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Abstract. The structure factors $S(Q)$ of liquid tellurium measured by pulsed neutron diffraction at 490, 670 and 800 °C have been analysed using a method based on a short-chain model. The $S(Q)$ and the pair distribution functions $g(r)$ could be explained using this model. The mean chain length estimated for each temperature is rather short: about 14, 8, and 6 (Te atoms/chain) at 490, 670 and 800 °C, respectively. The enthalpy of scission of a Te–Te bond in the liquid state is estimated to be 14.5 kcal (g atom)$^{-1}$ (0.63 eV). A rough estimation of the mean chain length of Se–Te liquid alloys as a function of the temperature and concentration suggests that an anomalous volume contraction may be related to a shortening of Se–Te mixed chains.

1. Introduction

The local structure of liquid tellurium (Te) has received considerable attention because of its characteristic behaviour regarding electronic and thermodynamic properties. A structural evolution from a two-fold atomic configuration to a three-fold one in liquid Te with increasing temperature has been proposed by Cabane and Friedel [1] based on the neutron diffraction data of Tourand and Breuil [2]. Many x-ray [3, 4] and neutron [5–10] diffraction measurements on liquid Te have been carried out since. The x-ray results seemed to support the data of Tourand and Breuil. Recently, Enderby and Barnes [11] examined all of these diffraction data, and concluded that recent neutron diffraction data [5–10] were in general agreement with each other, but *totally* disagreed with the earlier measurements [2–4] upon which the Cabane and Friedel model was based. Takeda *et al* [7] have, however, reported that the temperature dependence of their neutron diffraction data could be explained by a gradual transition from a two-fold coordinated ordering (non-metallic) to a three-fold coordination (metallic), which is basically similar to the Cabane and Friedel model. Menelle *et al* [9, 10] examined the local structure of supercooled liquid Te and found a significant decrease in the first coordination number in the supercooled state. They suggested a distinct origin for one of the three atoms of the first coordinated shell. The local structure of liquid Te, especially the three-fold atomic configuration, seems to be still subject to controversy.

The short-chain model may be one of the simplest structural models for liquid Te, since the Te atoms form long chains in the crystalline state. It seems, however, that this model has not been examined in detail. We believe that it would be worthwhile to examine whether or not it can explain quantitatively the local structure of liquid Te. It is commonly observed in the pair distribution functions $g(r)$ of liquid Te that there is

a substantial penetration of the first coordination shell by non-bonded Te atoms [11]. This penetration prevents one from estimating an accurate number of covalent bonds and, therefore, from estimating the mean chain length if chains exist. The separation of bonded Te atoms from non-bonded Te atoms in the first coordination shell seems to be essential.

It is generally hard to decompose the bonded and non-bonded atoms with sufficient accuracy. However, if the structural unit in the liquid is given, the determination of the local structure and, therefore, the decomposition of the first shell may be made by applying the same technique as used in analyses of the orientational correlations in molecular liquids [12]. Unfortunately, the structure of the short chains of Te is not uniquely defined, except for very short range, since various conformations of chains may be statistically possible [13]. We therefore choose a Te$_2$ dimer as a definite structural unit in liquid Te. Moss and Price [14] have shown that a random packing of Se$_2$ dimers can simulate quite well the $S(Q)$ of amorphous selenium if all the dimers are aligned. Their investigation supports the present choice of the Te$_2$ dimer as being the structural unit in liquid Te.

The analytical procedure is as follows: initially, all of the Te$_2$ dimers are distributed at random; they are then polymerized into short chains and redistributed so as to reproduce the experimental $S(Q)$. From this procedure we can estimate an average conformation of the chains (bond length, bond angle and dihedral angle), the mean chain length, and interchain configurations. As a result, a decomposition of the first coordination shell into the intrachain and interchain distributions may be made.

The purpose of this paper is to examine the validity of the short-chain model to describe the local structure in liquid Te. In order to obtain the structure factors $S(Q)$ to high Q, pulsed neutron diffraction experiments were carried out.

2. Experimental details and results

The structure factors $S(Q)$ for liquid Te were measured by pulsed neutron diffraction using the $S(Q)$ instrument (HIT) installed at the pulsed neutron source at the National Laboratory for High Energy Physics (KEK), Tsukuba. A Te sample of 99.9999% purity was sealed in a thin-walled silica glass cell (8 mm in inner diameter and 0.35 mm in wall thickness). The $S(Q)$ measurements were made at three temperatures (490, 670 and 800 °C). The $S(Q)$ was obtained from the scattered intensity after standard corrections [15], such as subtraction of the cell intensity with attenuation corrections [16], multiple scattering [17] and normalization to the cross-section using a vanadium standard. The number density ρ of liquid Te was taken from [18]. The experimental points of $S(Q)$ measured at the three temperatures are shown together with smooth fits in figure 1. The smoothed curves are used for the following analysis.

The pair distribution functions $g(r)$ are shown in figure 2, which are calculated from Fourier transforms of the structure factors $S(Q)$ truncated at about 18 Å^{-1}. The dashed line in the $g(r)$ plots for $r \leqslant 2.5$ Å is noise and/or artifact due to truncation. The $g(r)$ curves are essentially in good agreement with those of other recent neutron measurements [7, 10]. The definition of the coordination number n for liquid Te is ambiguous, as described in the previous section. However, if one defines it as being the integration from the leading edge of the first peak (typically
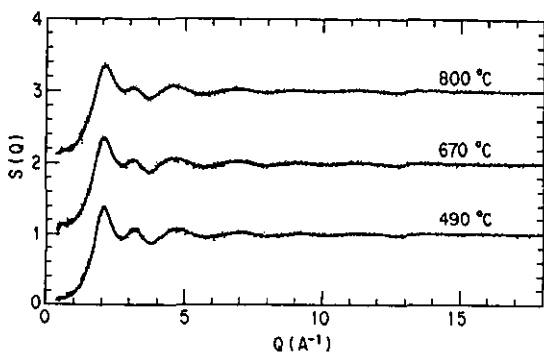
Figure 1. Experimental structure factors $S(Q)$ for liquid tellurium measured at 490, 670 and 800 °C. The points represent the unsmoothed data and the full curves are smooth fits. The upper two curves are shifted in the vertical direction for clarity.
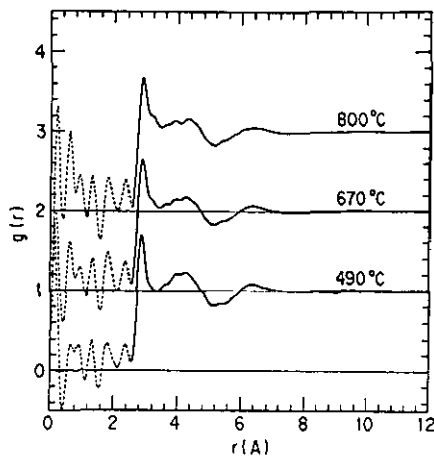
Figure 2. Experimental pair distribution functions $g(r)$ for liquid tellurium at 490, 670 and 800 °C. The upper two curves are shifted in the vertical direction for clarity.

2.56 Å) to the first minimum of $g(r)$ (typically 3.44 Å) the values of n are calculated to be 2.9, 3.0, and 3.2 in order of increasing temperature, while the integration from the same value as described above to the first minimum of $4\pi r^2 \rho g(r)$, instead of $g(r)$, typically 3.14 Å, gives n values of 2.0, 1.8, and 1.7 in order of increasing temperature. Since these values depend strongly on the definition of the region of integration, they are meaningless unless a decomposition of the first coordination shell is made.

3. A short-chain model

3.1. Method of analysis

We analyse the $S(Q)$ for liquid Te in a similar way as for liquid halogens. A Te_2 dimer was chosen as a basic structural unit, as described in section 1. Since the details concerning the method of analysis were fully described in [12, 19], only a brief description of the method is presented here. The structure factor $S(Q)$ for molecular liquids can be written as

$$S(Q) = S_u(Q) + \Delta S(Q) \tag{1}$$

where $S_u(Q)$ is the structure factor for a reference liquid in which Te_2 dimers are completely uncorrelated in orientation and $\Delta S(Q)$ is a correction term used to incorporate polymerization and orientational correlation effects. In the present case, we need at least two different correction terms, $\Delta S(Q)_{intra}$ and $\Delta S(Q)_{inter}$, since the Te_2 dimers are allowed to polymerize into the short Te_n chains and the chains are distributed so as not to overlap with each other. $\Delta S(Q)_{intra}$ is a correction for the polymerization, from which the mean chain length and the local chain conformation

are obtained. $\Delta S(Q)_{inter}$ is the correction for the distribution of chains, from which the interchain configurations are obtained.

$S_u(Q)$ is given by

$$S_u(Q) = F_1(Q) + F_u(Q)[S_c(Q) - 1] \tag{2}$$

where $F_1(Q)$ is the intradimer form factor; $F_u(Q)$ and $S_c(Q)$ are the interdimer form factor and the centre–centre structure factor respectively for completely uncorrelated dimers. $F_1(Q)$ and $F_u(Q)$ for Te_2 dimers have the same formulae as those defined for halogen molecules [12]. $S_c(Q)$ is assumed to be given by the structure factor for hard spheres $S_{hs}(Q)$ calculated by using a Percus–Yevick hard-sphere model [20] with two simple parameters: an effective diameter σ and a packing fraction η of Te_2 dimers. σ and η are related to each other through the definition $\eta = \pi(\rho/2)\sigma^3/6$, where ρ is the observed number density of Te atoms. An artificial damping factor Δ_{hs} is introduced in order to reduce oscillations in $S_{hs}(Q)$ persisting to very high Q [12].

Both the $\Delta S(Q)_{intra}$ and $\Delta S(Q)_{inter}$ are formally given in the same formula by [12, 19]

$$\Delta S(Q) = n_m \left[\frac{1}{2} \sum_{\alpha\beta} \langle \exp(iQ \cdot (R_c + r_\beta - r_\alpha)) \rangle \exp\left(-\frac{\Delta_{\alpha\beta}^2 Q^2}{2} \right) \right.$$
$$\left. - F_u(Q) \frac{\sin Q R_u}{Q R_u} \exp\left(-\frac{\Delta R_u^2 Q^2}{2} \right) \right] \tag{3}$$

where α labels an atom in the central Te_2 dimer, β labels an atom in a neighbouring dimer, $R_c + r_\beta - r_\alpha$ is the vector distance between atoms α and β (which depends on a relative orientation Ω of the two dimers), R_u is a distance between the centres of the two dimers in the reference liquid, and n_m ($m =$ intra or inter) is the number of equivalent dimers correlated in the same orientation as that specified above. n_{intra} is an important parameter, since the mean chain length is evaluated form this value. In order to define vector R_c and the orientation Ω of the second dimer, different coordinates are adopted for each of $\Delta S(Q)_{intra}$ and $\Delta S(Q)_{inter}$: for $\Delta S()_{intra}$, bond length l, bond angle θ_b, and dihedral angle ϕ_d are used; while for $\Delta S(Q)_{inter}$, polar coordinates R_c, Θ, and Φ (for the centre of the second dimer) and tilting angle θ (for the direction of the axis of the second dimer) are used. The fluctuation of the atomic spacing between atoms α and β, $\Delta_{\alpha\beta}$, is evaluated from the fluctuations in the above-mentioned coordinates.

The number of the nearest neighbour Te atoms n_1 in the chain is obtained from the value of n_{intra} using

$$n_1 = 1 + n_{intra}/2. \tag{4}$$

The mean chain length $\langle L \rangle$, which is defined as the mean number of atoms involved in one chain, is given by

$$\langle L \rangle = 4/(2 - n_{intra}). \tag{5}$$

In the following the most probable local conformation of the chains, the mean chain length and the interchain configuration are estimated by fitting (1) with (2) and (3) to the experimental $S(Q)$ using a non-linear least-squares method [21].

3.2. Fitting results

Figure 3 compares the fitted structure factor $S(Q)$ with the experimental one measured at 490 °C. The agreement between the two $S(Q)$'s is reasonably good. In the figure, the structure factors ($S_u(Q)$, $\Delta S(Q)_{intra}$ and $\Delta S(Q)_{inter}$) are also shown. The structure factor for randomly distributed Te_2 dimers, $S_u(Q)$, is considerably modified by the two correction terms ($\Delta S(Q)_{intra}$ and $\Delta S(Q)_{inter}$) in the Q region from 1 to 4 Å^{-1}. The first peak of $S(Q)$ and the dip following this peak are closely related to the interchain correction term $\Delta S(Q)_{inter}$, while the second peak and the second dip are related to the intrachain correction term $\Delta S(Q)_{intra}$. The fitted parameters are listed in tables 1 and 2.

Table 1. Intrachain structure parameters: the bond length l, its fluctuation Δl, the bond angle θ_b, its fluctuation $\Delta\theta_b$, the dihedral angle ϕ_d, its fluctuation $\Delta\phi_d$ and the number of the nearest neighbour dimers in a chain n_{intra}.

| T (°C)	l (Å)	Δl (deg)	θ_b (deg)	ϕ_d (deg)	$\Delta\theta_b$ (deg)	$\Delta\phi_d$ (dimers)	n_{intra}
490	2.886	0.19	103.6	108.0	8.3	7.5	1.72
	±0.005	±0.005	±1.2	±6.1	±2.5	±15.4	±0.06
670	2.889	0.19	103.7	103.9	8.2	2.1	1.46
	±0.005	±0.005	±1.2	±6.1	±2.8	±18.4	±0.06
800	2.890	0.19	105.3	96.4	8.1	3.1	1.36
	±0.005	±0.005	±2.3	±7.3	±3.2	±18.9	±0.06

Table 2. Interchain structure parameters: the effective diameter of Te_2 dimiers σ, the packing fraction η, the dumping factor Δ_{hs}, the polar coordinates for the centre of correlated dimer R_c, Θ and Φ, the tilting angle of correlated dimer θ, its fluctuation $\Delta\theta$, and the number of correlated dimers in the equivalent configuration n_{inter}.

T (°C)	σ (Å)	η	Δ_{hs} (Å)	R_c (Å)	Θ (deg)	Φ (deg)	θ (deg)	$\Delta\theta$ (deg)	n_{inter} (dimers)
490	3.83	0.402	0.58	4.20	61.4	0	11.3	0.1	3.0
	±0.02		±0.02	±0.03	±0.8	±72	±1.1	±5.3	±0.16
670	3.85	0.399	0.58	4.16	61.9	0	12.6	1.2	2.68
	±0.02		±0.02	±0.03	±0.9	±73	±1.1	±9.7	±0.14
800	3.84	0.385	0.57	4.14	61.9	0	12.6	1.3	2.61
	±0.02		±0.02	±0.03	±0.9	±76	±1.6	±9.8	±0.15

The pair distribution function $g(r)$ calculated from the fitted $S(Q)$ and that from the experimental $S(Q)$ are compared in figure 4. The agreement between both $g(r)$'s is fairly good. The fitted $g(r)$ comprises three different atomic distributions (curves (a), (b) and (c)), as shown in figure 4: curve (a) is the intrachain atomic distribution, which is given by the Fourier transform of both the intradimer form factor $F_1(Q)$ and the first term of $\Delta S(Q)_{intra}$; curve (b) is the atomic distribution between the correlated chains, which is given by the Fourier transform of the first terms of $\Delta S(Q)_{inter}$; curve (c) is the atomic distribution between the uncorrelated chains, which is given by the Fourier transform of three terms ($F_u(Q)[S_c(Q)-1]$ and the second terms in both $\Delta S(Q)_{intra}$ and $\Delta S(Q)_{inter}$). It is clearly seen that there
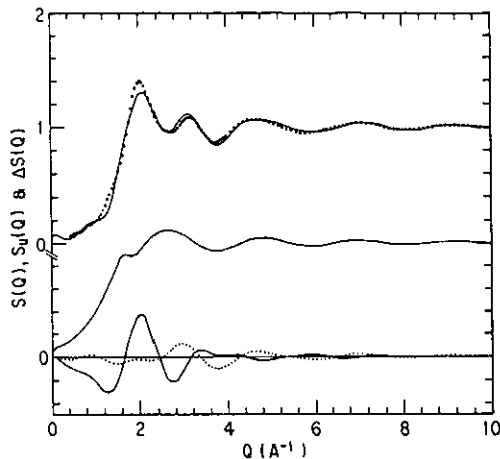
Figure 3. Fit of the structure factor $S(Q)$ for liquid tellurium at 490 °C. The dots are the experimental $S(Q)$ and the solid curve is the fitted $S(Q)$. The lower three curves denote $S_u(Q)$ (thin solid curve), $\Delta S(Q)_{intra}$ (dotted curve) and $\Delta S(Q)_{inter}$ (thick solid curve).
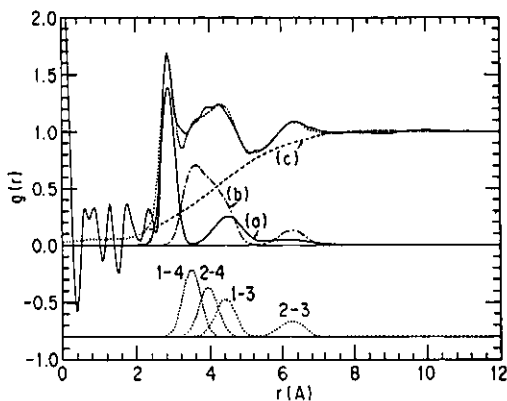
Figure 4. Comparison of the experimental pair distribution function $g(r)$ (solid curve) with the fitted one (dotted curve) for liquid tellurium at 490 °C. Curve (a) is the intrachain distribution, (b) the interchain distribution between correlated chains, and (c) the interchain distribution between uncorrelated chains. The decomposition of curve (b) into four different atomic pairs defined in figure 5 is shown in the lower part of the figure.

is considerable penetration of the first shell by non-bonded Te atoms which originate both from the correlated chains (curve (b)) and the uncorrelated chains (curve (c)).

The very local structure of liquid Te at 490 °C estimated from the present analysis is schematically drawn in figure 5. The values of R_c, Θ, Φ, θ, and n_{inter} listed in table 2 suggest that about three Te$_2$ dimers in the different chains are correlated in a staggered parallel orientation around a Te$_2$ dimer of the central chain. The mean chain length $\langle L \rangle$ calculated from (5) with the value of n_{intra} listed in table 1 is 14 Te atoms/chain. A very short chain length is estimated. The number of bonded Te atoms (n_1, the area under the first peak of curve (a) in figure 4) calculated from (4) is 1.86. As listed in table 1, the bond length l is 2.886 Å, which is slightly longer than 2.835 Å for the helical chain in the crystalline state [22], while the bond angle ($\theta_b = 103.6°$) and the dihedral angle ($\phi_d = 108°$) are rather similar to the coreresponding values of the crystalline state, i.e. $\theta_b = 103.2°$ and $\phi_d = 100.8°$ [22].

The second broad peak of the experimental $g(r)$ loacted at ~ 4 Å in figure 4 is attributed to two different origins: the intrachain second neighbours (curve (a)) and the interchain atomic distribution between the correlated chains (curve (b)). Both are superimposed on the smooth atomic distribution of uncorrelated dimers (curve (c)). The atomic distribution of curve (b) comprises three different atomic pairs (1–4, 2–4, and 1–3 in figure 5) which are drawn in the lower part of figure 4. The third peak of the experimental $g(r)$, located at ~ 6 Å, is attributed to the interchain third neighbours. The 1–4 pair has the shortest interchain atomic separation, about 3.5 Å; the counterpart in the crystalline state is 3.495 Å [22].

There are some discrepancies between the model and the experimental data in

$\langle L \rangle \sim 14$
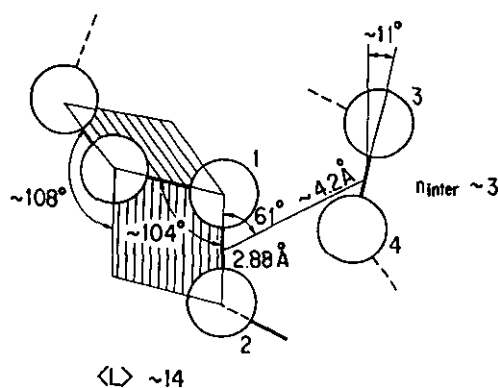
Figure 5. Schematic drawing of the local structure in liquid tellurium at 490 °C estimated from the short-chain model. The intrachain structure is given on the left, and the interchain structure is given on the right. Two other correlated dimers exist which are equivalent to those labelled 3 and 4, but are not shown in the figure. Uncorrelated dimers are not shown. The atomic distribution for each of the 1–3, 1–4, 2–3, and 2–4 pairs is shown in the lower part of figure 4.
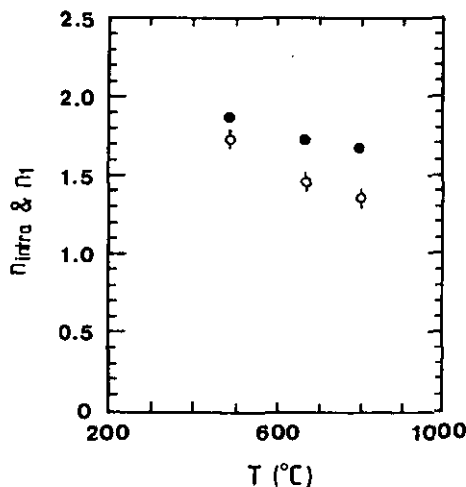
Figure 6. Temperature dependence of n_{intra} (open circles) and n_1 (solid circles).

figures 3 and 4. The height of the first peak of the fitted $S(Q)$ is slightly lower than that of the experimental $S(Q)$. This discrepancy in Q space may be related to a discrepancy in r space at large r (> 8 Å), where the fitted $g(r)$ is damped too fast compared with the experimental $g(r)$, as shown in figure 4. This implies that an initial distribution of uncorrelated Te_2 dimers in a reference liquid is too random and a longer range correlation may exist between the chains in liquid Te. Another discrepancy is found in $g(r)$ at about 3.2 Å, where the fitted $g(r)$ has a deeper dip compared with the experimental $g(r)$. It is not clear whether this discrepancy is significant, or is simply due to the experimental error.

Similar analyses have been made for liquid Te at 670 and 800 °C. The local structure of liquid Te estimated for all three temperatures seems to be essentially similar, since the fitted values of parameters listed in tables 1 and 2 are similar at the three temperatures. One of the exceptions is the value of n_{intra}, which decreases significantly with increasing temperature (figure 6). The number of nearest neighbour Te atoms in a chain n_1 calculated from (4) is also plotted in figure 6. The quality of the fits may be judged by the error of the mean square R, which is defined by $R = [\sum(S_{obs}(Q) - S_{calc}(Q))^2/(N - p)]^{1/2}$, where N is the number of data points and p is the number of fitting parameters. In this case $N = 200$ and $p = 20$. The fits to $S(Q)$ are equally good at all temperatures, since the values of R for the three temperatures are almost the same: $R = 0.035(490 °C)$, $0.036(670 °C)$ and $0.038(800 °C)$.

4. Discussion

One of the interesting results obtained in this analysis is the value of n_{intra}, which is considerably smaller than 2 (the value for an infinite chain) and decreases with increasing temperature (figure 6). The average chain length $\langle L \rangle$ evaluated from (5) is plotted as a function of $1/T$ in figure 7. The values of $\langle L \rangle$ reported for liquid Se [23] by means of NMR measurements are also plotted. A simple expression for the temperature dependence of $\langle L \rangle$ is [13, 24]

$$\langle L \rangle (\langle L \rangle - 1) = A \exp(\Delta H_{sc}/RT) \qquad (6)$$

where ΔH_{sc} is the enthalpy of scission of a Te–Te bond in the liquid state and A is an entropy term. The solid lines in figure 7 are the calculated values from (6) with ΔH_{sc}(Te–Te) = 14.5 kcal (g atom)$^{-1}$ (0.63 eV) for liquid Te and Δ_{sc}(Se–Se) = 29 kcal (g atom)$^{-1}$ (1.3 eV) for liquid Se which is a typical value reported in [13, 23]. A constant value of $A = 0.012$ [13] is assumed for both liquids.
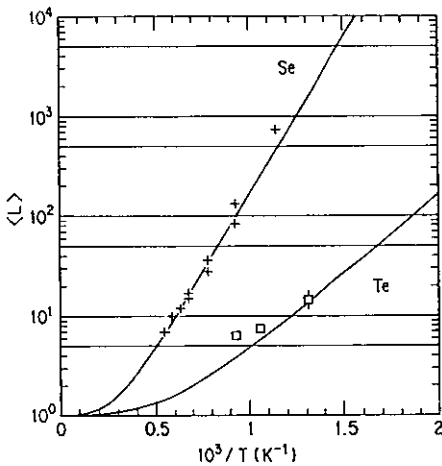
Figure 7. Plot of the mean chain lengths $\langle L \rangle$ estimated for liquid tellurium (squares) as a function of $1/T$. The values of $\langle L \rangle$ for liquid selenium (pluses) [23] are also shown. The solid curves are calculations using (6) with ΔH_{sc}(Te–Te)=14.5 and ΔH_{sc}(Se–Se)=29 kcal (g atom)$^{-1}$ respectively.
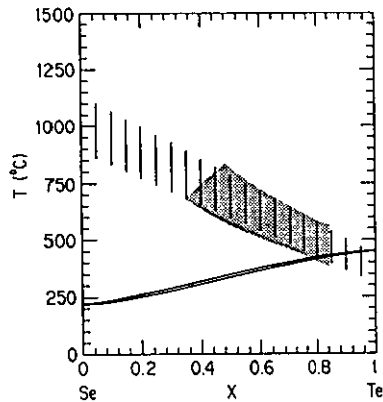
Figure 8. Temperature and concentration dependence of the chain length estimated from (6) and (7) in Se$_{1-x}$–Te$_x$ alloys. The hatched area indicates the region where the mean chain length ranges from 20 to 60 (atoms/chain). The shaded area indicates the region where an anomalous volume contraction is observed [18]. The two solid curves indicate the liquidus and solidus of the alloy.

As clearly shown by curve (c) in figure 4, there is considerable penetration of the first coordination shell by the non-bonded Te atoms belonging to the uncorrelated chains, although curve (c) may be somewhat erroneous because the tail of the curve extends far below the first coordination shell, which is physically unacceptable. Nevertheless, we think that most of the penetration of curve (c) is meaningful. We do not presently have any conclusive explanation for the origin of this distribution. One possible explanation is the Te atoms distributed around the atoms located at the

chain ends, which may play an important role in the thermodynamic and electronic properties of liquid Te when the chain length becomes very short. Another possible explanation is the three-fold bonding Te atoms which we have ignored entirely in this analysis. Even though the latter explanation is correct, it is likely that the concentration of the three-fold bonding atoms is much smaller than that of two-fold bonding atoms in the temperature range studied here.

It may be concluded that the short-chain model could explain the local structure in liquid Te as far as the static structure is concerned. However, whether or not many other properties, such as the electronic, thermodynamic, and mass transporting properties, of liquid Te can also be explained by this model has not been examined. In contrast, the structural model originally proposed by Cabane and Friedel [1] took into account not only the structure, but also many other properties, although Cutler [25] raised a question concerning the electronic structure derived from their model. The present results seem not to contradict Cutler's argument [25] that the concentration of three-fold bonded Te atoms is smaller than the concentration of dangling bonds.

One of the properties directly related to atomic structure is density. Liquid Te and its alloys with Se exhibit an anomalous volume contraction over a somewhat wide temperature range, which shifts to higher temperatures with increasing Se content [18]. It may be interesting to examine qualitatively whether or not the anomalous volume contraction of liquid Se_{1-x}-Te_x alloys is interpreted by the short-chain model. X-ray diffraction [26] and Mössbauer [27, 28] studies on Se_{1-x}-Te_x solid alloys have suggested that the solid alloys form disordered copolymers, except for one at the equiatomic composition which forms ordered copolymers. In order to make a rough estimate of the mean chain length in Se–Te liquid alloys, we simply assume that the liquid alloys also form disordered copolymers as do the solid alloys. Assuming, furthermore, that ΔH_{sc}(Te–Te) and ΔH_{sc}(Se–Se) are independent of the alloy concentration, we may have a crude expression for the enthalpy of scission $\Delta H_{sc}(x)$ in $Se_{1-x}Te_x$ liquid alloys,

$$\Delta H_{sc}(x) = (1-x)^2 \Delta H_{sc}(\text{Se–Se}) + 2x(1-x)\,\Delta H_{sc}(\text{Se–Te}) + x^2\,\Delta H_{sc}(\text{Te–Te})$$

(7)

where ΔH_{sc}(Se–Te) is the enthalpy of the scission of the Se–Te bond and is assumed to be given by $[\Delta H_{sc}(\text{Se–Se}) + \Delta H_{sc}(\text{Te–Te})]/2$ for simplicity, although there are some indications that the Se–Te bond is slightly stronger than the average by about 0.07 eV or more [27, 29]. From (6) and (7) we can roughly estimate the temperature and concentration dependence of the mean chain length $\langle L \rangle$ in Se_{1-x}-Te_x liquid alloys. The hatched area in figure 8 is the region where the estimated value of $\langle L \rangle$ ranges from 20 to 60 (atoms/chain). The temperature region where the anomalous volume contraction was observed [18] is shown by the shaded area in figure 8. It is surprising that both areas are in good coincidence with each other despite the crudeness of the present treatment. This simple consideration suggests that the anomalous volume contraction is related to the shortening of the chains. It may be interesting to note that the semiconductor–metal transition occurs within a similar temperature range of the anomalous volume contraction [30]. This also suggests that the semiconductor–metal transition may be related to the chain shortening.

5. Conclusion

The structure factors $S(Q)$ of liquid Te measured by pulsed neutron diffraction

at 490, 670 and 800 °C were analysed using the short-chain model. The structure factors $S(Q)$ and pair distribution functions $g(r)$ could be explained by this model. The mean chain length estimated in this analysis is rather short: about 14, 8, and 6 (atoms/chain) at 490, 670 and 800 °C, respectively. Very local intrachain and interchain atomic configurations were also estimated. The enthalpy of scission of a Te–Te bond was estimated to be 14.5 kcal (g atom)$^{-1}$ (0.63 eV) from an analysis of the temperature dependence of the chain length. The simple consideration of the mean chain length in liquid Se–Te alloys suggests that the anomalous volume contraction could be interpreted as being a consequence of chain shortening.

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