Poster Presentation

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Usage of Debye scattering equation for diffraction calculation of nanomaterials

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It is known, that the physicochemical properties of materials are defined directly by features of the structure and morphology. Studying of atomic structure and nanostructure of such small objects is an actual problem. X-ray diffraction method can be used for this purpose. Anisotropic broadening of the diffraction peaks, redistribution of the intensities or appearance of diffuse scattering can appear for nanomaterials. Standard X-ray diffraction techniques are often not applicable in this case.

These tasks can be solved by the Debye Function Analysis (DFA) method, based on Debye scattering equation (DSE). 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.

Possibilities of modelling diffraction patterns by the DFA by our software [1] will be shown for specific examples of various nanocrystalline materials. It is public-domain software available on the website: www.sourceforge.net/projects/dianna.

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[1] Yatsenko, D.A. & Tsybulya, S.V. Bull. (2012). Russ. Acad. Sci.: Phys. 76, 382-384.

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