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Study of Local Structure of $Fe_{84}B_{16}$ Amorphous Alloy by Electron Diffraction

V. Hrabčáková[a,*], Š. Michalik[b], K.B. Borisenko[c], V. Girman[a], V. Nemcová[a] and P. Sovák[a]

[a]Institute of Physics, Faculty of Sciences, P. J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovakia
[b]ELI – Beamlines, Institute of Physics of the ASCR, v.v.i., Na Slovance 2, 182 21 Praha 8, The Czech Republic
[c]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH United Kingdom

Local atomic structure in $Fe_{84}B_{16}$ metallic glass, prepared by melt-spinning technique in He atmosphere, was studied by electron diffraction (ED) reduced density function (RDF) analysis. RDF curves were also obtained from X-ray diffraction (XRD) patterns and compared with the data from ED. Atomic reduced density functions, G(r), calculated from ED and XRD patterns showed good agreement. Atomic structure model has been fitted to the experimental ED data using Reverse Monte Carlo (RMC) simulation.

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1. Introduction

The $Fe_{84}B_{16}$ alloy is a typical amorphous metal-metalloid system with eutectic concentration. This alloy has excellent magnetic properties such as large saturation magnetization, Invar-like characteristics (low thermal expansion over a wide range of temperatures) and simple composition which is advantageous for structural modeling [1]. The main aim of this work is to investigate the local atomic structure of the as-quenched $Fe_{84}B_{16}$ using electron diffraction (ED) and Reverse Monte Carlo (RMC) simulation.

2. Methods

The amorphous ribbons (2 mm width, 25–28 μm thickness) were prepared by arc melting from pure elements (Fe–99.98% and B–99.99%) in Ar atmosphere and subsequent melt-spinning in He atmosphere. Selected area electron diffraction (SAED) patterns were obtained in JEOL JEM 2100F UHR microscope with FEG cathode at 200 kV accelerating voltage. Calibration of diffraction patterns was performed using Au nanoparticles on carbon film. X-ray diffraction was performed at the BW5 beamline station in DESY centre in Hamburg. Averaged atomic model of the local structure of the studied sample was created by the RMC simulation.

3. Results

Experimental diffraction patterns obtained from ED were converted first to the reduced scattering intensity $\varphi(q)$ (1).

*corresponding author; e-mail: valentina.hrabcakova@upjs.sk

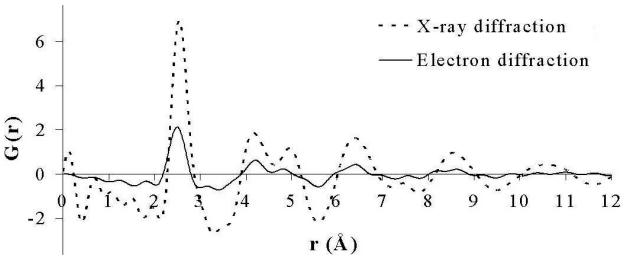

Fig. 1. Comparison of $G(r)$ calculated from XRD and ED experimental data.

$$\varphi(q) = \left[\frac{I(q) - Nf^2(q)}{Nf^2(q)}\right] q, \tag{1}$$

where $I(q)$ is the total scattering intensity and $Nf^2(q)$ is atomic scattering intensity including any intensity related to scattering from the instrument (scattering on aperture, sample holder etc.).

Reduced density function $G(r)$ was obtained from $\varphi(q)$ by Fourier transformation (2) [2].

$$G(r) = 4\int_0^\infty \varphi(q)\sin(qr)\,\mathrm{d}q. \tag{2}$$

XRD data were converted to $G(r)$ using PDFgetX2 software. The $G(r)$ curves from ED and XRD experiments are compared in Fig. 1. Profiles of the curves are typical for metallic glasses. Both $G(r)$ curves are composed of broad first peak, split second peak and smaller peaks at longer distances. The most intensive first peak is located at 2.52 Å (ED) and at 2.55 Å (XRD), showing a relatively good agreement between the two methods. The second peak and its shoulder are at 4.23 Å and 4.83 Å for ED and at 4.16 Å and 4.96 Å for XRD. RMC simulation is a basic method for modelling of structures of liquids and glasses. We used this technique to refine a 3D structural model from 2D diffraction data obtained by ED. In the

first step an initial approximation of an atomic model of the material was created. This model consisted of 1000 atoms (840 Fe and 160 B atoms) randomly placed in a cubic cell with defined density (6.7 g/cm^3). Then the atomic configuration of the model was optimized to minimize the difference between the $G(r)$ curves obtained from ED and the model. The details about the RMC algorithm can be found elsewhere [3].

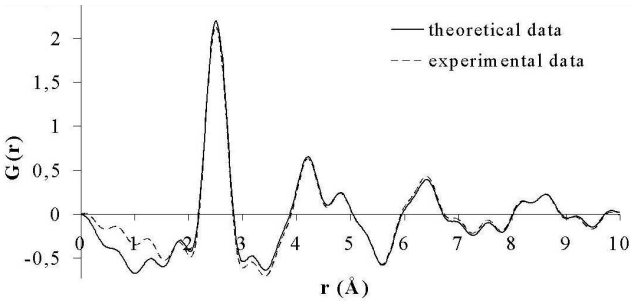

Fig. 2. Agreement between $G(r)$ curves from theoretical model and experimental data obtained by TEM.

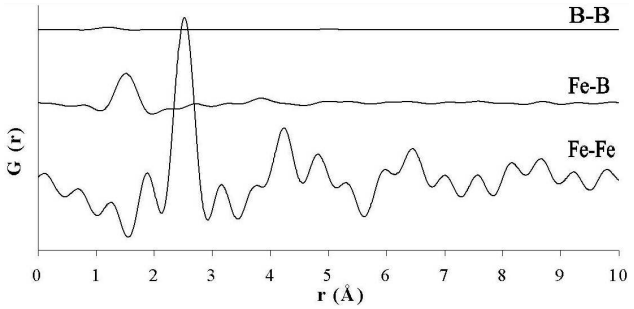

Fig. 3. Partial pair distribution function $G(r)$, calculated from structural model refined in the RMC simulations. B-B pair correlation function appears almost featureless, because of boron's weak contribution to electron scattering.

The $G(r)$ computed from the final simulated 3D model is in good accordance with the experimental $G(r)$ obtained from ED data as can be seen in Fig. 2. The refined model allows calculation of partial pair distribution functions, average bond lengths and their occurrences. In the final atomic model there are 79% Fe-Fe bonds, 18% Fe-B bonds and 2% B-B bonds. Average bond lengths are 2.48 ± 0.25 Å , 1.73 ± 0.37 Å and 1.29 ± 0.23 Å for Fe-Fe, Fe-B and B-B bonds, respectively. In the analysis the atoms were considered to form a bond if the distance between them was shorter than a sum of the respective covalent radii and a tolerance of 0.5 Å. The crystalline structure of $Fe_{84}B_{16}$ should include α-Fe and Fe_2B phases according to Fe-B phase diagram. The lattice parameter and closest distances between two Fe atoms in α-Fe are 2.866 Å, 2.482 Å, respectively (Crystallography Open Database ID 9008536) [4]. The average Fe-Fe bond length from the refined model agrees well with that in α-Fe phase. However, the Fe-Fe (3.035 Å, 3.045 Å) and Fe-B (3.101 Å) bond lengths in Fe_2B (COD ID 1510682) [4] do not fit to any of the major peak positions in the experimental $G(r)$ curves. It was observed, however, that as-quenched binary Fe-B alloys with near eutectic composition typically separate into nanoscale α-Fe and Fe_3B phases [5]. The Fe-Fe and Fe-B bond lengths in crystalline Fe_3B are 2.58 Å and 2.07 Å, respectively [6]. The bond lengths from this phase agree considerably better with the corresponding bond lengths in our refined model (2.48 ± 0.25 Å, 1.73 ± 0.37 Å, respectively), taking the wide distribution of bonds in the amorphous material into account.

4. Conclusions

ED technique and RDF analysis were used for $Fe_{84}B_{16}$ local structure characterisation. The results from the refined theoretical model suggest that the material contains building blocks corresponding to α-Fe and Fe_3B phases in the local atomic structure.

Acknowledgments

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