EXAFS study of liquid Se-Te mixture

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Introduction

Liquid (l-) Se-Te mixtures have attracted considerable interest because they have covalently bonded chain structure and undergo the semiconductor to metal (S-M) transition at high temperature. Previous EXAFS studies on l-Se-Te mixtures have been carried out by Tamura *et al*[1]. However, their study at 2.5 GeV operation in PF was not sufficient enough in S/N ratio. In the present study we have measured EXAFS spectra at 3.0 GeV operation in which the S/N ratio is much better than those at 2.5 GeV operation. In this paper the changes of the local structure for around Te atoms l-Se-Te mixtures near the S-M transition are reported.

Experimental

The mixtures were prepared by weighing 99.999% pure Se and Te in silica glass ampoules sealed under vacuum. More detailed procedure of sample preparation is described elsewhere[2]. X-ray absorption spectra of Te *K*-edge (31.8 keV) were obtained at BL-10B. An electron beam energy was 3.0 GeV and a stored ring current was 200 mA. Si(311) channel-cut crystal monochromator was used. X-ray absorption spectra were recorded in transmission mode. The samples were put in a quartz cell with appropriate length. The EXAFS interference function was extracted from the absorption spectra and was Fourier transformed by the program of XANADU code described elsewhere[3]. In order to obtain the structural parameters, the EXAFS function was fitted by non-linear least-squares method to the theoretical function, in which theoretical parameters were calculated by FEFF 6 code[4].

Results and Discussion

The previous EXAFS analysis indicates that the short chains in l-Te with metalic nature are composed of the same number of short (~2.80A) and long (~2.95A) covalent bonds and that the long bonds vanish in the semiconducting state at low temperature [5]. In this report we performed 2-shell (Te-Se and Te-Te) fitting. Figure 1 shows temperature variation of the coordination numbers around Te atoms for l-$Se_{40}Te_{60}$. Open circles indicate the coordination number of Se around Te atoms ~2.56A ($N_{Te\text{-}Se}$), open squares Te around Te at ~2.77A ($N_{Te\text{-}Te}$) and closed circles total coordination number (N_{tot}). The values of N_{tot} are about 2.0 at temperature range from 375 to 500C, suggesting that the l-$Se_{40}Te_{60}$ mixture is composed of the chain structure with covalent bonding in this temperature region. With increasing temperature from 500 to 600 C, the value of N_{Total} decreases from 2.0 to 1.5. It is suggested that the S-M transition is accompanied by the appearance of the short chain. More detail analyses are in progress.

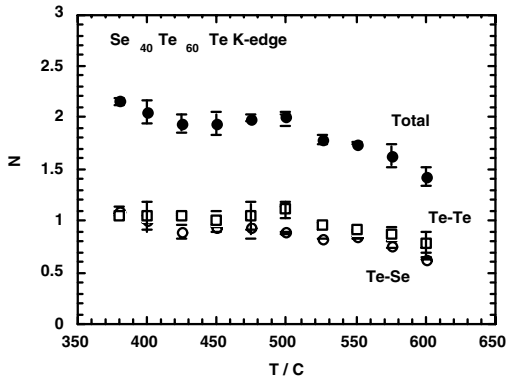

Fig. 1. Temperature variation of the coordination number around Te atoms for l-$Se_{40}Te_{60}$.

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