Structure and physical properties of Mg-based metallic glasses prepared by a melt spinning technique

Š. Michalik¹, K. Kušnírová², Z. Molčanová², M. Šulíková³, P. Jóvári⁴, K. Saks⁵

¹Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0DE, United Kingdom, ²Institute of Materials Research of SAS, Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovakia, ³Department of Medical and Clinical Biophysics, Faculty of Medicine, Pavol Jozef Šafárik University in Košice, Trieda SNP1, 040 11 Košice, Slovakia, ⁴Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, PO Box 49, 1525 Budapest, Hungary, ⁵Faculty of Materials, Metallurgy and Recycling, Technical University of Košice, Letná 9, 042 00 Košice, Slovakia stefan.michalik@diamond.ac.uk

Keywords: Mg-based metallic glasses, X-ray and neutron total scattering, RMC simulations, Voronoi analysis

Over the last three decades an intensive material science research is aiming at the preparation of new Mg-based metallic glasses (MGs) suitable for various engineering applications [1-3]. Recently, two very different suggestions were made proposing Mg-based MGs as suitable materials for hydrogen storage [4] as well as promising candidates for biomedical purposes [5]. By a melt spinning technique, we prepared a series of ternary and quaternary Mg-Ce-(Ni,Cu) MGs intended for hydrogen storage applications and determined their absorption reaching up to ~ 5.0 wt% H storage capacity for the best composition. We also fabricated a series of Mg-Zn-Ca and Mg-Zn-Sr ribbon shaped MGs to serve as precursors for design of future highly alloyed systems with tuned mechanical properties and dissociation rate in human body [6]. While physical properties of Mg-based metallic glasses can routinely be found in literature, the detailed structure characterisation of their short-range ordering based on measurements is far from being standardly present. In our work we combine synchrotron based high energy X-ray diffraction and neutron diffraction to characterise the amorphous structure of above-mentioned Mg-based MGs by means of atomic pair distribution functions. Figure 1(a) demonstrates decomposition of the first maximum of neutron and X-ray total reduced atomic pair functions, $D_N(r)$ and $D_X(r)$ into three Gaussian functions representing ZnZn, MgZn and MgMg pairs for Mg$_{50}$Zn$_{43}$Ca$_{7}$, Mg$_{60}$Zn$_{43}$Ca$_{7}$ and Mg$_{70}$Zn$_{23}$Ca$_{7}$ MGs [7]. To extend our description of the local atomic arrangement, we combine the experimental data with the Reverse Monte Carlo simulations and the obtained 3D configurations are subject of intensive topological analysis. Figure 1(b) shows results of distributions of coordination numbers based on Voronoi analysis for ternary Mg-Ni-Ce MGs.

![Figure 1](image_url)

Figure 1. (a) Decomposition of the first $D_X(r)$ and $D_N(r)$ into three Gaussians representing ZnZn, MgZn and MgMg pairs for Mg$_{50}$Zn$_{43}$Ca$_{7}$, Mg$_{60}$Zn$_{43}$Ca$_{7}$ and Mg$_{70}$Zn$_{23}$Ca$_{7}$ MGs. (b) Fraction distribution of Mg-, Ni- and Ce-centred Voronoi cells based on their total coordination number for Mg$_{70}$Ni$_{20}$Ce$_{10}$, Mg$_{80}$Ni$_{10}$Ce$_{10}$ and Mg$_{90}$Ni$_{0}$Ce$_{10}$ MGs.