XAS STUDY OF CARBON COATED Fe AND Fe_3O_4 DERIVED NANOPARTICLES

K. Schneider [1*], **Cz. Kapusta** [1], **D.A. Zajac** [2,3], **C.I. Marquina** [4], **and M.R. Ibarra** [4]

[1] Faculty of Physics and Applied Computer Science, AGH University of Science&Technology, 30-059 Kraków, Poland
[2] Hasylab at DESY, D22607 Hamburg, Germany
[3] Institute of Nuclear Physics, Polish Academy of Sciences, 31-342 Kraków, Poland
[4] Instituto Nanociencias de Aragon, Universidad de Zaragoza, Spain

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**) e-mail: kryschna@agh.edu.pl*

Results of a XAS study of new magnetic nanoparticle materials derived from iron metal and iron oxide are presented. The materials have potential biomedical applications, *e.g.* as contrast agents in MRI. Several samples of carbon coated nanoparticles have been obtained by arc melting of graphite electrodes willed with metallic Fe or magnetite. Three fractions of nanoparticles from different places of the furnace: top, walls and bottom have been collected.

In order to determine the local structure and the Fe valence state in the materials, the X-ray absorption spectroscopy in the XANES and EXAFS range was used. The experiments were performed at the Fe:K edge at room temperature in Hasylab/DESY, Hamburg. Metallic Fe, hematite, maghemite and magnetite were used as references.

The edge energy and shape in the spectra of the Fe and Fe_3O_4 derived nanoparticle materials are similar to those of metallic iron (Fig. 1). This reveals a reduction of magnetite to metallic iron by carbon upon arc melting.

The contents of different iron species in the materials studied determined from the linear combination fits of their spectra with those of the reference samples using the least squares method in the Ifeffit pack software are presented in Table 1.

Table 1. Percentage contents of different iron species in the materials studied.

sample	Fe	α-Fe_2O_3	γ-Fe_2O_3	Fe_3O_4
Fe_3O_4 top	99.1	0	3.9	0
Fe_3O_4 walls	95.9	0	7.7	0
Fe_3O_4 bottom	93.8	0	9.1	0
Fe top	97.1	2.9	0	0
Fe walls	95.3	4.7	0	0
Fe bottom	92.0	8.0	0	0

The Fourier transforms of the EXAFS functions obtained from the Fe:K edge spectra of the magnetite derived nanoparticle materials reveal their close similarity to that of metallic Fe and are unlike to that of magnetite (Fig. 2). Also the Fourier transforms of the EXAFS functions of the iron derived nanoparticle materials are similar to that of metallic Fe. However, the distance of the 1st neighbour peak is of 0.2 Å smaller than that in the Fe metal. This suggests a compression of the lattice, possibly due to incorporation of carbon atoms which have their radius smaller than that of iron.

Preliminary MRI experiments performed on water suspensions of the materials studied idicate their high efficiency in increasing the T2 and T2* contrasts.

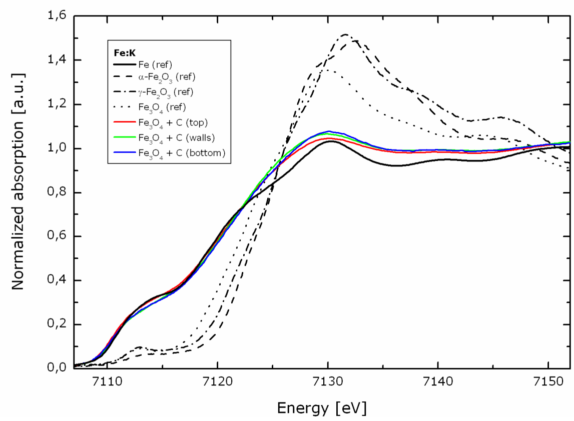

Figure 1. XANES spectra at the Fe: K edge of the carbon coated nanoparticle materials together with the spectra of the reference samples.

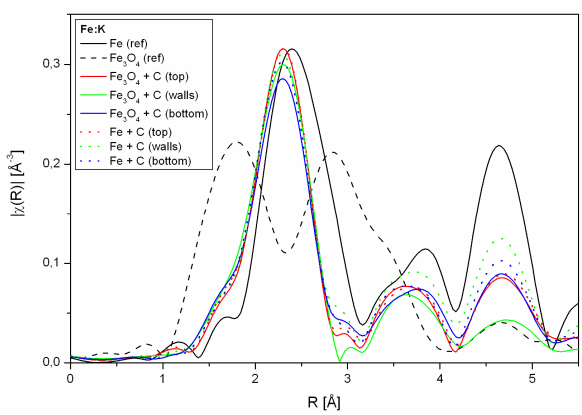

Figure 2. Fourier transforms of the Fe:K edge EXAFS functions of carbon coated Fe and Fe_3O_4 derived nanoparticle materials.