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Lattice distortions and phase transitions in Tl-based thermoelectric materials

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1 Introduction

Ternary Tl-compounds with TlSe-type structure attract much attention because of their extremely large thermoelectric power, small thermal conductivity, and relatively large electrical conductivity. Thus, these materials, such as $TlInSe_2$ and $TlGaTe_2$, are foreseen as a member of a new class of thermoelectric materials [1].

$TlGaTe_2$ has a rather complex tetragonal chain structure at room temperature, which can be described as a set of $GaTe_4$ chains extended along the *c*-axis and connected with each other through one dimensional chains of Tl atoms (normal (N) phase). At temperatures lower than 290K, the positions of Tl atoms are believed to deviate from the periodicity of the $GaTe_4$ frameworks, indicating an incommensurate (IC) phase [2]. With the further decrease of temperature, another phase transition from IC to commensurate (C) phases is expected to occur at about 100 K. These phase transitions cause the degree of positional order of the Tl atoms and strongly affects thermoelectric properties of this material.

In this study, we have started a series of structural measurements on $TlGaTe_2$ by means of x-ray diffraction, XAFS, and x-ray fluorescence holography at low temperatures down to 30K, where the N-IC-C phase transition takes place.

2 Experiment

Single crystal $TlGaTe_2$ was grown by a modified Bridgeman method [1]. The well-ground powder of the sample was mixed with BN and pressed into a pellet with a diameter of 13 mm.

The Ga *K* edge (10.367 keV) and Tl L_{III} edge (12.657 keV) XAFS spectra were measured at BL9C of the PF, and the Te *K* edge (31.811 keV) spectra at NW10A of the PF-AR.

3 Results and Discussion

Figure 1 shows the Ga *K* XAFS signal (upper) and its Fourier transform (lower) of $TlGaTe_2$ at 30 K. As seen in the figure, good quality of the XAFS signal was obtained in the C phase. The similar qualities of the data were obtained in all of the edges at low temperatures.

With increasing temperature beyond 100K, the quality of the Tl L_{III} edge XAFS data gets worse, which is not due to the temperature effect only, but spatial fluctuations of the Tl atoms may set in at about 100K, which may be related to the C-IC phase transition. Detailed analyses of the present XAFS results are now in progress.

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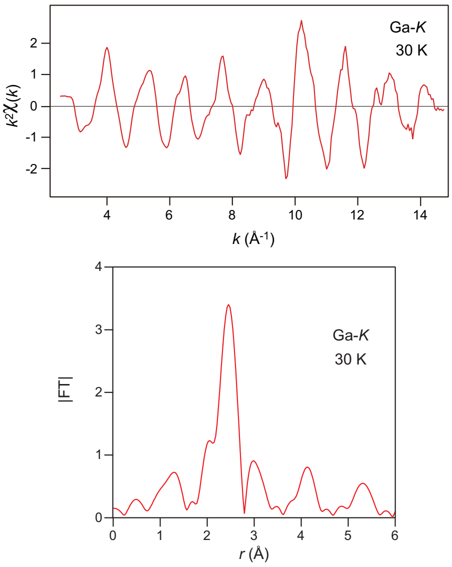

Fig. 1: Ga *K* XAFS signal (upper) and its Fourier transform (lower) of $TlGaTe_2$ at 30 K.

References

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