Analysis of the Structure Factor of Liquid Tin in the Wide Temperature Range

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Abstract

The structure factors, S(Q), of liquid tin was obtained by neutron diffraction last year. Analysis of this S(Q) was performed in comparison with the use of hard sphere model. The radial distribution function g(r) was calculated from the S(Q), then the first coordination numbers were estimated by the standard regime.

Introduction

In this project, one of the important purposes is to clarify the diffusion mechanism of atom in liquid state. It is considered diffusion of atoms in liquid deeply relates to its liquid structure. For example, if short range order, such as chemical bonding, exist in liquid state, the motion of atoms is affected by their environment. Then, the diffusion coefficient will differ from that of simple liquid whose structure is well reproduced by the hard sphere model. In order to clarify a relation between the diffusion coefficient and the liquid structure, the study of the structures of group IVB elements is substantial for such purpose. Solid silicon and germanium have diamond type structure with covalent bonds and show semiconductive character. On the other hand lead has closed packed cubic type structure and show metallic character. Solid tin has intermediate character between metal and semiconductor, which has metallic type structure at its high temperature phase and diamond-like structure at lower temperatures. For liquid silicon and germanium, it is well known that there exists pronounced 'shoulder' in the high-Q side of the first peak of the structure factor, S(Q). The shoulder in liquid state is the most pronounced for silicon and less pronounced for heavier elements. There is no shoulder for the S(Q) of liquid lead. For the liquid tin, less pronounced shoulder is present near the melting point. It can be easily considered that these shoulders are related to the complex feature in liquid state, which may be relevant to semiconductive character in the solid state. As for the first coordination number, silicon and germanium have 6-8 nearest neighbor atoms around an atom while lead has

10-12 atoms at the melting point. In this report, the variation of the structure of liquid tin in wide temperature range is discussed in terms of shoulder of S(Q) and the first coordination number.

The structure factors of liquid tin have already been obtained by neutron scattering experiments at temperatures of 573K, 773K and 1073K, 1373K, 1473K, 1673K and 1873K until last year. Neutron scattering data were corrected by the standard procedure, which include corrections of absorption [1] and multiple scattering [2], subtraction of inelastic effect (Placzek correction) [3], and normalization of scattering intensity. As a result, structure factors, S(Q), of liquid tin in wide temperature range were obtained. In addition, the radial distribution functions, g(r)'s, were also evaluated from obtained S(Q)'s, then first coordination numbers were calculated.

S(Q) and g(r) of liquid tin

Fig.1 shows the S(Q) obtained from neutron scattering experiment. The radial distribution

$$g(r) = 1 + \frac{1}{2\pi^2 \rho_0 r} \int_{Q\min}^{Q\max} Q[S(Q) - 1]\sin[Qr]dQ$$

functions, g(r)'s, were calculated by the relation described below.

ρ_0 : number density of atoms ($Å^{-3}$)

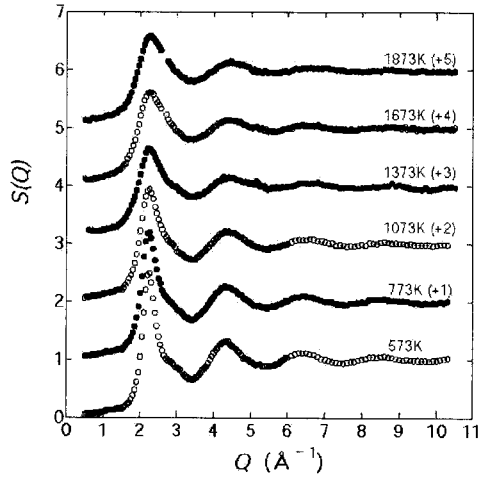

Fig.1 Structure factor of liquid tin.

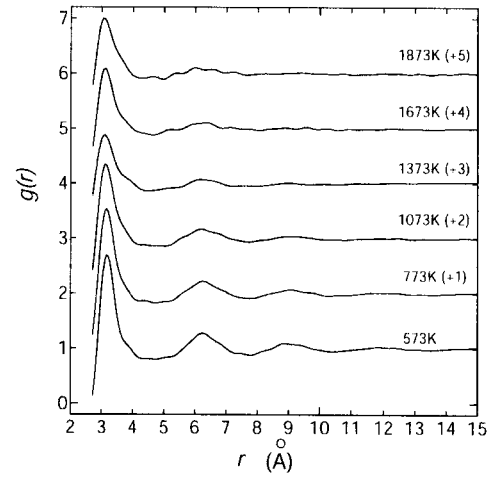

Fig.2 Radial distribution function of liquid tin.

Q-range of integration was from Q_{min}=0.5 $Å^{-1}$ to Q_{max}=10.5 $Å^{-1}$ corresponding to the range of the neutron scattering experiment. The g(r) of liquid tin was shown in Fig.2. Estimation of the first coordination number, n, was performed with the relation described below [4].

$$n = \int_{r_0}^{r_m} 4\pi\rho_0 r^2 g(r)dr$$

Integration was performed from r_0, where $4\pi\rho_0 r^2 g(r)$ reached to 0 in the low r range, to r_m where the $4\pi\rho_0 r^2 g(r)$ has the first minimum on the high-r side of the first peak.

Results and Discussions

A comparison between the experimental S(Q) and the hard sphere structure factor is a effective for a fundamental understanding of liquid metals. The hard sphere structure factor is characterized by random distribution of atoms and shows the following features [4].

- The first peak of the structure factor is symmetrical.
- The ratio (Q_2/Q_1) of the position of the second peak (Q_2) to that of the first peak (Q_1) is about 1.86.

The characteristics of the present S(Q) is shown in Table 1. The ratios (Q_2/Q_1) are deviated from 1.86 at the measured temperature range, therefore it is considered that there exists anisotropic distribution of atoms in liquid tin even at the temperatures up to 1873K. As for the first peak, it is not symmetrical or the 'shoulder' seems to be present from 573K to 1873K. These results confirm that the complex character of the structure in liquid tin will be present up to high temperature of 1873K. However, the estimated first coordination number, shown in Fig.3, is 10.7 at the melting point and reduces monotonously with increasing temperature. These values of coordination number, which are in correspondence with that of simple liquid metal, suggest that liquid tin has a nearly closed packed structure. It is concluded that liquid tin has a nearly closed packed atomic distribution but there are some complexity such as anisotropy, which has been recently clarified by means of molecular dynamics simulation [5].

Table 1 The characteristics of the present S(Q) of liquid tin.

T (K)	Q_1	$S(Q_1)$	Q_2	$S(Q_2)$	Q_2/Q_1	$S(Q_2)/S(Q_1)$
573	2.234	2.498	4.308	1.309	1.93	0.524
773	2.232	2.198	4.303	1.269	1.93	0.577
1073	2.238	1.936	4.31	1.215	1.93	0.628
1373	2.220	1.649	4.399	1.149	1.98	0.697
1673	2.266	1.616	4.4	1.144	1.94	0.708
1873	2.27	1.581	4.45	1.153	1.96	0.729

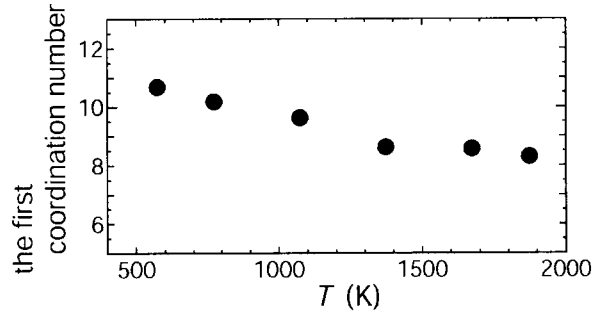

Fig.3 The estimated first coordination number of liquid tin.

Summary

In this year, the analysis of the structure of liquid tin was performed with the use of S(Q) from the neutron scattering experiments and derived g(r). The ratio, Q_2/Q_1, deviate from the hard sphere model and 'shoulder' exist even in the high temperature liquid of 1873K. Therefore, it is considered that there exists the complex character in liquid tin even at 1873K.

References

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