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► To cite this version:

T. Miyanaga, H. Hoshino, H. Ikemoto, M. Yuza, I. Yamamoto, et al.. EXAFS of Liquid As-Te Mixtures. Journal de Physique IV Proceedings, 1997, 7 (C2), pp.C2-1001-C2-1002. 10.1051/jp4:19972115 . jpa-00255173

HAL Id: jpa-00255173

<https://hal.science/jpa-00255173>

Submitted on 1 Jan 1997

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EXAFS of Liquid As-Te Mixtures

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Abstract. The EXAFS measurements on As and Te *K*-edges of liquid As_2Te_3 have been carried out in the temperature range including the supercooled liquid state down to 330°C . By curve-fitting analyses with two-shell model the bond lengths and the coordination numbers were determined. It is suggested that As atoms within a chain bridge neighbouring chains with decreasing temperature and the network structure with three-fold coordinated As and two-fold coordinated Te is formed near the glass transition temperature.

1. INTRODUCTION

An important part of the recent scientific effort on liquid chalcogenides has been directed towards the glass transition. In the present paper, we have tried to get information on the change in local structure using EXAFS technique when liquid As_2Te_3 is supercooled down to the glass transition temperature.

2. EXPERIMENTAL

The mixture was prepared in the same way as described elsewhere [1]. The liquid As_2Te_3 specimen was kept in thin quartz cell with thickness of $50\ \mu\text{m}$. The EXAFS experiments were made on As and Te *K*-edges of liquid As_2Te_3 at 500 , 400 , 370 , 350 and 330°C , the latter three temperatures correspond to the supercooled liquid state of As_2Te_3 (m.p. 380°C). The EXAFS absorption spectra were recorded in transmission mode at BL-10B station of the Photon Factory in Tsukuba by using Si(311) channel-cut monochromator with a beam energy of $3.0\ \text{GeV}$ and the storage ring current from 160 to $200\ \text{mA}$.

Figure 1: The magnitudes of the Fourier transformation of phase corrected $k\chi(k)$, $|F(r)|$, obtained around the central As atom (a) and Te atom (b) for liquid As_2Te_3 at different temperatures.

3. RESULTS AND DISCUSSION

The EXAFS oscillations $\chi(k)$ were clearly detected up to $12\text{\AA}^{-1}$ in the spectra. To derive the structural parameters, the two-shell curve-fitting analysis was carried out in the k range from 3 to $12\text{\AA}^{-1}$ by using the theoretical parameters calculated by the FEFF code [2,3]. Figure 1 shows $|F(r)|$ around the central As (a) and Te (b) atoms for liquid As_2Te_3 at different temperatures including supercooling states, which was obtained by the Fourier transformation of phase corrected $k\chi(k)$. The main peaks and shoulders in Fig. 1(a) correspond to As-Te covalent bonds and As-As bonds. The two peaks in Fig. 1(b) are associated with Te-As and Te-Te bonds. From the curve-fitting analyses, the As-Te bond length is estimated to be $2.62\text{\AA}$, the As-As bond length $2.46\text{\AA}$ and the Te-Te bond length $2.75\text{\AA}$. The bond lengths are independent of temperature within experimental errors.

It is interesting to study how the local structure of liquid As_2Te_3 changes when the liquid specimen is cooled down to the glass transition temperature $T_g(130^\circ\text{C})$ [4] via the melting point $T_m(380^\circ\text{C})$. However, it is difficult to get the glassy state unless the rate of cooling is fast because the glass forming ability for As_2Te_3 is rather poor. The temperature dependence of the coordination numbers, N , around the central As and Te atoms is shown in Figs. 2(a) and 2(b), respectively. The solid points in Figs. 2(a) and 2(b) are N obtained for amorphous As_2Te_3 at 25°C by Ma *et al.* [4]; the total N for the central As atom is 3.0 and that for the central Te 2.4. Nearly the same amounts of As-As and Te-Te bonds do exist in the liquid state, suggesting that the arrangement of unlike atom is not chemically ordered. The numbers of As-Te bonds around the central As atom, $N_{\text{As-Te}}$ and those of Te-As bonds around the central Te atom, $N_{\text{Te-As}}$ rapidly increase with decreasing temperature, while the rate of increase in $N_{\text{As-As}}$ and $N_{\text{Te-Te}}$ is small. The correlation between the neighbouring chains becomes stronger when fluctuations of the interchain coupling reduce with decreasing temperature and the diffusive motions of atoms are frozen below T_g . The rapid increases of $N_{\text{As-Te}}$ and $N_{\text{Te-As}}$ encourage us to believe that As atoms within a chain bridge the neighbouring chains and the two dimensional network with three-fold coordinated As and two-fold coordinated Te is formed near T_g , though the temperature range in the present measurements covers only the supercooled region down to 330°C , not near T_g .

Figure 2: Variation with temperature of the coordination numbers N around the central As atom (a) and Te atom (b) determined by curve-fitting of the EXAFS data for liquid As_2Te_3 . The solid points at 25°C are N for amorphous As_2Te_3 from Ref. [4]. Lines are drawn as guides for the eye.

Acknowledgements

This work is partly indebted to Nippon Sheet Glass Foundation for Materials Science and Engineering for financial support. The authors are grateful to Dr. H. Sakane (Yamanashi University) for his support on the EXAFS experiments.

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