A NEW COMPUTER CODE USED FOR THE NANOSTRUCTURE ANALYSIS OF ADVANCED MATERIALS USING POWDER X-RAY DIFFRACTION TECHNIQUE

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Abstract

The goal of the contribution consists in realizing a versatile software system in Maple 10 language based on Generalized Fermi Function (GFF) and other distributions for approximation of the experimental X-ray line profiles (XRLP) and processing them in order to investigate global structure of advanced nanomaterials. This objective is achieved by implementing the physical concepts regarding the X-ray diffraction on imperfect nanostructure based on generalization of the Warren-Averbach theory. The software system is capable of determining average crystallite size, microstrain of the lattice, the effective crystallite size, the microstrain as lattice disorder, the particle size and microstrain distribution functions and stacking fault probability by analyzing the position, the shape and the broadening of XRDLPs. A large variety of graphical option is available after each processing stage. The global structure are for supported Pd (Pd/SiO2, Pd/TiO2 and Pd/Al2O3) catalysts used in H/D isotopic exchange and CO oxidation reactions are illustrated.

Keywords: computer code, nanostructure analysis, X-ray diffraction

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