# Structural Study of Liquid Iron by X-Ray Diffraction†

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Until now, the liquid structures of many pure metals and their alloys have been studied by many investigators.

However, the diffraction study of the iron group is very difficult because of their high melting points and active chemical reactivities. The X-ray studies of the iron group in the liquid state, therefore, are only reported by Ruppersberg and Seeman[1], Spector[2], and Schmidt-Prange and Kohlhaus[3]. On the other hand, the neutron diffraction analyses are performed by Waseda, Suzuki, Tamaki and Takeuchi[4], and Waseda and Suzuki[5]. In this paper, the X-ray diffraction study of liquid iron was reported as a divisional studies for structures and physical properties of liquid metals in our laboratory.

The X-ray diffractometer has been reported in detail in the previous paper[6]. Iron of 99.99% purity was contained in a high grade alumina crucible of 25mm width by 20mm length, and melted in a reducing atmosphere of 90%He–10%$H_2$. The temperature of the sample was measured with a 0.3mm$\phi$ $PtRh_6$-$PtRh_{30}$ thermocouple. The intensities from 90° to 10° ($2\theta$) were measured with the scan speed of 1°/min. The $MoK_\alpha$ radiation was used.

The area of the irradiated surface did not exceed 9mm×7mm which was almost flat. The sample could be scarcely hold at the temperature above its melting point above three hours in this measurement. The curved graphite monochrometer which reflected the beam strongly in comparison with the LiF monochrometer was used for the monochromatization of the diffracted beam, though its ability for resolution was not so high.

The observed intensities were corrected for background and polarization, but the absorption correction was not carried out because of the flatness of the sample surface. The method on analysis was the same as described in the previous paper[6]. The intensity data less than 12.0 of $k=4\pi\sin\theta/\lambda$ were contained in this analysis. The normalization constant was obtained by averaging both the results of the high angle region method and the Krogh-Moe-Norman method ($\gamma=0.008$)[7]. The following values were used: the parameter of Cromer & Waber[8] for the atomic scattering factors f(k), the parameter of Cromer & Mann[9] for the incoherent scattering terms $I_{inc}^{eu}$ (k), and the result of Saito, Amatatu & Watanabe[10] for the mean atomic density of liquid iron $\rho_0$.

The absolute intensity curve $I_{coh}^{eu}$(k) and the interference function a(k) are shown in **Fig. 1.** The position and height of the first speak of the a(k) is 2.99 and 2.06 respectively. The a(k) curve deviated upward from 1.0 in the high angle region. This may be attributed to the limitation of the measuring time and the insufficient background correction.

The radial distribution function (RDF) $4\pi r^2\rho_0 g(r)$, which gives the informations of the liquid structure, could be obtained by the following relation

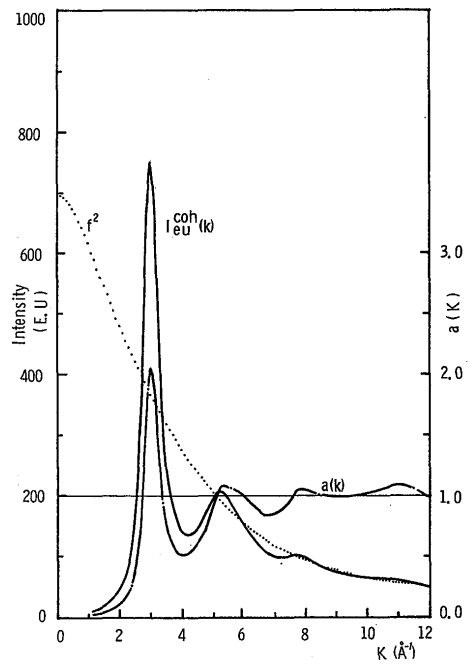


Fig. 1. Absolute intensity curve and interference function of liquid iron at 1570°C.

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

where r is the distance from the origin atom and g(r) is the pair correlation function (PCF). The resulting RDF and PCF are shown in **Fig. 2.** The position of the first peak in the RDF gives the nearest neighbour distance $r_A$. The number of atoms in the first coordination cell is obtained by integrating the first peak. This is called the coordination number CN. The CN depends on the ways of taking the integration area as shown in **Fig. 3.** The ways that have been usually used are as follows;

A : the trailing edge of the first peak in the RDF is made symmetrical with the leading edge.

B : a perpendicular is dropped from the first minimum on the RDF to the r-axis.

C : the trailing edge is extrapolated as a straight line.

The results are summarized in **Table 1.** The CN of liquid iron is about 10, as seen in Table 1.

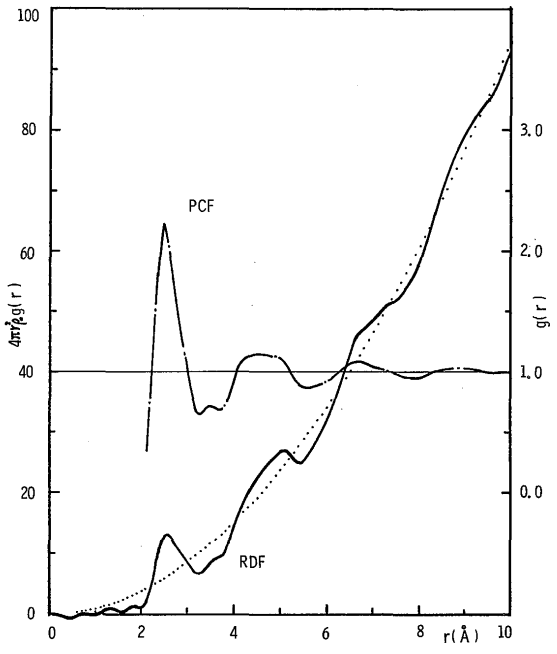


Fig. 2. Radial distribution function and pair correlation function of liquid iron at 1570°C.

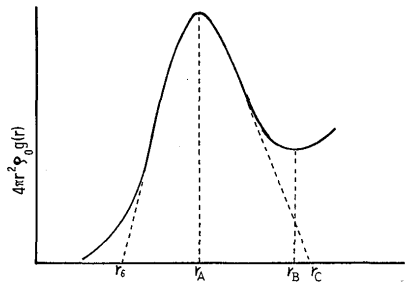


Fig. 3. Different methods of defining the integration area of the first peak in the radial distribution function.

It is an interesting problem whether the liquid structure of iron is the fcc like structure or the bcc like structure. If the liquid structure of iron is the fcc like structure, there is one coordination zone with twelve atoms. On the other hand, there are two coordination zones with eight and six atoms respectively in the first coordination cell, if it is the bcc like structure. The first peak therefore should be more asymmetric in the case of bcc like structure than in the case of fcc like structure. Spektor[2] concluded that the packing of the first cell of liquid iron is that of fcc type from the consideration of the shape of the first peak in the RDF and the CN. It is difficult, however, to speculate the liquid structure of iron from this result.

The a(k) was calculated using the theory of Percus & Yevick[11] concerning a hard sphere model. The observed and calculated a(k) curves are shown in **Fig. 4.** The main property is reappeared in the

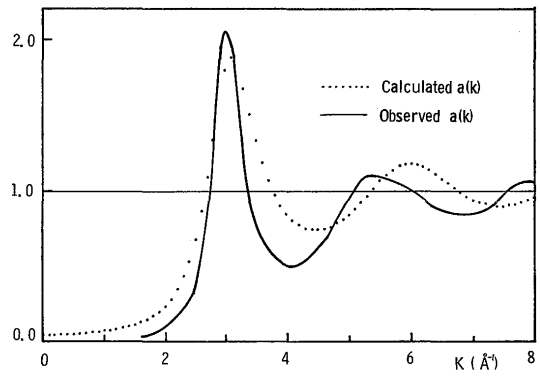


Fig. 4. Observed and calculated interference function of liquid iron at 1570°C.

Table 1. Results of liquid iron.

| Reference | Temp. (°C) | I(k) $k_{max}$ (Å$^{-1}$) | I(k) $k_1$ (Å$^{-1}$) | RDF $r_A$ (Å) | RDF CN (Atoms) A | B | C |
|---|---|---|---|---|---|---|---|
| This work | 1570 | 12.0 | 2.99 | 2.54 | 6.9 | 10.3 | 10.7 |
| Ruppersberg & Seeman[1] | — | 13.0 | — | 2.52 | 8.2 | — | — |
| Spektor[2] | — | — | 2.98 | 2.58 | — | — | — |
| Schmitz-pranghe & Kohlhaas[3] | 1550 | 12.5 | — | 2.58 | 9.2 | 11.6 | — |
| Waseda & Suzuki[5]* | 1620 | 9.0 | 2.97 | 2.58 | — | 9.5 | 9.0 |

* Neutron diffraction method

calculated curve, using the proper values for the density and the radius of the hard sphere. This shows that the major property of the RDF and a(k) curve is determined by the packing geometry of atoms in the liquid state.

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