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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 l-Se-Te mixtures near the S-M transition are reported. Our discussions focus on the temperature variation of the coordination numbers around Te atoms.

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 is 3.0 GeV and a stored ring current is 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 suggests that the short chains in l-Te with metalic nature are composed of the same number of short (~2.80Å) and long (~2.95Å) covalent bonds and that the long bonds vanish in the semiconducting state at low temperature[5]. Figure 1 shows temperature variation of the coordination numbers around Te atoms for l-Se$_{10}$Te$_{90}$. Open circles indicate the coordination number of Se around Te atoms (N$_{\text{Te-Se}}$), open squares Te around Te at ~2.77Å (N$_{\text{Te-Te(short)}}$) and open triangles at ~2.95Å (N$_{\text{Te-Te(long)}}$) and closed circles total coordination number (N$_{\text{tot}}$). The values of N$_{\text{tot}}$ are about 2.1 and nearly independent of temperature, suggesting that the l-Se$_{10}$Te$_{90}$ mixture is composed of the chain structure with covalent bonding. The values of N$_{\text{Te-Se}}$ are almost constant. With increasing temperature the value of N$_{\text{Te-Te(short)}}$ decreases from 1.7 at 400°C to 1.3 at 550°Cand N$_{\text{Te-Te(long)}}$ increases from 0.3 at 400°C to 0.8 at 550°C, which indicates that the l-Se$_{10}$Te$_{90}$ mixture becomes metallic at higher temperatures. It is found that the contribution due to the long Te-Te bond in the l-Se$_{10}$Te$_{90}$ is larger than that in the l-Se$_{20}$Te$_{80}$[6].

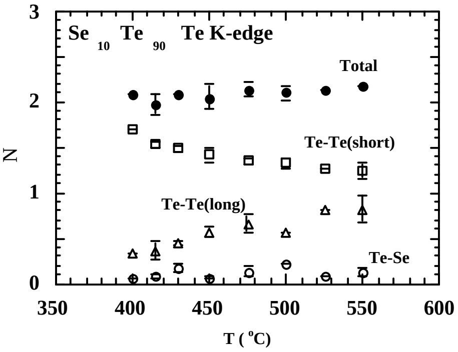

Fig. 1. Temperature variation of the coordination number around Te atoms for l-Se$_{10}$Te$_{90}$. Open circles indicate the coordination number of Se around Te atoms(N$_{\text{Te-Se}}$), open squares Te around Te at ~2.77 Å (N$_{\text{Te-Te(short)}}$) and open triangles at ~2.95 Å (N$_{\text{Te-Te(long)}}$) and closed circles total coordination number (N$_{\text{tot}}$).

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