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XAFS studies of $TlInSe_2$ and spatial fluctuations in the incommensurate-commensurate phase transition range

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Introduction

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

$TlInSe_2$ has a rather complex tetragonal layer-chain structure (space group I4/mcm) at room temperature, which can be described as a set of $InSe_4$ chains extended along the *c*-axis and connected with each other through one dimensional chains of Tl atoms. At room temperature, Tl atoms are believed to deviate from the periodicity of the $InSe_4$ frameworks, showing an incommensurate (IC) phase. From our recent x-ray fluorescence holography (XFH) experiment at room temperature, it was found that the Tl atoms have extremely large spatial fluctuations, which were discussed in relation to the IC phase of this material [2,3].

In this study, we have started to investigate a series of structural measurements of $TlInSe_2$ by means of XFH, x-ray diffraction (XD), and XFH at low temperatures down to 25 K, where an IC-commensurate phase transition takes place.

Experimental procedure

Single crystalline $TlInSe_2$ was grown by a modified Bridgeman method [1]. The XAFS experiments were performed in the temperature range down to 25 K close to the Tl L_{II} edge at BL9C/PF and the In K edge at NW10A/PF-AR.

Results and discussion

Figure 1 shows the In K XAFS signal (upper) and its Fourier transform (lower) of $TlInSe_2$ measured at room temperature. As seen in the figure, good quality of the XAFS signal was obtained, and the same qualities of the data were in the whole temperature range. The first prominent peak indicates the first neighboring Se atoms, and the second peak corresponds to the Tl atoms. Since the Se K and Tl L_{III} XAFS signals merge into the Tl L_{II} XAFS signal, however, careful analyses are necessary to discuss the local structures around the Tl atoms.

Recent powder XD experiments revealed that the intensity and peak position of only the (231) Bragg peak highly change with decreasing temperature down to 200 K [4]. This finding may be related to temperature dependence of the positional fluctuations of Tl atoms in the IC phase. Detailed analysis of the present XAFS data are now in progress.

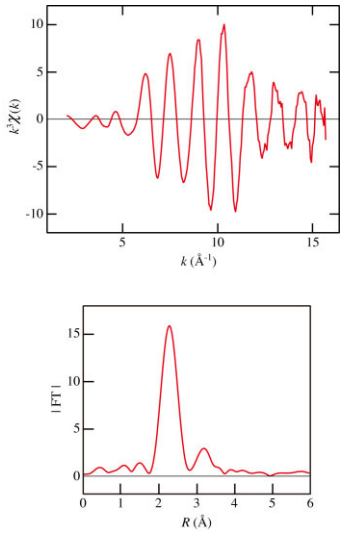

Figure 1. In K XAFS signal (upper) and its Fourier-transform (lower) of $TlInSe_2$ measured at room temperature.

References

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