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METALLIC GLASSES

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ON THE STRUCTURE OF IRON-BORON  
METALLIC GLASSES

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#### АННОТАЦИЯ

Была определена интерференционная функция  $I(K)$  металлического стекла  $Fe_{100-x}B_x$  ( $x = 15,8; 19,6$  и  $23,1$ ) в области вектора рассеяния от  $0,5$  до  $14 \text{ \AA}^{-1}$  с применением излучения  $Mo K_\alpha$  в симметричной трансмиссионной геометрии. Во всех трех случаях была определена также и функция парной корреляции  $g(r)$ , что хорошо совпадает с результатами как рентгеновских, так и нейтронно-дифракционных измерений, опубликованных в литературе. Структуру второго пика в  $g(r)$  можно считать "нормальной".

#### KIVONAT

$Mo K_\alpha$  sugárzás felhasználásával szimmetrikus transzmissziós geometriai elrendezésben meghatároztuk a  $Fe_{100-x}B_x$  ( $x = 15,8, 19,6$  és  $23,1$ ) fémüvegek  $I(K)$  interferenciafüggvényét a  $0,5$  és  $14 \text{ \AA}^{-1}$  közötti szórásvektor tartományban. Mindhárom esetben meghatároztuk a  $g(r)$  párkorrelációs függvényt. Jó egyezésben a Fukunaga et al. röntgen- és Cowlam et al. neutrodiffrakciós méréseinek eredményeivel,  $g(r)$  második csúcának szerkezetét "normális"-nak találtuk.

## ABSTRACT

The interference function,  $I(K)$  of glassy  $\text{Fe}_{100-x}\text{B}_x$  ( $x = 15.8, 19.6$  and  $23.1$ ) alloys was determined in the wave vector range between  $0.5$  and  $14 \text{ \AA}^{-1}$  using Mo K $\alpha$  radiation in symmetric transmission geometry. The pair correlation,  $g(r)$  was determined in all the cases. In agreement both with X-ray [2] and neutron diffraction [3] investigations the second peak splitting in  $g(r)$  is "normal".

## INTRODUCTION

Up till now three different investigations have been published on iron-boron metallic glasses [1,2,3]. Waseda and Chen [1] claimed that the reduced pair correlation function of the hypoeutectic iron-boron metallic glasses is very similar to the one of the dense random packing of hard spheres, that is, the so-called shoulder is higher than the second peak. On the other hand, according to Fukunaga et al. [2] and Cowlam et al. [3] the structure of iron-boron glasses is normal even in the low boron concentration range. In this contribution, our aim is to show that as to the structural properties, the iron-boron glasses behave "normally", like the other transition metal-metalloid glasses [4].

## EXPERIMENTAL

The glassy  $\text{Fe}_{100-x}\text{B}_x$  ( $x = 15.8, 19.6$  and  $23.1$ ) ribbons were prepared by rapid quenching from the melt at the Central Research Institute for Physics, Budapest. The thickness of the ribbons was around  $25 \mu\text{m}$ . The ribbons were cut to pieces and samples with  $10$  by  $10$  mm surface were prepared. The as-cast ribbons were chemically

analysed by a Varian atomic absorption spectrophotometer. The density of the samples was found to be 7.3, 7.2 and 7.0 g/ml for  $x = 15.8, 19.6$  and  $23.1$ , respectively, by the Archimedean method. These values are somewhat smaller than those by Waseda and Chen [1].

The intensity curves were measured in symmetrical transmission geometry using an MZ-1 type Seifert diffractometer and  $\text{Mo K}_\alpha$  radiation. The measurements were made at the Central Research Institute for Chemistry, Budapest. The LiF crystal-monochromator was located in the primary beam because this arrangement makes the Compton correction relatively simple. The intensity was determined in the scattering vector range  $K = 0.5-14.0 \text{ \AA}^{-1}$ . The scattering vector was changed by 0.05, 0.1 and  $0.25 \text{ \AA}^{-1}$  steps in the intervals 0.5-5, 5-10 and 10-14  $\text{ \AA}^{-1}$ , respectively.

The X-ray intensity,  $I_{\text{coh}}(K)$ , coherently scattered by more than one species of atoms can be written as

$$I_{\text{coh}}(K) = \langle f^2 \rangle + \langle f^2 \rangle \int_0^\infty 4\pi r^2 [\rho(r) - \rho_0] \frac{\sin Kr}{Kr} dr \quad (1)$$

where  $\langle f^2 \rangle = \sum_i c_i f_i^2$ ,  $\langle f \rangle = \sum_i c_i f_i$  and  $K, c_i, f_i$  are the scattering vector, the concentration and the atomic scattering factor of the  $i$ -th kind of atoms,  $\rho(r)$  is the radial density function and  $\rho_0$  is the average number density of atoms.

As the total interference function  $I(K)$  is defined by

$$I(K) = [I_{\text{coh}}(K) - \langle f^2 \rangle + \langle f \rangle^2] / \langle f \rangle^2, \quad (2)$$

the total pair correlation function,  $g(r)$  can be evaluated as the Fourier transform of  $I(K)$  by the following relation

$$g(r) = 1 + \frac{1}{2\pi^2 r \rho_0} \int_0^\infty K [I(K) - 1] \sin Kr dK. \quad (3)$$

The observed intensity ( $I_{\text{obs}}$  in arbitrary units) must be corrected for background, absorption and polarization.

The background intensity, such as the air scattering and the sample-holder scattering, was measured without the sample and then subtracted from the observed intensity.

As symmetrical transmission arrangement was used we applied Alexander's absorption correction [5] and the polarization correction factor given by Whittaker [6] and converted the corrected intensity to absolute units by both Krogh-Moe-Normann [7] and high-angle [8] methods. The difference between the two normalization factors was within 2 per cent.

The monochromator was located in the primary beam, so the incoherent intensity could be calculated using the fitting parameters reported by Hajdu [9]. The data processing was carried out on an R-40 computer. In this procedure a modified version of a FORTRAN-IV program by Hajdu and Radnai [10] was used.

## RESULTS

After the normalization of the corrected coherent intensities (see Fig. 1), the total interference functions are obtained (Fig. 2). In Tables 1a and b the peak positions and the relative peak heights of the total interference functions are summarized.

Table 1a. The peak positions in I(K)

$c_B$ at. %	$K_1 (\text{\AA}^{-1})$	$K_2 (\text{\AA}^{-1})$	$K_3 (\text{\AA}^{-1})$	$K_4 (\text{\AA}^{-1})$	Ref.
15.8	3.09 <sub>2</sub>	5.23 <sub>2</sub>	6.13 <sub>8</sub>	7.80	
19.6	3.10 <sub>2</sub>	5.22 <sub>0</sub>	6.19 <sub>2</sub>	7.80	
23.1	3.11 <sub>0</sub>	5.22 <sub>2</sub>	6.23 <sub>7</sub>	7.85	
11.5	3.08				[2]
14.1	3.08				[2]
16.8	3.11 <sub>5</sub>				[2]
19.6	3.12				[2]
22.6	3.13				[2]
16	2.99	5.26	6.10		[1]
20	3.01	5.26	6.10		[1]
25	2.98	5.23	6.10		[1]
17	3.15	5.28	6.13		[3]

Table 1b. The peak heights in I(K)

$c_B$ at.%	$I(K_1)$	$I(K_2)/I(K_1)$	$I(K_3)/I(K_1)$	$I(K_4)/I(K_1)$	Ref.
15.8	3.83	0.48	0.24	0.34 <sub>5</sub>	
19.6	3.71	0.50	0.27	0.36	
23.1	3.53	0.53	0.26	0.36 <sub>8</sub>	
11.5	3.38				[2]
14.1	3.46				[2]
16.8	3.36				[2]
19.6	3.14				[2]
22.6	3.14				[2]
16	3.20				[1]
20	3.10				[1]
25	3.02				[1]

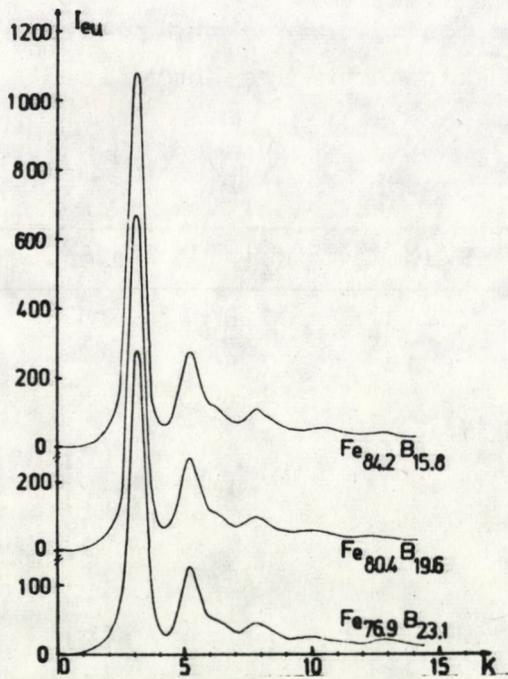


Fig. 1. Coherently scattered intensity for  $Fe_{100-x}B_x$  glasses

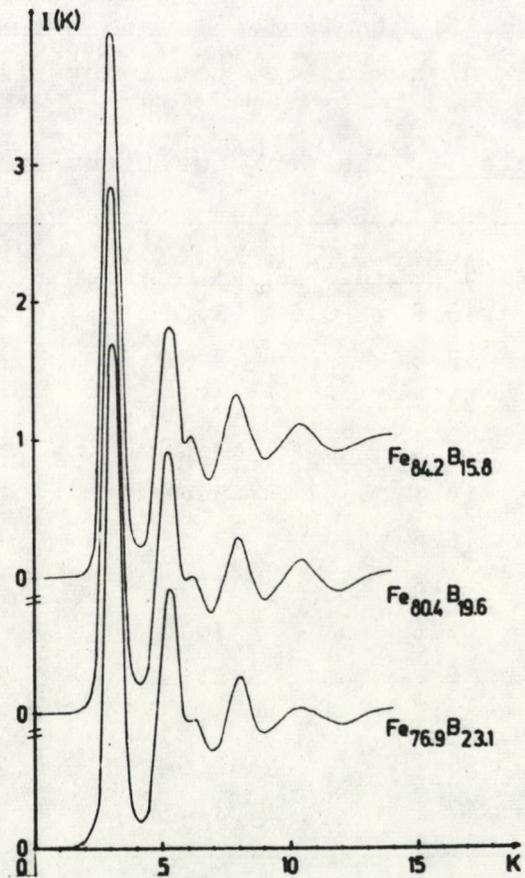


Fig. 2. The total interference function of  $Fe_{100-x}B_x$  glasses.

With increasing boron concentration the height of the first peak of the interference function gradually decreases, its width gradually increases. Similarly, there is a gradual change in the reduced interference function,  $F(K) = K(I(K)-1)$ , that is shown in

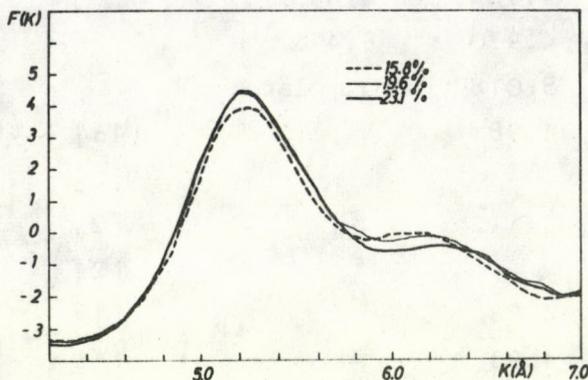


Fig. 3. The reduced interference function,  $F(K) = K(I(K)-1)$ , in the shoulder region.

$g(r)$  were obtained using (3). In Table 2 the peak positions in  $g(r)$  are given. For the sake of simplicity in Fig. 4 the pair-correlation functions for  $c_B = 15.6$  at% and 23.1 at% are only shown. One can clearly see that even in the case of low boron concentration alloy,  $c_B = 15.6$  at%, the second peak is higher than the shoulder, i.e. the structure remains "normal" similarly to any other transition metal-metalloid glass.

Fig. 3. These changes with decreasing boron content can be explained by assuming increasing distortions in trigonal prismatic packing proposed by Gaskell [12]. However, no peculiarities show up at 20 per cent in the distortions.

By Fourier transforming the reduced total interference functions the total pair-correlation functions,

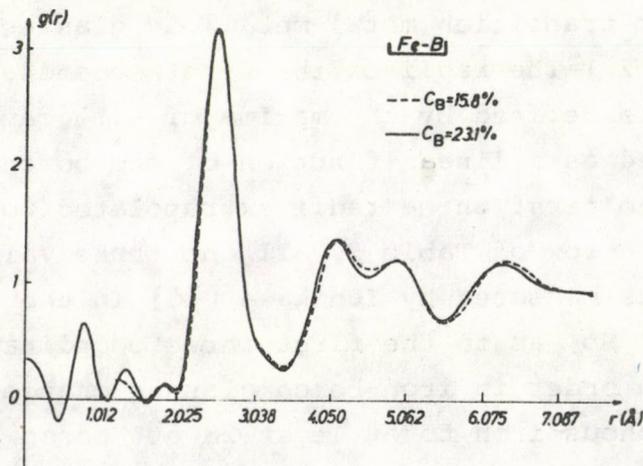


Fig. 4. The total pair correlation functions for  $Fe_{84.4}B_{15.6}$  and  $Fe_{76.9}B_{23.1}$  glasses.

Table 2. Peak positions in  $g(r)$

$c_B$ at%	$R_1$ (Å)	$R_2$ (Å)	$R_3$ (Å)	$R_4$ (Å)	Ref.
15.8	2.560	4.183	4.985	6.428	
19.6	2.559	4.166	4.981	6.443	
23.1	2.567	4.150	4.970	6.412	
0	2.544	4.254	5.018	Extrapolated	
0	2.54	4.25	4.98		[13]
16.8	2.537				[2]
19.6	2.554				[2]
22.6	2.546				[2]
16	2.58	4.40	4.88		[1]
20	2.57	4.37	4.93		[1]
25	2.62	4.33	4.90		[1]

## CONCLUSIONS

1.) In good agreement with the measurements of Tohoku group [2], we have found that the diffraction pattern and the total pair correlation function of iron-boron glasses are similar to the other transition metal-metalloid glasses.

2.) The radii of the first, second and third coordination shells defined by the maxima of  $g(r)$  can be extremely well represented as a linear function of the boron content,  $c_B$ . The values of the first three radii extrapolated to  $c_B = 0$  are given in the fourth row of Table 2. All the three values are very close to the values measured by Ichikawa [13] in the case of pure amorphous iron. So, as to the first three coordination shells, the short range order in iron-boron glasses changes smoothly from the pure amorphous iron to at least 23 at% boron content.

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