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Preferred orientation studies on nanomaterials

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In nanotechnology, knowledge of the structure and composition of the materials studied is a key requirement for understanding materials properties at a small distance. One of the important parameters to be investigated is the preferred orientation of the crystallites in the nanosample. Understanding the preferred orientation gives insight in the growth, deposition or synthesis of the materials and in the materials properties.

Since the dimensions of X-ray wavelengths are in the same order as the sizes of nanostructures, X-ray diffraction is an important tool for the nanoscientist. X-ray diffractograms hold a wealth of structural information of the nanomaterials, including preferred orientation. In this study we give an overview of texture studies performed on different types of nanomaterials, both in reflection and transmission geometries.

Texture studies on ZnO nanobelts, grown on sapphire substrates with assistance of gold particles, revealed an epitaxial relationship with the substrate depending on the conditions of the growth process.

Transmission texture studies are very useful in the structural analysis of highly oriented polymer foils and fibers. Using the transmission geometry information about in-plane orientations of crystallites can be obtained. This information is essential in understanding the materials properties of the polymers studied.

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Nanostructure and peculiarities of X-ray powder diffraction patterns of low temperature Al₂O₃ polymorphs

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Al₂O₃, traditionally referred to as alumina, plays high technological importance since it is widely used for producing different kinds of ceramics, wide set of catalysts for numerous industrial chemical processes, adsorbents, coatings, soft abrasives, etc. Only α-Al₂O₃ (corundum) is the stable oxide whereas γ-, δ-, η-, θ-, χ- and κ- derivatives are considered to be metastable; they are formed gradually upon the dehydration of different hydroxides and oxyhydroxides [1]. Low temperature alumina polymorphs, γ-, η-, χ-Al₂O₃, were synthesized and studied by high resolution transmission electron microscopy and X-ray powder diffraction along with computer simulation of the diffraction patterns. An approach to the investigation of highly imperfect nanocrystalline compounds based on the simulation of X-ray powder diffraction pattern and involving a model of one-dimensionally disordered crystal [2] has been used. Planar defects lying on the {111}, {110} and {100} planes and being the origin of the broadening of X-ray diffraction peaks in different forms of aluminium oxide have been revealed. In addition to providing strong experimental support for the imperfect character of the specimens structure, these results demonstrate the possibility of using nanosized crystalline domain with spinel structure, regularly shaped and having specified developed face and bounding surfaces, for description of the nanostructure of whole variety of low temperature aluminas. Definite kinds of the line shape broadening observed in the X-ray diffraction patterns of these materials originate from the different types of packing of nanocrystalline domains accompanied by subsequent formation of planar defects inside oxide particles. It was found that γ-, η- and χ-Al₂O₃ differ from each other by the crystallographic shape of the building blocks (nanodomains with size about 2 - 3 nm), character of their stacking with each other and types of the faulting arising upon their assembly into extended oxide structure.

[1] Lippens B.C., Stegarda J.J. *Physical and Chemical Aspects of Adsorbents and Catalysts* (Academic Press, New York). 1970. 171 p.

[2] Tsybulya S. V., Cherepanova S. V., Kryukova G. N. (2004). *Diffraction Analysis of the Microstructure of Materials*, edited by E. J. Mittemeijer and P. Scardi, 2004, pp. 92-123. Berlin-Tokyo: Springer Verlag.