Oral Contributions

[MS26 - 05] Residual Strain in -Fe2O3 Nanoparticles Embedded in SiO2 Matrix. Petr Brazda[1], Petr Bezdicka[2], D. Niznansky[3], and J. Vejpravova[4].

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Discovery of giant 2 T coercivity at room temperature of ε-Fe_2O_3 in 2004 [1] stimulated interest of material scientists in this youngest and metastable ferric oxide polymorph. It crystallizes in orthorhombic crystal system and its structure is described in P$na2_1$ space group [2]. Samples containing less than 10 wt. % of other iron oxide polymorphs are difficult to prepare due to the fact that ε-Fe_2O_3 is stable only in the form of nanoparticles with diameter of a few tens of nanometres. A standard preparation technique of high-purity ε-Fe_2O_3 nanoparticles uses Fe_2O_3/amorphous-SiO_2 system prepared by a sol-gel method[2], where the nanoparticles are synthesized by annealing the gel at temperatures about 1000°C. Homogeneous iron distribution in the amorphous-SiO_2 matrix is crucial for preparation of very pure samples. We have modified this sol-gel method by using a single molecular precursor for the matrix and the nanoparticles [3], which improved the phase purity up to 95 wt. % under optimal annealing conditions. Presumably different thermal expansion coefficients of the matrix and the nanoparticles materials imply a possibility of existence of a residual strain in the nanocomposite after high-temperature sample treatment. However, nothing is known about this macro-strain. The presence and magnitude of the residual strain has been evaluated using shifts of the lattice parameters of the ε-Fe_2O_3 nanoparticles embedded in the SiO_2 matrix in comparison to the lattice parameters of the bare nanoparticles obtained by a removal of the SiO_2 matrix using NaOH water solution. The data pool consists of several hundred diffractograms measured using Cu $K\alpha_{1,2}$ and/or Co $K\alpha_{1,2}$ radiations in the 2θ range between 10 and 90° as a routine scan and a scan using the range from 10 to 130° for more precise lattice parameters determination. Several samples were measured with internal standard reference material SRM 640c. The standard deviations of the lattice parameter values were estimated from the standard deviations the values obtained within the groups of samples prepared under the same conditions. These standard deviations are approximately five times higher than the standard deviations estimated for a precision of the lattice parameters determination. The obtained values of the lattice para¬meters of the bare ε-Fe_2O_3 nanoparticles are a = 5.0908(8) Å, b = 8.7842(15) Å and c = 9.475(2) Å. The lattice parameters of nanoparticles embedded in the SiO2 matrix lie within the ranges of 5.100 – 5.105 Å for the a parameter, 8.790 – 8.794 Å for the b parameter and 9.465 – 9.473 Å for the c parameter. The level of the residual strain depends mainly on the annealing regime. The results clearly states that the values of the a and b lattice parameters are increased in comparison to the relaxed ones while the lattice parameter c is decreased. As we have not observed any Fe-O-Si stretching modes in the infrared spectra of the material, the phenomenon may be explained solely by the anisotropic elastic modulus of ε-Fe_2O_3.

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