L-04 **Tue. 01. 09., 15^{00}-15^{40}**

Wide-angle X-ray scattering and Reverse Monte Carlo studies of $Fe_{80}B_{20}$, $Co_{80}B_{20}$, $Mg_{60}Cu_{30}Y_{10}$ metallic glasses

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Keywords: synchrotron radiation, metallic glasses, wide-angle X-ray scattering, Reverse Monte Carlo

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The atomic scale structure of $Fe_{80}B_{20}$, $Co_{80}B_{20}$ and $Mg_{60}Cu_{30}Y_{10}$ metallic glasses has been studied using the wide-angle X-ray scattering and reverse Monte Carlo methods. The $Fe_{80}B_{20}$ and $Co_{80}B_{20}$ samples were prepared in the form of amorphous ribbons with thickness of 0.03 mm and width of 5 mm by the "chill-block melt spinning technique under the argon protective atmosphere. The bulk $Mg_{60}Cu_{30}Y_{10}$ glass was obtained by injection of the Mg-Cu-Y melted material in the proportion 60:30:10 into a copper mold by a pressure casting method.

The wide-angle X-ray scattering measurements were performed on the ID31 beam-line at the European Synchrotron Radiation Facility, Grenoble, France. The incident beam energy of 31 keV yielding the wavelength of 0.4 Å was used in this experiment. The scattered intensities were recorded to the maximum value of the scattering vector $Q = 4\pi\sin\theta/\lambda$ = 23 Å^{-1}, where 2θ is the scattering angle and λ is the wavelength.

As the atomic scale structure of the investigated materials cannot be described using formalism of crystallography an approach based on the Reverse Monte Carlo [1] fitting procedure was used. In this method Marcov chain sampling with the Metropolis accelerating algorithm [2] allows generation of three dimensional particle configuration that is consistent with the experimentally measured structure factor. The fit quality is evaluated by a standard χ^2 test in which the experimental errors are taken into account.

In our previous paper [3] the local atomic arrangement in the $Fe_{80}B_{20}$ glass was compared with those of the Fe_3B, $Fe_{23}B_6$ and bcc Fe crystalline phases. From this comparison it has been concluded that the local structure of the crystalline counterparts is not consistent with the experimental data for glassy $Fe_{80}B_{20}$.

The Reverse Monte Carlo method applied for the $Fe_{80}B_{20}$, $Co_{80}B_{20}$ and $Mg_{60}Cu_{30}Y_{10}$ metallic glasses allowed obtaining perfect fit to the experimental structure factors and to the experimental pair distribution functions. Resemblance of the local structure, which extends up to approximately 20 Å, to the icosahedral and trigonal prism configurations is discussed. The Reverse Monte Carlo results are compared with high-resolution transmission electron microscopy observations. From this comparison it can be concluded that both methods lead to consistent description of the local atomic arrangement in the investigated materials.

Acknowledgments: This work was supported by the National Science Centre under the research project No.: 2011/03/D/ST8/04138.

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