Supplemental material to the article

XMCD study of local magnetic and structural properties of microcrystalline NdFeB-based alloys

Extended X-ray Absorption Fine Structure (EXAFS) studies of $Nd_{10.4}Zr_{4.0}Fe_{79.2}B_{6.4}$ alloy were performed at beamline BM23 of the European

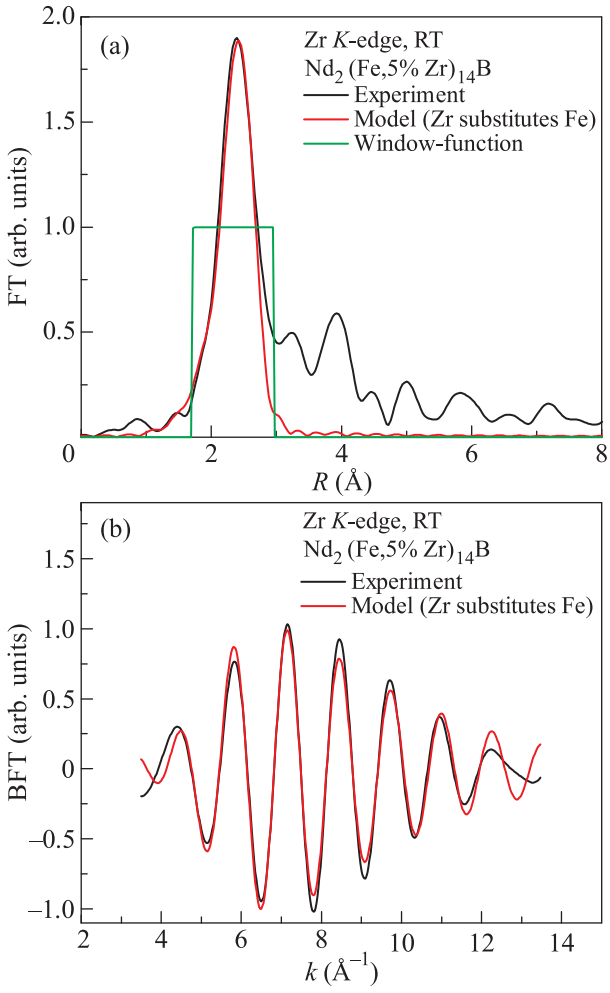

Figure 1: Fourier transform (FT) modulus (a) and Back-Fourier transform (BFT) (b) of experimental and model K-Zr EXAFS function $\chi(k)k^2$ for $Nd_{10.4}Zr_{4.0}Fe_{79.2}B_{6.4}$ sample

Synchrotron Radiation Facility (ESRF), Grenoble, France [1]. High-quality EXAFS spectra above the K-edge of zirconium were acquired at room temperature in fluorescence mode using a 13-element Ge detector. Experimental data were analyzed

with VIPER program package [2] using back-scattering amplitude and phase shifts calculated by FEFF-8.20 code [3]. The structural information for modeling the spectra was taken from [4].

The experimental K-Zr EXAFS function $\chi(k)k^2$ was Fourier transformed in the momentum range $k = 3.5{-}13.5\,\text{Å}^{-1}$ (see black line in the upper panel of Fig. 1). After that we isolated the first coordination shell $R = 1.8{-}3.0\,\text{Å}$ using square window function and conducted Back-Fourier Transform (BFT) (see black line in the lower panel of Fig. 1). The simulation of this filtering experimental EXAFS function was performed in the frame of model in which Zr atoms substitutes Fe atoms in their lattice positions, i.e. has the same local environment. A rather good agreement of the model curve (red lines in both panels of Fig. 1) with experimental data confirms that Zr atoms indeed occupy predominantly the Fe positions in $Nd_2Fe_{14}B$ matrix.

References

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