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Combined EXAFS and X-Ray Scattering Investigation of Amorphous Zr-Based Alloys

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Abstract. EXAFS spectra for all K absorption edges and X-ray scattering data have been obtained on an amorphous Fe-Zr sample prepared by mechanical alloying and a rapidly quenched Co-Zr one. Partial pair distribution functions have been determined as a solution of an inverse ill-posed problem for the system of integral equations describing combined experimental data. For Fe-Zr and Co-Zr amorphous alloys we find a high degree of chemical order and also non-Gaussian nearest neighbour distribution.

1. INTRODUCTION

Amorphous alloys formed by two transition elements have been widely interested because of their interesting structural, electronic and magnetic properties. The investigation of the magnetic properties shows that $\text{Fe}_x\text{Zr}_{1-x}$ and $\text{Co}_x\text{Zr}_{1-x}$ alloys are paramagnetic and superconducting at high Zr concentration [1]. At reduced Zr-content superconductivity is suppressed and the alloys become inhomogeneous ferromagnets [1,2] at $x=0.35$ for Fe and $x=0.55$ for Co. For low Zr concentrations, there is an interesting contrast between Co-Zr and Fe-Zr alloys. For $\text{Fe}_x\text{Zr}_{1-x}$ at $x>0.85$ a complex spin structure is described as a spin glass phase. Co-rich $\text{Co}_x\text{Zr}_{1-x}$ alloys remain strong ferromagnets [2].

We present here an application of combined EXAFS and X-ray scattering data to obtain short range order information for $\text{Fe}_{67}\text{Zr}_{33}$ and $\text{Co}_{90}\text{Zr}_{10}$ amorphous alloys. We use a regularization method of solving the system of integral equations describing experimental data sets [3].

2. EXPERIMENTAL AND RESULTS

Amorphous $\text{Fe}_{67}\text{Zr}_{33}$ alloy has been obtained by mechanical alloying after 17h milling starting from pure elemental powders [4]. The $\text{Co}_{90}\text{Zr}_{10}$ amorphous ribbons are produced by conventional melt spinning [5].

All measurements were performed in Ekaterinburg using laboratory EXAFS spectrometer with variable curvature bent crystal and X-ray diffractometer. Experimental Zr K-spectra were corrected on core level width ($\Gamma=3.7$ eV) by special deconvolution method. This procedure was included in preliminary experimental data processing [6].

To obtain the partial pair correlation functions (PCFs) $g_{ij}(r)$ of binary amorphous alloy, we use the combination of the three experimental data on X-ray scattering and absorption: the X-ray total structure factor, $s \in [1..16. \text{\AA}^{-1}]$; the first element EXAFS, the second element EXAFS, $k \in [3..13. \text{\AA}^{-1}]$. A full description of the mathematical scheme can be found in Ref. [3].

As a solution of the system of the integral equations we present partial PCFs for $\text{Fe}_{67}\text{Zr}_{33}$ (Fig. 1a) and $\text{Co}_{90}\text{Zr}_{10}$ (Fig. 1b) amorphous alloys. Characteristics of the first coordination shell of partial PCFs for amorphous alloys and their crystalline references are given in Table 1.

Table 1: Characteristics of the first peak of the partial pair correlation functions for amorphous alloys $\text{Fe}_{67}\text{Zr}_{33}$, $\text{Co}_{90}\text{Zr}_{10}$ and their references – crystalline Fe_2Zr and Co_2Zr . (r – the first interatomic distance, error $\Delta r = \pm 0.02 \text{\AA}$; α – asymmetry parameter, $\Delta \alpha = \pm 0.1$; N – coordination number, $\Delta N = \pm 0.2$ at.)

	Fe – Zr alloys									Co – Zr alloys					
	Fe-Fe			Fe-Zr			Zr-Zr			Co-Co			Co-Zr		
	$r, \text{\AA}$	α	$N, \text{at.}$	$r, \text{\AA}$	α	$N, \text{at.}$	$r, \text{\AA}$	α	$N, \text{at.}$	$r, \text{\AA}$	α	$N, \text{at.}$	$r, \text{\AA}$	α	$N, \text{at.}$
amorphous	2.48	1.1	5.7	2.83	1.1	3.9	3.14	1.1	4.9	2.42	1.2	10.9	2.79	1.0	1.5
crystalline	2.50	1.0	6.	2.93	1.0	6.	3.06	1.0	4.	2.43	1.0	9.1	2.88	1.0	3.3

Figure 1: Partial pair correlation functions for Fe-Zr (a) and Co-Zr (b) systems: theoretical functions for crystal (points line) and experimental ones for amorphous alloys (solid line).

3. DISCUSSION

For $\text{Fe}_{67}\text{Zr}_{33}$ amorphous alloy the Fe-Fe bond length is found to be practically the same as in the crystal, whereas the Fe-Zr bond length is shorter and the Zr-Zr one is more longer. For $\text{Co}_{90}\text{Zr}_{10}$ alloy the curve $g_{\text{Co-Co}}$ is similar to the crystalline one as far as the fourth coordination shell. The Co atoms are surrounded the Zr atoms like in crystal (asymmetry coefficient defined as a ratio of the right-hand and left-hand half-widths on the half-amplitude, $\alpha=1$) and form a peculiar unit with a perfect configuration. A correlation between the Zr atoms is absent. As a consequence, the interatomic distance Co-Zr becomes shorter than in crystal.

In numerical simulations of the partial PCFs of TM-TM glasses it was shown [7] that attractive forces between TM-Zr atoms resulting from the strong covalent d-d interactions are expressed in terms of d-d transfer integral and the bond-order defined as the difference in the number of d-electrons in bonding and antibonding states. From our results short range order in amorphous $\text{Fe}_{67}\text{Zr}_{33}$ and $\text{Co}_{90}\text{Zr}_{10}$ is reasonably chemically ordered. The distance TM-Zr is shorter than the crystal value.

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