Thermoelectric properties of Al-based ternary chalcopyrites: TAlTe$_2$ (T = Cu, Ag)

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[Introduction] Recently we demonstrated that Ga-based ternary chalcopyrite materials, TGaTe$_2$ (T = Cu, Ag)[1,2] have excellent thermoelectric properties, such as the very low lattice thermal conductivity below 0.7 Wm^{-1}K^{-1} at 900 K.[2] This small lattice thermal conductivity of CuGaTe$_2$ allowed us to obtain a very large value of dimensionless figure of merit zT exceeding 1.4. In this study, we employed Al as a substitute for Ge because it is abundant and hence much cheaper than Ga. We also considered that it might cause a widening of band gap to increase the value of Seebeck coefficient S, power factor PF, and zT.[3]

[Experimental procedure] Polycrystalline bulk materials of nominal compositions with TAlTe$_2$ (T = Cu, Ag) were synthesized by conventional solid state reaction. The obtained ingots were pulverized using an agate mortar and then sintered under argon atmosphere by a hot-pressing method. The structure of prepared samples was investigated by means of high temperature powder XRD, HR-TEM, and EPMA. Their thermal stability was studied using TG-DTA and DSC, and the electrical resistivity and thermal conductivity were precisely measured using conventional 4-probe method and laser flash method, respectively.

[Results and discussion] The good agreement between calculated and measured powder XRD patterns shown in Fig.1 indicated that we succeeded in synthesizing polycrystalline chalcopyrite samples free from the precipitation of secondary phases at CuAlTe$_2$ and AgAlTe$_2$. We found that these samples possess extremely low lattice thermal conductivity in the same manner as TGaTe$_2$ (T = Cu, Ag)[1,2]. We also revealed that the electrical resistivity of AgAlTe$_2$ shows a sudden increase at around 550 K with increasing temperature, while such a unusual behavior of electrical resistivity was not observable for CuAlTe$_2$.

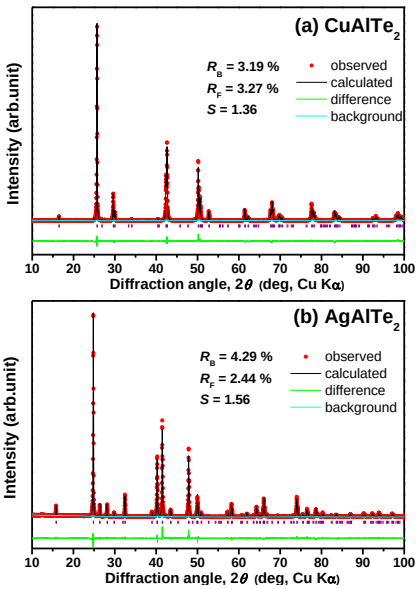

Fig. 1. Powder XRD data for polycrystalline samples with nominal composition TAlTe$_2$ (T = Cu, Ag) obtained from Rietveld refinement.

References

1. A. Yusufu, K. Kurosaki *et al.*, *Appl. Phys. Lett.* **99**, 061920 (2011).

2. T. Plirdpring, K. Kurosaki *et al*, *Adv. Mater.* **24**, 3622-3626 (2012).

3. I. V. Bodnar'*et al*., *Inorg. Mater*. **39**, 10-14 (2003)