MS23-P13 Simulation of X-ray diffraction scattering for nanostructured aluminum oxides

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The metastable g-, h-, c-Al_2O_3 polymorphs prepared by low-temperature decomposition of the various aluminum hydroxides are the nanocrystalline systems with complex hierarchical nanostructure [1]. They are widely used as catalysts and supports. Therefore, the investigation of the relationship between physicochemical properties, atomic structure and nanostructure of materials is an actual problem.

However, the structure determination of alumina by the powder scattering data is a significant challenge due to the complexity of the diffraction patterns. Specific shape of primary nanocrystallites and their type of coherent ordering in the nanostructure are cause of significant and, moreover, anisotropic broadening of the diffraction peaks. The purpose of this report is the illustration of possibilities of the method associated with the creation of an nanostructured systems and the subsequent calculation of the diffraction pattern.

The method is based on the Debye equitation and known in the literature as Debye Function Analysis (DFA) [2]. It is full-profile method which is applicable for any an arbitrary atoms collection, and therefore can be used for crystalline materials or nano-structured objects. The calculations were performed on the DIANNA program [3], which is public-domain software and available on the website: www.sourceforge.net/projects/dianna.

This work is supported by Russian Science Foundation project N 14-23-00037.

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Keywords: X-ray analysis, XRD, modeling, nanostructure, Debye scattering equitation, DFA

MS23-P14 Structure determination of molecular nanocomposites by combining pair distribution function analysis and solid-state NMR

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Transparent mesoporous silica monoliths of well controlled porosity and a narrow pore size distribution around 6 nm have been used to elaborate sodium nitroprusside (SNP) nanocomposites. The obtained nanomaterials could be characterised using X-ray total scattering coupled to atomic pair distribution function analysis (PDF) and solid-state NMR spectroscopy. The PDF analysis allows for a structural description of the confined species as well as for the identification of various existing phases: SNP isolated molecules and SNP crystalline nanoparticles. The model obtained suggests that the nanocrystals have the same molecular structure as the bulk crystalline material and measure about 6 nm in diameter. This result is quite exceptional since the space available inside the pores is only about ten times the size of the molecules. The multi-nuclei Solid State NMR investigation confirms the structural model proposed by the PDF analysis and assigns the isolated molecules to dynamic disorder of a solvated phase. The latter approach additionally provides quantitative information on the relative ratio between the dynamic molecules and the rigid nanocrystals. This result is exploited to study the evolution of the two confined SNP phases with respect to solvating water molecules. We show that the confined SNP nanocrystals can be easily dissolved when storing the nanocomposites at increasing atmospheric relative humidity.

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