Apparatus for X-ray Diffraction of Liquid Metals and Several Results

Apparatus for X-ray Diffraction of Liquid Metals and Several Results*

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Synopsis

A high temperature attachment for X-ray diffraction of liquid metals has been built enabling liquid metal sample to be measured at temperatures up to 1000°C in vacuum, whilst scanning angles from 0 to 130° of 2θ.

The usefulness of this apparatus was demonstrated by obtaining the structure factors of liquid Al, Pb, Sn, and Bi at several temperatures from the measured X-ray intensities and a comparison was made with those found in earlier works.

Numerical values of the structure factors obtained in this work were illustrated.

I. Introduction

X-ray diffraction is one of the most important methods that may be employed to study the liquid structure of metals. A most important prerequisite for this kind of studies is a small furnace which can be attached on a θ-θ diffractometer[1]. But such furnaces are not commercially available.

From this reason, it would be desirable to construct the special furnace for X-ray diffraction study of liquid metals. The purpose of this report is to present a new apparatus for X-ray measurements of liquid metals and several results obtained by this apparatus.

II. Design of furnace chamber and heating system

Photograph of the furnace chamber is shown in Fig. 1 and Fig. 2 is the detailed drawing of a high temperature furnace chamber for X-ray diffraction study of liquid metals. This chamber is constructed of two parts, enclosure-part and base-part, which are made of brass. Two water-cooled-copper electrodes are attached to the base-part with neoprene plate and bakelite as a vacuum shield and electrical insulator.

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* The **204th** report of the Research Institute of Mineral Dressing and Metallurgy; A part of this work has been presented in Physica Status Solidi, **49** (1972), 339.

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(1) K. Furukawa, Sci. Rep. RITU., **A12** (1960), 368.

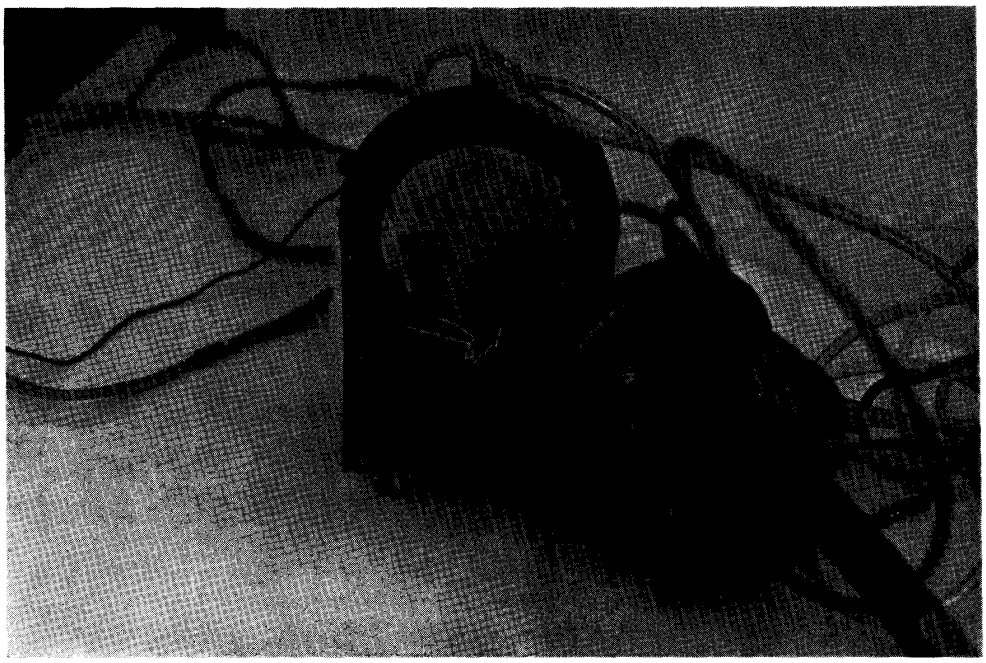

Fig. 1. Photograph of furnace chamber.

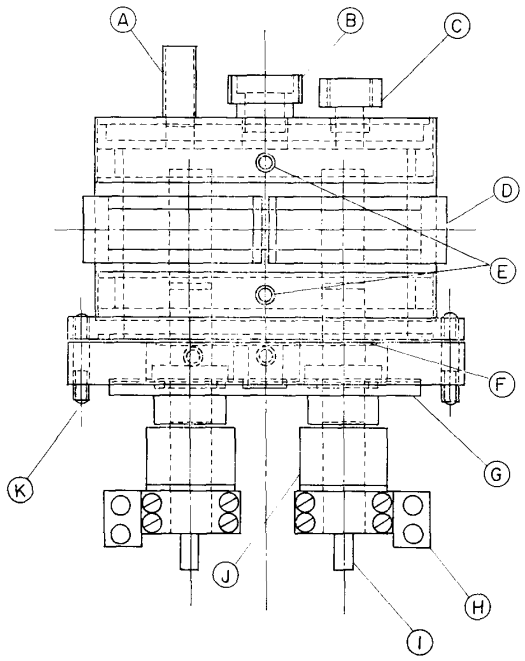

Fig. 2. Diagrams of furnace chamber.
A duct to vacuum, B window, C leak valve, D X-ray window, E water-cooling duct, F packing, G insulator, H electrode, I water-cooling duct for electrode (in), J water-cooling duct for electrode (out), K connecting parts.

The slot of 14 mm wide through the water-cooled enclosure wall allows passage of X-ray beam. The opening is covered by 0.3 mm thick beryllium window which is held with a neoprene-gasket.

Easily replaceable inner cover of 0.039 mm zirconium foil is held against the

wall of the chamber by the dowel pins. This arrangement protects the beryllium window from heat and contamination, whilst ensuring a filtered Mo-K_α X-ray beam. For Cu-K_α X-ray beam this cover of 0.020 mm nickel foil is prepared. This enclosure-part is attached to the base-part with an O-ring seal and four dowel bolt-nut.

A vacuum of 10^{-4} Torr can be obtained in this chamber at room temperature through a hole in the enclosure-part.

The specimen stage with sample is fixed. But the whole furnace chamber can be adjusted by the elevation and azimuth controls so that the liquid sample surface can be made horizontal and can be set at the level of the diffractometer axis.

A boron nitride (BN) crucible size is 30 mm$\times$20 mm$\times$2 mm which makes it possible to obtain a fairly flat surface area, about 10 mm$\times$10 mm, regardless of the surface tension of the metals and alloys under investigation. This BN crucible is placed on the heating block.

The heating block is made of alumina block into which a SYTT (Fe–25%Cr–4%Al–1%Y) wire of 0.5 mm diameter is densely inserted with spiral elaboration resistant element as shown in Fig. 3. Temperatures up to 1000°C can be easily obtained in vacuum, and up to 800°C in Ar–10%H_2 mixture. No attempt to run higher than 1000°C was made, but it is hoped that on introduction of a Pt wire with spiral elaboration temperatures up to at least 1300°C in vacuum can be obtained without altering the other furnace assembly.

The sample temperature was measured by a Pt-Pt, Rh thermocouple of 0.3 mm diameter, which was inserted into a hole in the side of BN crucible. This thermo-

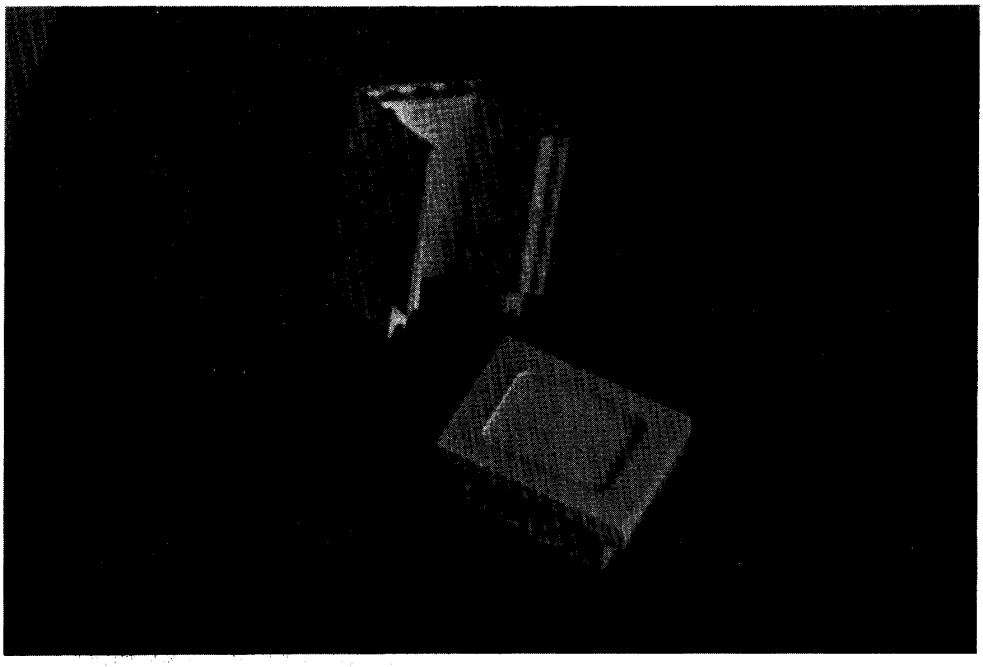

Fig. 3. Photograph of heating block and BN crucible.

couple was calibrated by measuring the melting points of the pure Sn, Pb, Al, and Ag. Sample temperature was maintained to within ±5°C for more than 10 hours required for the course of the experiment. The BN crucible is a very good heat conductor and hence reading of temperature on the thermocouple showed the agreement with the melting points of the pure metals within ±5°C.

III. Experimental test

1. Operating procedures

The experimental arrangement for the measurement of the scattered X-ray intensities of liquid metals was identical to the one described in a previous paper[2]. A few additional details are given below.

All data were obtained with Mo-K_α radiation at 60 kV and 20 mA. To obtain the absolute of X-ray source, a combination of K_β-filter and pulse-height analyzer was used. Positioning of the filter in the diffracted beam eliminated most of the extraneous radiation from the sample.

Measurements were taken at intervals of 15′ over the angular range (θ) between 4° and 20°, and at intervals of 30′ between 20° and 43°. This angular range corresponds to a range from $K_{min}=1.30$ Å^{-1} to $K_{max}=12.0$ Å^{-1}. The obtained data correspond to an average of three runs at each measurement.

The liquid metal samples were prepared by 99.9% Al, 99.999% Sn, 99.9999% Pb, and 99.9999 Bi and Ar–10%H_2 mixture was used. Before each run the sample was heated to 800°C, where oxide was reduced by the atmosphere used and then brought to the desired temperature within ±5°C.

2. Analysis of intensity patterns

The method on the analysis of the observed intensity data was the same as described in the previous paper[2]. The essential features are given below.

The observed intensities were corrected for background and polarization. The distribution of atoms as a function of the radial distance r for a given reference atom, $4\pi r^2\rho_0 g(r)$, can be obtained from X-ray intensity $I(K)$ scattered coherently by N atoms with atomic scattering factor f as a function of K, by means of the well-known relation[2];

$$4\pi r^2\rho_0 g(r) = 4\pi r^2\rho_0 + \frac{2r}{\pi}\int_0^\infty K\,[a(K)-1]\sin(K\cdot r)\,dK\,, \tag{1}$$

and

$$a(K) = \frac{I(K)}{Nf^2}\,, \tag{2}$$

where ρ_0 is the average density of atoms, $g(r)$ is the pair correlation function, $a(K)$ is the structure factor, $K=4\pi\sin\theta/\lambda$ where 2θ is the angle between the incident and diffracted X-rays and λ is the wave-length.

(2) Y. Waseda and K. Suzuki, Phys. Stat. Sol., **40** (1970), 183.

In order to convert the observed counts into electron units (normalization) the Krogh-Moe-Norman's method[3],[4] with the dispersion corrected scattering factor of Cromer[5] was used in this work. In this normalization the incoherent scattering was eliminated.

The observed intensity curves at small K value less than 1.30 Å^{-1} have been smoothly extrapolated to the value of $K=0.0$ Å^{-1} with reference to the value of $a(0)$ which is connected with the coherent small-angle scattering due to the isothermal compressibility. This relation is

$$\lim_{K\to 0} a(K) = a(0) = \rho_0 \chi_T kT\,, \tag{3}$$

where k is the Boltzmann constant, χ_T is the isothermal compressibility, ρ_0 is the average density of atoms, and T is the absolute temperature. We used the isothermal compressibility calculated from the sound velocity observed by Kleppa[6] and Filippov et al.[7] As shown in the previous paper,[2] the uncertainty in this extrapolation is insignificant, since the contribution to the radial distribution function (RDF) from the region of small K is considerably small[1]. Our measurements being confined up to $K\simeq 12.0$ Å^{-1}, we performed the Fourier transformation between $a(K)$ and $g(r)$ to eliminate the spurious ripples in the radial distribution function.

The numerical calculation was performed on the NEAC-2200, MODEL 700, Computer Center, Tôhoku University.

3. Several results obtained by this apparatus

Fig. 4 ~ Fig. 7 show the structure factors and the pair correlation functions for liquid Al, Pb, Sn, and Bi at several temperatures from the measured X-ray intensities.

The results of liquid Al are quite similar to those of Fessler, Kaplow, and Averbach[8] by X-ray diffraction.

The structure factors, including the temperature dependence of the structure factor, of liquid Pb obtained in this work are in general accord with those of North, Enderby, and Egelstaff[9] by neutron diffraction.

The structure factors of liquid Sn are in general agreement with those found by North, Enderby, and Egelstaff[9] (neutron diffraction) and Furukawa et al.[10] (X-ray diffraction). A new experimental information obtained from this work is the structure factor at 700°C. At this temperature a broadening of the peaks is

(3) J. Krogh-Moe, Acta Cryst., **9** (1956), 351.
(4) N. Norman, Acta Cryst., **10** (1957), 370.
(5) D.T. Cromer, Acta Cryst., **18** (1965), 17.
(6) O.J. Kleppa, J. Chem. Phys., **18** (1950), 1331.
(7) S.I. Filippov, N.B. Kazakov, and L.A. Prounin, Izv. Vyshiku. Chern. Met., **9** (1966), 8: Chem. Abstracts, **65** (1966), 1410d.
(8) R.R. Fessler, R. Kaplow, and B.L. Averbach, Phys. Rev., **150** (1966), 34.
(9) D.M. North, J.E. Enderby, and P.A. Egelstaff, J. Phys., C**1** (1968), 1075.
(10) K. Furukawa, B.R. Orton, J. Hamor, and J.I. Williams, Phil. Mag., **8** (1963), 141.

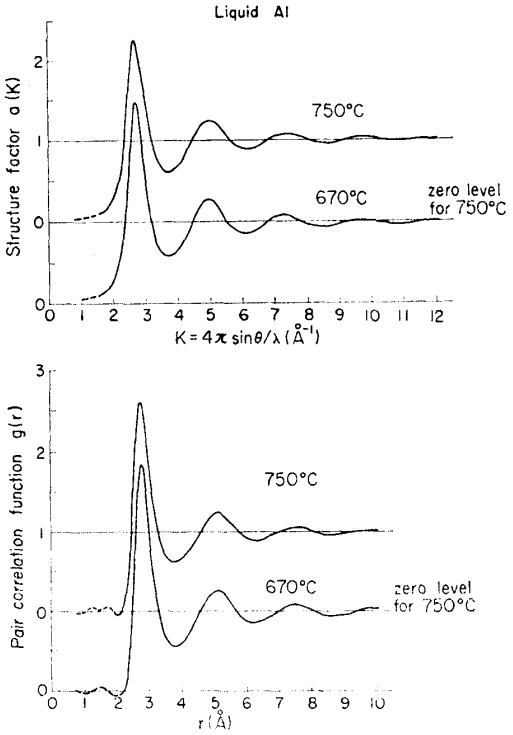

Fig. 4. Structure factors and pair correlation functions of liquid Al.

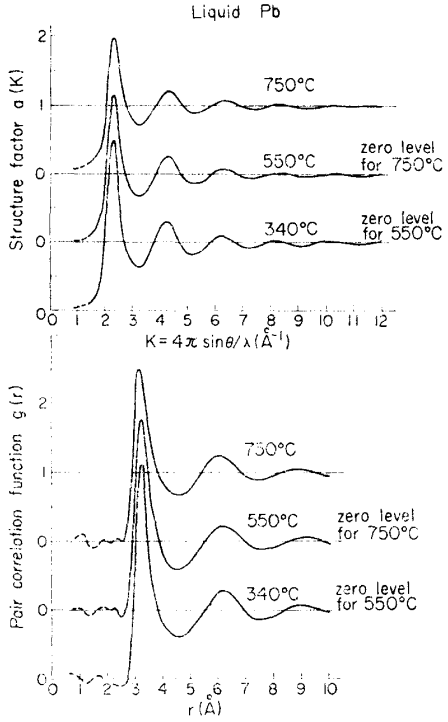

Fig. 5. Structure factors and pair correlation functions of liquid Pb.

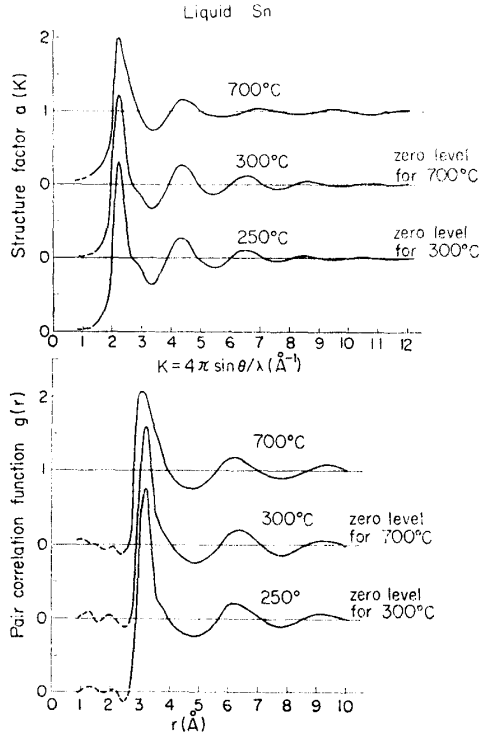

Fig. 6. Structure factors and pair correlation functions of liquid Sn.

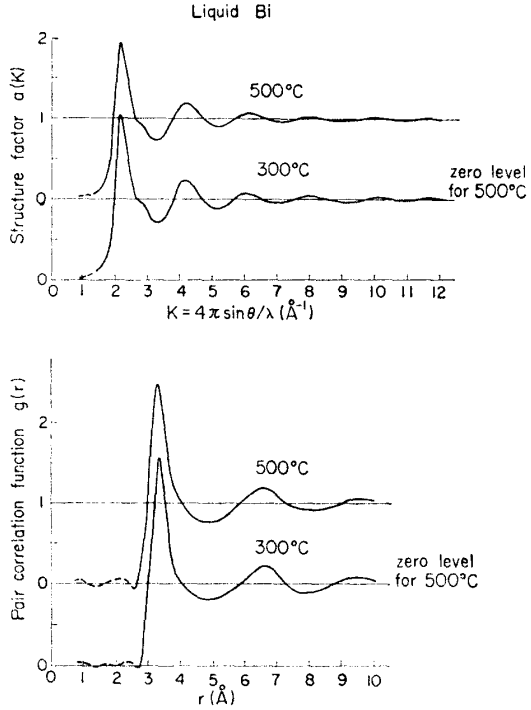

Fig. 7. Structure factors and pair correlation functions of liquid Bi.

Table 1. Numerical values of the structure factors of liquid Al.

Temp. (°C) K Å^{-1}	670 $a(K)$ Å^{-1}	750 $a(K)$ Å^{-1}	Temp. (°C) K Å^{-1}	670 $a(K)$ Å^{-1}	750 $a(K)$ Å^{-1}
0.00	0.017*	0.018*	5.40	1.086	1.122
1.30	* * *	* * *	5.60	0.977	1.013
1.40	* * *	* * *	5.80	0.899	0.935
1.50	0.090	0.092	6.00	0.864	0.890
1.60	0.110	0.113	6.20	0.851	0.882
1.70	0.138	0.138	6.40	0.888	0.991
1.80	0.170	0.171	6.60	0.949	0.962
1.90	0.210	0.215	6.80	1.010	1.010
2.00	0.308	0.285	7.00	1.065	1.040
2.10	0.390	0.400	7.20	1.090	1.068
2.20	0.498	0.584	7.40	1.093	1.072
2.30	0.739	0.823	7.60	1.068	1.047
2.40	1.183	1.160	7.80	1.024	1.020
2.50	1.761	1.686	8.00	0.991	0.999
2.60	2.264	2.205	8.20	0.959	0.966
2.70	2.475	2.271	8.40	0.940	0.954
2.80	2.316	2.143	8.60	0.944	0.958
2.90	1.901	1.874	8.80	0.957	0.969
3.00	1.440	1.487	9.00	0.989	0.990
3.10	1.095	1.141	9.20	1.017	1.012
3.20	0.900	0.940	9.40	1.027	1.020
3.30	0.791	0.826	9.60	1.036	1.022
3.40	0.700	0.723	9.80	1.030	1.021
3.50	0.614	0.653	10.00	1.018	1.021
3.60	0.561	0.618	10.20	1.008	1.011
3.70	0.559	0.607	10.40	0.989	0.999
3.80	0.594	0.620	10.60	0.983	0.992
3.90	0.635	0.645	10.80	0.983	0.988
4.00	0.671	0.697	11.00	0.979	0.989
4.20	0.786	0.775	11.20	0.986	0.990
4.40	0.976	0.926	11.40	0.998	0.994
4.60	1.137	1.094	11.60	1.013	0.998
4.80	1.257	1.216	11.80	1.020	1.005
5.00	1.280	1.253	12.00	1.007	1.011
5.20	1.194	1.200			

* $a(0) = \rho_0 \chi_T kT$

found and the subsidiary maximum is not specified but it seems that the asymmetry of the first peak is still maintained.

Fig. 7 shows the structure factors of liquid Bi at 300° and 500°C. In the case of liquid Bi the subsidiary maximum on the high angle side of the first peak was observed at two temperatures. It has been confirmed that this subsidiary maximum disappears at higher than 800°C by neutron diffraction[11].

From these results, the apparatus for X-ray diffraction of liquid metals described in this paper will be useful for the structural studies of metals and alloys in the liquid state.

Recent advances[12] in the structure and electronic properties of liquid metals undoubtedly indicate that the structure factor is one of the most important

(11) Y. Waseda and K. Suzuki, unpublished.

Table 2. Numerical values of the structure factors of liquid Pb.

Temp. (°C)	340	550	750	Temp. (°C)	340	550	750
K Å^{-1}	$a(K)$ Å^{-1}	$a(K)$ Å^{-1}	$a(K)$ Å^{-1}	K Å^{-1}	$a(K)$ Å^{-1}	$a(K)$ Å^{-1}	$a(K)$ Å^{-1}
0.00	0.009*	0.012*	0.014*	5.40	0.875	0.881	0.905
1.30	0.079	0.096	0.137	5.60	0.941	0.938	0.948
1.40	0.097	0.117	0.162	5.80	1.013	0.999	0.998
1.50	0.120	0.149	0.188	6.00	1.094	1.048	1.037
1.60	0.159	0.188	0.233	6.20	1.116	1.071	1.060
1.70	0.242	0.260	0.296	6.40	1.064	1.062	1.065
1.80	0.380	0.385	0.395	6.60	1.039	1.024	1.043
1.90	0.624	0.643	0.642	6.80	0.973	0.990	1.006
2.00	1.207	1.231	1.240	7.00	0.943	0.960	0.968
2.10	1.920	1.622	1.683	7.20	0.930	0.943	0.957
2.20	2.400	2.083	1.931	7.40	0.942	0.950	0.953
2.30	2.482	2.145	1.987	7.60	0.975	0.972	0.962
2.40	2.048	1.814	1.782	7.80	1.003	0.993	0.983
2.50	1.511	1.458	1.466	8.00	1.037	1.016	1.016
2.60	1.082	1.157	1.223	8.20	1.051	1.034	1.023
2.70	0.862	0.979	1.037	8.40	1.042	1.041	1.024
2.80	0.786	0.860	0.907	8.60	1.025	1.032	1.015
2.90	0.736	0.781	0.811	8.80	0.991	1.011	0.993
3.00	0.664	0.626	0.759	9.00	0.970	0.992	0.979
3.10	0.598	0.694	0.730	9.20	0.968	0.981	0.975
3.20	0.583	0.681	0.716	9.40	0.971	0.980	0.978
3.30	0.622	0.684	0.718	9.60	0.991	0.981	0.980
3.40	0.682	0.712	0.737	9.80	1.006	0.998	0.992
3.50	0.740	0.753	0.780	10.00	1.014	1.008	1.002
3.60	0.807	0.816	0.838	10.20	1.021	1.017	1.017
3.70	0.899	0.888	0.904	10.40	1.017	1.020	1.021
3.80	1.016	0.976	0.967	10.60	1.012	1.017	1.013
3.90	1.133	1.063	1.032	10.80	1.000	0.998	1.002
4.00	1.225	1.148	1.101	11.00	0.985	0.981	0.991
4.20	1.307	1.246	1.193	11.20	0.987	0.977	0.980
4.40	1.247	1.221	1.192	11.40	0.987	0.980	0.995
4.60	1.066	1.087	1.089	11.60	0.991	0.993	1.003
4.80	0.933	0.948	0.990	11.80	1.009	1.004	1.012
5.00	0.869	0.880	0.921	12.00	1.011	1.019	1.005
5.20	0.832	0.859	0.893				

* $a(0) = \rho_0 \chi_T kT$.

informations to discuss these properties. But generally, the figures on the structure factor for liquid metals in the papers previously reported are considerably small. Therefore, for example, the attempt of the electrical resistivity calculation is in danger of containing the ambiguous error due to the error in the structural information obtained from these small figures. Hence, it seems that the numerical values of the structure factors of liquid metals are very useful for the quantitative calculations of a variety of the properties in liquid metals.

Table 1 ~ Table 5 show the numerical values of the structure factors obtained in this work together with those of liquid Hg[2] and liquid Bi[11]. We wish these

(12) P.D. Adams, H.A. Davies, and S.G. Epstein (editors): The Properties of Liquid Metals (Brookhaven conference), Taylor and Francis, 1967; Adv. Phys., **16** (1967), 147.

Table 3. Numerical values of the structure factors of liquid Sn.

Temp. (°C) K Å^{-1}	250 $a(K)$ Å^{-1}	300 $a(K)$ Å^{-1}	700 $a(K)$ Å^{-1}	Temp. (°C) $a(K)$ Å^{-1}	250 $a(K)$ Å^{-1}	300 $a(K)$ Å^{-1}	700 $a(K)$ Å^{-1}
0.00	0.007*	0.007*	0.011*	5.40	0.871	0.876	0.964
1.30	0.047	0.047	0.125	5.60	0.884	0.881	0.946
1.40	0.067	0.064	0.158	5.80	0.931	0.929	0.938
1.50	0.105	0.106	0.199	6.00	1.002	1.007	0.958
1.60	0.157	0.158	0.254	6.20	1.068	1.057	0.979
1.70	0.243	0.235	0.331	6.40	1.111	1.098	1.008
1.80	0.401	0.389	0.425	6.60	1.091	1.096	1.029
1.90	0.640	0.645	0.698	6.80	1.036	1.044	1.038
2.00	1.193	1.263	1.275	7.00	0.997	1.000	1.042
2.10	1.937	1.971	1.943	7.20	0.960	0.963	1.026
2.20	2.298	2.224	2.010	7.40	0.938	0.945	1.008
2.30	2.135	2.073	1.894	7.60	0.941	0.949	0.994
2.40	1.747	2.662	1.688	7.80	0.959	0.956	0.981
2.50	1.328	1.363	1.440	8.00	0.994	0.984	0.978
2.60	1.069	1.105	1.276	8.20	1.026	1.016	0.974
2.70	0.992	1.008	1.193	8.40	1.045	1.034	0.977
2.80	0.994	0.988	1.123	8.60	1.046	1.044	0.991
2.90	0.965	0.952	1.021	8.80	1.023	1.035	1.002
3.00	0.877	0.873	0.900	9.00	1.002	1.014	1.016
3.10	0.772	0.784	0.806	9.20	0.985	0.993	1.023
3.20	0.702	0.720	0.761	9.40	0.975	0.975	1.020
3.30	0.676	0.691	0.752	9.60	0.979	0.971	1.017
3.40	0.679	0.684	0.753	9.80	0.980	0.973	1.005
3.50	0.698	0.694	0.755	10.00	0.990	0.985	0.994
3.60	0.739	0.729	0.769	10.20	1.008	1.007	0.987
3.70	0.809	0.795	0.806	10.40	1.016	1.015	0.978
3.80	0.899	0.886	0.863	10.60	1.020	1.019	0.984
3.90	0.991	0.983	0.927	10.80	1.014	1.020	0.993
4.00	1.071	1.071	0.990	11.00	1.000	1.009	0.996
4.20	1.205	1.204	1.110	11.20	0.996	0.998	1.005
4.40	1.261	1.239	1.169	11.40	0.991	0.989	1.012
4.60	1.161	1.166	1.122	11.60	0.987	0.984	1.019
4.80	1.034	1.066	1.065	11.80	0.994	0.991	1.019
5.00	0.958	0.960	1.016	12.00	1.001	0.999	1.002
5.20	0.895	0.885	0.973				

* $a(0) = \rho_0 \chi_T kT$

detailed structural informations for several liquid metals at various temperatures illustrated would give a contribution to the progress of the study of liquid metals.

Acknowledgments

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The assistance of the Computer Center, Tôhoku University, is also gratefully acknowledged.

Table 4. Numerical values of the structure factors of liquid Bi.

Tepm. (°C) K Å^{-1}	300† $a(K)$ Å^{-1}	500† $a(K)$ Å^{-1}	550‡ $a(K)$ Å^{-1}	800‡ $a(K)$ Å^{-1}	950‡ $a(K)$ Å^{-1}
0.00	0.010*	0.013*	0.014*	0.018*	0.020*
1.20	* * *	* * *	0.050	0.072	0.080
1.30	0.065	0.060	0.061	0.090	0.107
1.40	0.092	0.083	0.080	0.121	0.122
1.50	0.131	0.122	0.113	0.154	0.186
1.60	0.186	0.184	0.182	0.202	0.231
1.70	0.395	0.291	0.294	0.324	0.344
1.80	0.591	0.528	0.521	0.563	0.605
1.90	1.034	0.998	1.002	1.041	1.082
2.00	1.581	1.583	1.560	1.557	1.571
2.10	2.035	1.940	1.882	1.813	1.740
2.20	1.975	1.832	1.821	1.734	1.688
2.30	1.778	1.604	1.594	1.536	1.513
2.40	1.396	1.338	1.332	1.318	1.369
2.50	1.096	1.135	1.141	1.144	1.214
2.60	0.965	0.990	0.998	1.030	1.091
2.70	0.946	0.941	0.938	0.962	1.000
2.80	0.935	0.901	0.897	0.913	0.943
2.90	0.876	0.862	0.856	0.868	0.882
3.00	0.791	0.801	0.811	0.823	0.839
3.10	0.731	0.752	0.765	0.802	0.822
3.20	0.718	0.738	0.760	0.797	0.820
3.30	0.735	0.740	0.763	0.807	0.837
3.40	0.757	0.773	0.800	0.841	0.865
3.50	0.783	0.817	0.842	0.882	0.913
3.60	0.835	0.869	0.898	0.933	0.962
3.70	0.925	0.941	0.961	0.986	1.013
3.80	1.041	1.033	1.027	1.043	1.062
3.90	1.149	1.110	1.106	1.100	1.102
4.00	1.221	1.178	1.147	1.132	1.124
4.20	1.231	1.187	1.180	1.158	1.143
4.40	1.129	1.112	1.133	1.130	1.122
4.60	1.014	1.027	1.049	1.069	1.078
4.80	0.942	0.954	0.961	0.992	1.020
5.00	0.893	0.912	0.920	0.945	0.976
5.20	0.883	0.902	0.921	0.928	0.947
5.40	0.926	0.936	0.939	0.941	0.940
5.60	0.980	0.982	0.972	0.969	0.957
5.80	1.042	1.033	1.017	0.999	0.976
6.00	1.085	1.070	1.049	1.024	0.999
6.20	1.076	1.068	1.060	1.042	1.017
6.40	1.039	1.042	1.060	1.047	1.037
6.60	0.992	1.007	1.039	1.040	1.039
6.80	0.958	0.980	1.009	1.020	1.037
7.00	0.954	0.968	0.986	1.007	1.028
7.20	0.963	0.960	0.978	0.988	1.018
7.40	0.985	0.978	0.981	0.982	1.000
7.60	1.008	0.997	0.989	0.980	0.992
7.80	1.024	1.016	1.012	0.982	0.980
8.00	1.034	1.023	1.020	0.998	0.980
8.20	1.022	1.020	1.022	1.003	0.982
8.40	1.001	1.009	1.014	1.009	0.993
8.60	0.989	0.993	1.002	1.011	0.999
8.80	0.979	0.980	0.995	1.002	1.010
9.00	0.983	0.976	0.980	0.998	1.010

* $a(0) = \rho_0 \chi_T kT$ † X-ray diffraction, ‡ neutron diffraction.

Table 5. Numerical values of the structure factors of liquid Hg.

Temp. (°C)	−35	15	80	Temp. (°C)	−35	15	80
K Å^{-1}	$a(K)$ Å^{-1}	$a(K)$ Å^{-1}	$a(K)$ Å^{-1}	K Å^{-1}	$a(K)$ Å^{-1}	$a(K)$ Å^{-1}	$a(K)$ Å^{-1}
0.00	0.006*	0.007*	0.010*	5.60	0.803	0.806	0.808
1.50	0.100	0.101	0.101	5.80	0.844	0.843	0.845
1.60	0.132	0.132	0.133	6.00	0.893	0.894	0.901
1.70	0.183	0.183	0.183	6.20	0.954	0.956	0.956
1.80	0.233	0.234	0.234	6.40	1.027	1.026	1.028
1.90	0.345	0.346	0.347	6.60	1.088	1.087	1.091
2.00	0.610	0.609	0.611	6.80	1.118	1.118	1.121
2.10	1.210	1.209	1.213	7.00	1.068	1.067	1.070
2.20	1.975	1.960	1.965	7.20	0.985	0.986	0.987
2.30	2.539	2.438	2.413	7.40	0.936	0.935	0.938
2.40	2.332	2.297	2.298	7.60	0.915	0.914	0.916
2.50	1.793	1.787	1.793	7.80	0.914	0.915	0.915
2.60	1.534	1.534	1.537	8.00	0.926	0.924	0.928
2.70	1.332	1.330	1.334	8.20	0.966	0.965	0.967
2.80	1.128	1.127	1.130	8.40	1.006	1.006	1.009
2.90	0.944	0.945	0.946	8.60	1.045	1.047	1.047
3.00	0.803	0.802	0.804	8.80	1.057	1.057	1.059
3.10	0.721	0.721	0.723	6.00	1.057	1.058	1.060
3.20	0.660	0.660	0.661	9.20	1.036	1.036	1.037
3.30	0.640	0.640	0.641	9.40	1.007	1.002	1.010
3.40	0.620	0.620	0.621	9.60	0.985	0.985	0.987
3.50	0.630	0.630	0.632	9.80	0.986	0.986	0.989
3.60	0.640	0.640	0.641	10.00	0.985	0.985	0.990
3.70	0.681	0.681	0.683	10.20	0.984	0.986	0.989
3.80	0.722	0.721	0.722	10.40	0.997	0.996	0.997
3.90	0.803	0.802	0.805	10.60	1.005	1.006	1.007
4.00	0.873	0.874	0.875	10.80	1.018	1.017	0.943
4.20	1.076	1.078	1.079	11.00	1.027	1.027	0.950
4.40	1.290	1.294	1.292	11.20	1.027	1.026	1.028
4.60	1.311	1.314	1.313	11.40	1.006	1.007	1.009
4.80	1.179	1.178	1.182	11.60	0.997	0.990	1.000
5.00	0.996	0.995	0.998	11.80	0.985	0.987	0.987
5.20	0.863	0.864	0.865	12.00	0.964	0.966	0.964
5.40	0.803	0.803	0.805				

* $a(0) = \rho_0 \chi_T kT$