The Structure of Liquid Copper†

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The studies for structures and physical properties of liquid metals have been undertaken in our laboratory. The structures of liquid copper have scantly been reported yet. Therefore the x-ray analysis of liquid copper was carried out, simaltaneously with the effeciency test of our x-ray diffractometer at a high temperature.

The diffractometer has been reported in detail in the previous paper[1]. Copper of 99.5% purity supplied by B. C. S. was used. The sample was contained in high purity alumina crucible of 20mm width by 25mm length. Molybudenum foil of 0.1mm thickness was used for a sample stage. A thin foil of aluminum (30μ) was held inside the chamber to protect the beryllium window from the thermal radiation, Temperature was measured by a 0.3ϕmm $PtRh_6$-$PtRh_{30}$ thermocouple. The thermocouple was inserted into a hole located in the corner of the clucible.

The chamber was at first evacuated to 10^{-3}mmHg to clean up its inside. Then a reducing gas of Ar-10%H_2 was flowed through the chamber to maintain an oxide free liquid surface. It was found necessary to heat the liquid copper above 1200°C to reduce the surface oxide. Diffraction data were obtained with Mo-Kα radiation, using a graphite curved monochromator. Measurements were carried out at intervals of 1/2°(2θ) between 10° and 80°, and at intervals of 1° between 80° and 120°. The maximum irradiated area of the sample surface (about 10mm×10mm) was seemed to be almost flat, as the area of the sample (25mm×20mm) was sufficiently large. Therefore the absorption correction was constant throughout.

The method on analysis was the same as deseribed in the previous paper[1]. The observed intensities were corrected for background and polarization, The data less than 12.0 of $k=4\pi\sin\theta/\lambda$ were used in this work. The normalization constant was calculated by averaging both the results of the high angle region method and the Krogh-Moe-Norman method ($\gamma=0.008$). The atomic scattering factors for neutral copper were used those given by Cromer & Waber[2], and the Compton scattering factors were refered to the values given by Cromer & Mann[3]. The radial distribution function (RDF) $4\pi r^2\rho(r)$ could be obtained by the following relations

$$4\pi r^2\rho(r)=4\pi r^2\rho_0+\frac{2r}{\pi}\int_0^\infty k[I(k)-1]\sin(kr)\,dk$$

and

$$I(k)=I_{eu}^{coh}(k)/f^2(k)$$

where ρ_0 is the mean atomic density, and I (k) is the interference function.

The absolute intensities I_{eu}^{coh} and the interference function are shown in **Fig. 1.** The resulting radial distribution function is shown in **Fig. 2.**

The peak positions and heights of the interference function are listed in **Table 1** together with those of other works. The maximum and minimum positions of the peaks agree approximately with each other. The third minimum appears clearly but a fourth peak exists very ambiguously in this work. The amplitude

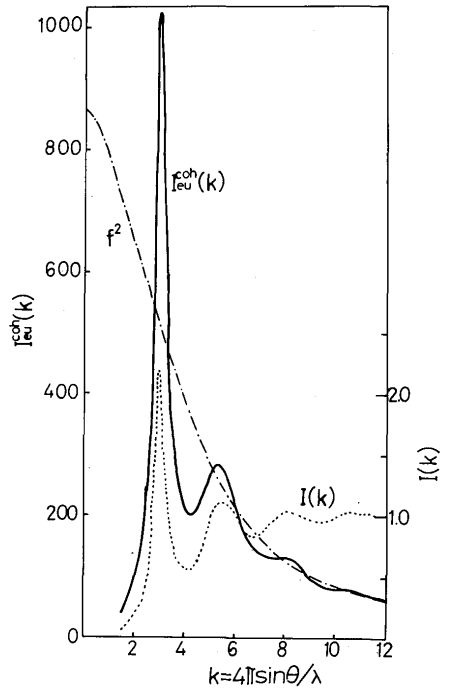

Fig. 1. The absolute intensity function $I_{eu}^{coh}(k)$ and interference function I(k).

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Table 1. Summary of interference functions for liquid copper.

References \ k (Å^{-1})	k_{1max}	k_{1min}	k_{2max}	k_{2min}	k_{3max}	k_{max}	Temp. (°C)
Wagner, Ocken & Joshi[4]*	2.96 (1.83)**	3.95 (0.61)	5.35 (1.15)	6.80 (0.85)	8.20 (1.06)	12.0	1125
Breuil & Tourand[6]***	3.00 (2.41)	4.05 (0.63)	5.44 (1.26)	6.72 (0.87)	8.01 (1.10)	9.4	1150
present work	2.97 (2.17)	4.10 (0.55)	5.50 (1.13)	6.80 (0.84)	8.15 (1.05)	12.0	1200

* These values were evaluated by authors.
** Interfarence functions I(k) were shown in parentheses.
*** Neutron diffraction.

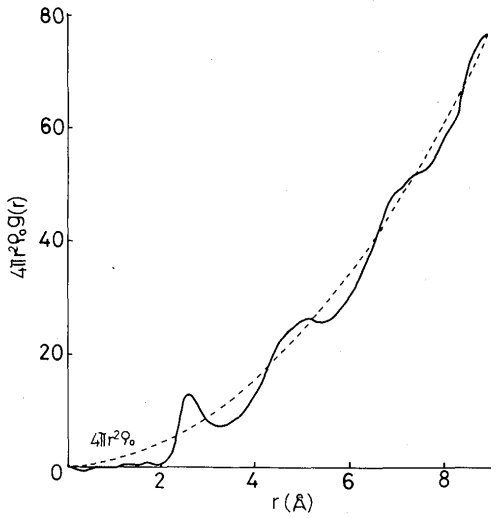

Fig. 2. The radial distribution function $4\pi r^2\rho(r)$.

appeared in the first peak in this work is more violent than that by Wagner, Ocken & Joshi[4], however the rest shapes are seemed to be in good agreement with their values.

In the radial distribution function, the nearest neighbour distance r_1=2.54 Å is insignificantly shorter than that for solid fcc copper (at 20°C)[5], and this value agrees with that of Breuil & Tourand[6]. The coordination number 10.3 was obtained by integrating the first speak of the RDF from r=2.04 to r=3.14. This value shows that liquid copper is less densely packed than soild copper.

References

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