high dimensionless figure of merit, ZT=1.3 at 670 K. The high thermoelectric performance of this material originates mainly from the extremely low-thermal conductivity. Recently, it has been reported that such an extremely low-thermal conductivity is attributed to the disordered structure of Zn atoms or rattling motion of Sb-dimmers along the c-axis. However, the origin of the extremely low-thermal conductivity still remains an unresolved problem. More recentrly, it has been revealed that the occupation of Zn atoms at the interstitial sites has also strong influence on the structural property as well as thermoelectric one. Especially, the alpha to beta structural transtion at 260 K is largely dependent on Zn composition. Thus, there are many problems left about the correlation between the structural and thermoelectric properties of Zn13Sb10 compound.

In this experiment, powder neutron diffraction measurements were performed to examine the detailed crystal structure of Zn13Sb10 compound to clarify the correlation between the structural and thermoelectric properties.

Polycrystalline ingots were prepared by gradient freeze (GF) and vacuum-melt to quench (VMQ) methods. The constituent elements of Zn(5N) and Sb(6N) with the stoichiometric ratio 13:10 were encapsulated in a double quartz ampoule under vacuum. The GF ingot was grown in a vertical GF furnace at the growth rate of 3 mm/day. On the other hand, the VMQ ingot was melted in an electric furnace for 2 days and then quenched into ice water. Neutron diffraction experiment was carried out at T1-3 HERMES in JRR-3M at room temperature with a wave length of 1.82646(6) A. The data were collected by an MFC mode.

Figure 1 shows the powder neutron diffraction profile and result of Rietvelt analysis of the Zn13Sb10 GF ingot at room temperature. The Rietveld analysis was performed by using a pattern profile fittig program RIETAN-2000. Any reflections from an impurity phase are not detected. All the reflection peaks can be indexed by assuming a rhombohedric hexagonal structure (R3-c). The lattice parameters determined by this analysis are in good agreement with that obtained by the previous X-ray diffraction experiment. The goodness of fit, S, is obtained to be 1.40 at present. However, the relative intensity of the reflection peaks is not well fitted. This may be due to the difference in occupation of Zn atom at the interstitial sites from the starting structure model proposed by other groups. More presice analysis is now under way to determine the site occupancy especially for Zn atoms and to discuss the correlation between structural and thermoelectric properties of Zn13Sb10 compound.

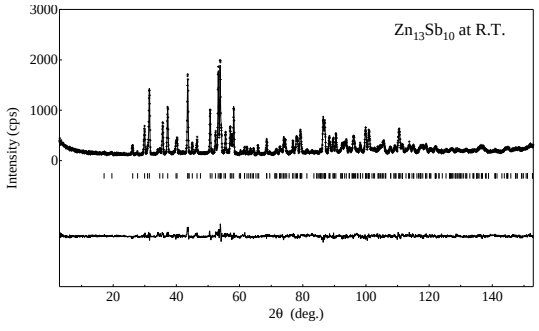

Fig. 1. Powder neutron diffraction profile and result of Rietveld analysis for Zn13Sb10 at room temperature.