

ANALYSIS OF THE FACTORS, INFLUENCING THE PRECISION OF SIMULATED X-RAY DIFFRACTION (REFLECTION) CURVES

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The reliability of information on investigated by x-rays sample depends very much on the utilized data interpretation techniques. The principal part of latter is the theory, which is used to simulate the physical processes during the penetration and interaction of x-rays with the matter. The theoretical part plays crucial role in the fitting procedures for sample parameters as well.

In the report, we give a comparative guide on calculation of x-ray diffraction (reflection) process, starting from the calculation of characteristics determining the interaction of x-rays with the matter (x-ray susceptibility, thermal vibrations of crystallographic lattice, etc) and ending with the simulation of signal recorded by detector. We discuss kinematical and dynamical approximations, Takagi-Taupin and direct summation of waves approaches in x-ray diffraction physics. The different algorithms for simulation of scattering process in multilayer structures are also considered in view of difference in the results of simulations. Finally, the influence of resolution effects and instrumental function on resulting x-ray intensity is shortly discussed.