

MS40-P05 | POSSIBILITIES OF THE X-RAY DIFFRACTION METHOD FOR THE STUDY OF ULTRADISPERSED SYSTEMS AND NANOPOWDERS

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It is known that the physical and chemical properties of ultradispersed systems and nanomaterials are defined by features of the atomic structure. For structural investigations X-ray diffraction analysis is one of the main methods. Diffraction patterns contain information on the structure and morphology of nanoparticles: the shape and size of crystallites, the presence of defects and microstresses of atomic order, the mutual orientation of the blocks and the inter-grain boundaries of structured systems.

This information can be obtained from diffraction data, but studying of atomic structure of such small objects is an actual problem. Often, the diffraction patterns of such samples cannot be fully analyzed by standard approaches (for example, the Rietveld method) that are related to the measurement of positions, intensities and widths of diffraction reflections without diffuse scattering consideration.

A more general method Debye Function Analysis (DFA) method based on Debye scattering equation (DSE) can be used. It is full-profile method which is applicable for any an arbitrary atoms collection, and therefore can be used for crystalline objects, non-crystalline materials or nanostructures. The method is the most general and does not require artificial corrections (in contrast to the method Rietveld).

Possibilities of modelling diffraction patterns by the DFA will be shown for examples of various nanocrystalline materials: hydroxides of magnesium and tungsten, layered structures, metastable forms of aluminum oxide, ultradispersed iron oxides et al.