Partial Atomic Distribution Functions of Liquid Fe\textsubscript{75}B\textsubscript{25}

N. Mattern\textsuperscript{a}, W. Matz\textsuperscript{b}, and H. Hermann\textsuperscript{a}

\textsuperscript{a} AdW der DDR, Zentralinstitut für Festkörperphysik und Werkstofforschung Dresden
\textsuperscript{b} AdW der DDR, Zentralinstitut für Kernforschung Rossendorf.

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Partial structure factors and atomic distribution functions for liquid Fe\textsubscript{75}B\textsubscript{25} were determined for the Fe–Fe and Fe–B pairs by means of X-ray and neutron diffraction. The experimental results show a strong chemical short-range order in the melt which is similar to that of amorphous Fe\textsubscript{75}B\textsubscript{25}.

Key words: liquid Fe–B – X-ray, neutron diffraction on liquid Fe–B – partial structure factors of liquid Fe–B – partial atomic distribution functions of liquid Fe–B – short-range order in liquid Fe–B.

1. Introduction

Until now only total atomic distribution functions of liquid Fe–B alloys were obtained by means of X-ray [1–3] and neutron diffraction [4]. This paper reports on the determination of partial structure factors of a Fe–B melt by combining X-ray and neutron diffraction. From the experimental results information is got concerning the chemical short-range order in liquid Fe\textsubscript{75}B\textsubscript{25}. On the other hand, the amorphous Fe\textsubscript{75}B\textsubscript{25} alloy can be prepared by the rapid quenching technique directly from the melt. The determination of partial radial distribution functions of amorphous Fe\textsubscript{75}B\textsubscript{25} [5] and Fe\textsubscript{80}B\textsubscript{20} [6] shows a strong chemical short-range order in the Fe–B glass. If the amorphous state is assumed to be a frozen in liquid it should be interesting to compare not only the total (see [3]) but also the partial pair correlation functions of liquid and amorphous Fe\textsubscript{75}B\textsubscript{25}.

2. Theoretical Background

From the diffraction experiment the total structure factor \(S(Q)\) is extracted (\(Q = 4\pi \sin \theta /\lambda\)). According to the Faber-Zimm definition [7], \(S(Q)\) is related to the coherent elastic scattering per atom \(I_{coh}\) by

\[
S(Q) = I_{coh} - \langle b^2 \rangle + \langle b \rangle^2 / \langle b \rangle^2.
\]

For a two-component alloy the mean values are given by \(\langle b \rangle = c_A b_A + c_B b_B\) and \(\langle b^2 \rangle = c_A b_A^2 + c_B b_B^2\), where \(c_i\) is the atomic concentration and \(b_i\) the coherent scattering length in the case of neutron diffraction

\[
S(Q) = \sum_i \sum_j W_{ij} S_{ij}(Q) = \frac{1}{\langle b \rangle^2} \left[ c_A b_A S_{AA}(Q) + 2 c_A c_B b_A b_B S_{AB}(Q) + c_B b_B S_{BB}(Q) \right].
\]

In order to evaluate \(S_{ij}(Q)\), three independent diffraction measurements are required with considerable differences in the weighting factors \(W_{ij}\). From the partial structure factors \(S_{ij}(Q)\) the partial atomic distribution functions \(G_{ij}(r)\) can be evaluated by the Fourier transform:

\[
G_{ij} = \frac{2}{\pi} \int_0^{Q_{max}} Q [S_{ij}(Q) - 1] \sin (Q r) d Q.
\]

From the partial atomic distribution functions partial coordination numbers \(N_{ij}\) (number of \(j\) atoms in the coordination shell around an \(i\) atom) can be calculated by

\[
N_{ij} = c_i \int_{r_i}^{r_j} [r G_{ij}(r) + 4 \pi r^2 \varrho_0] dr.
\]

In this equation \(\varrho_0\) represents the mean atomic number density.

3. Experimental

The neutron diffraction experiments on liquid Fe\textsubscript{75}B\textsubscript{25} were performed at a temperature of 1600 K.
The experiments were described in detail in [4]. The neutron diffraction patterns were recorded from \( Q = 2.5 \text{ nm}^{-1} \) up to \( Q = 89 \text{ nm}^{-1} \).

The X-ray diffraction measurement was performed at a temperature of 1573 K on a liquid sample with the same nominal composition. The structure factor was determined from this experiment in the \( Q \)-range \( 7 \text{ nm}^{-1} \leq Q \leq 125 \text{ nm}^{-1} \). For other experimental details cf. [3].

Although there was a small difference in the temperatures of the melts for neutron and X-ray diffraction it seems possible to use the data for the estimation of the partial structure factors. As shown by the X-ray and neutron diffraction experiments on liquid Fe\(_{75}\)B\(_{25}\) [3, 4] there is no strong temperature dependence of the structure factor in this temperature region.

The density of liquid Fe\(_{75}\)B\(_{25}\) was estimated to be \( \varrho_0 = 90.4 \text{ atoms/nm}^3 \) for a temperature of 1600 K [4].

4. Results and Discussion

The obtained total structure factors \( S(Q) \) for the two independent experiments are shown in Figure 1. The X-ray data are limited here to the \( Q \) range of the neutron diffraction experiments.

From the experimentally determined total structure factors the partial structure factors \( S_{ij}(Q) \) can be estimated. According to (2) we get for our experiments:

\[
S_N(Q) = 0.660 \, S_{FeFe}(Q) \\
+ 0.305 \, S_{FeB}(Q) + 0.035 \, S_{BB}(Q),
\]

\[
S_X(Q) = 0.883 \, S_{FeFe}(Q) \\
+ 0.113 \, S_{FeB}(Q) + 0.004 \, S_{BB}(Q).
\]

The coefficients \( W_{ij} \) for the X-ray experiment are given here for \( Q = 0 \). The very small weighting factor of \( S_{BB}(Q) \) indicates that this contribution may be neglected permitting errors in the same order of magnitude as the experimental ones. So the partial structure factors \( S_{FeFe}(Q) \) and \( S_{FeB}(Q) \) were evaluated from the modified Eq. (5) with \( Q \)-dependent \( W_{ij} \) values for the X-ray equation. The results are shown in Figure 2. The general behaviour of the partial structure factors in the melt is similar to that of the amorphous state according to [5] and [6]. But the amplitudes of the modulations are smaller, as it was expected from the higher mobility of atoms in the liquid state. The iron-iron partial structure factor is very similar to the total

Fig. 1. Total structure factors from the neutron and the X-ray diffraction experiments on liquid Fe\(_{75}\)B\(_{25}\).

Fig. 2. Partial structure factors for the Fe-Fe and Fe-B pairs of liquid Fe\(_{75}\)B\(_{25}\).
r_{ij}\text{Fe-Fe}/\text{nm} & N_{ij}\text{Fe-Fe} & r_{ij}\text{Fe-B}/\text{nm} & N_{ij}\text{Fe-B} \\
--- & --- & --- & --- \\
Liquid Fe_{75}B_{25} & 0.260 & 11.2 ± 0.3 & 0.225 & 2.8 ± 0.3 \\
amorphous Fe_{75}B_{25}[5] & 0.260 & 11.4 ± 0.6 & 0.218 & 2.7 ± 0.2 \\
tetr.b.c. Fe_{75}B & 0.261 & 10.7 & 0.222 & 3.0 \\
DRP-model Fe_{70}B_{25}[12] & & 9.7 & 2.0 \\

The parameters of the first neighbourhood of liquid Fe_{75}B_{25} are compared in Table 1 with those of amorphous Fe_{75}B_{25} given in [5]. From Table 1 it is visible that the typical data for the first neighbourhood of liquid and amorphous Fe_{75}B_{25} are very similar. Differences in the $G_{ij}(r)$ curves exist between the liquid and the amorphous state in the shape of the second peaks. In the melt the second peak of $G_{\text{FeB}}$ is not split and that of $G_{\text{FeFe}}$ shows a reversed shape with a shoulder on the left hand (Figure 3). The comparison of the total structure factors and the total atomic distribution functions of liquid and amorphous Fe-B alloys in [3] indicates that the amorphous state is not a simple frozen liquid. Structural changes arise during rapid quenching of the melt which result in a changed size and connection of structural units.

At present two important conceptual structure models for the local atomic order exist for transition-
metal-metalloid (T-M) glasses: (i) dense random packed (DRP) models for binary alloys and (ii) stereochemically defined models. Gaskell [9] reviewed the properties of these models in comparison with the essential experimental results of structural investigations. In spite of the apparent success in reproducing experimental total pair distribution functions, structure models of binary alloys which are based on central force atomic interactions [10–12] fail to reproduce the specific kind of chemical order present in T-M glasses [13]. For instance the number $N_{FeB}^1$ of boron atoms within the first coordination shell around iron atoms predicted by the DRP models [10–12] for amorphous Fe-B alloys is too low. In Table 1 the coordination numbers are given for the DRP model of Takacs [12] which are considerably smaller than the experimental values of amorphous and liquid Fe$_{75}$B$_{25}$. The stereochemically defined models are based on the assumption of the existence of the same local structural units in the amorphous and crystalline state of the alloy. Amorphous Fe$_{75}$B$_{25}$ crystallizes to metastable Fe$_3$B. The short-range order parameters of the Fe$_3$B phase given in Table 1 show good agreement with the experimental results within the errors. From the comparison of the data we can conclude that in liquid Fe$_{75}$B$_{25}$ the atomic arrangement within the first neighbourhood is similar to that of metastable Fe$_3$B.