Structure identification of Fe-Fe$_x$O$_y$ core shell nanoparticles and their time stability

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The structure identification of core-shell nanoparticles could be splitted into two parts. The first one was the structure of the core. In the literature two different structures of the core can be found: γ-Fe [1] and α-Fe[2]. The second one was the structure of the shell. Because iron is very reactive it is always covered by the oxide shell. Different structures of the oxide shell were reported: Fe$_3$O$_4$ [3], α-Fe$_2$O$_3$ [4], γ-Fe$_2$O$_3$[5] or the mixture of these oxides [2]. The long-time stability of Fe-Fe$_x$O$_y$ core shell nanoparticles was studied in [2] where the increase of oxide shell thickness was observed. On the other hand, it was observed that the core shell nanoparticles were complete oxidized after 26 hours [6].

In this contribution, the structure identification of Fe-Fe$_x$O$_y$ core shell nanoparticles were done by combination of X-ray diffraction and Mössbauer spectroscopy. The verification of structure indentification was done by computer simulation of powder X-ray diffraction pattern. The model of nanoparticle was created, and X-ray powder diffraction pattern was simulated using the Debye formula [7]. The long-time stability of the core shell nanoparticles was studied in period of 6 years. It has been found that the structure of the samples was not changed during this 6 years period. The powder X-ray diffraction data was fitted by program MStruct [8]. The program MStruct has special tool for refining bimodal distribution of particles. This tool was used for one sample, where the diffraction lines of oxide had exceptionally long tails (see Fig. 1). These long tails were originating from the core shell structure. After modelling the core shell particle and calculating the powder X-ray diffraction pattern by different methods, the best match was obtained by using the Debye formula and then the MStruct program.
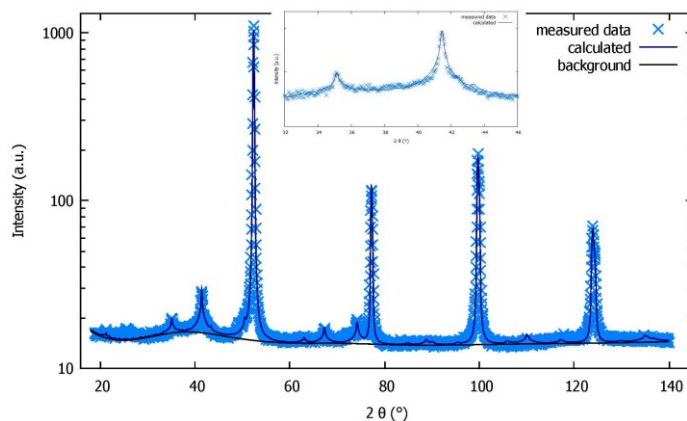
Figure 1. Comparison between measured PXRD pattern and pattern calculated by Debye formula (solid line)

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