Rietveld refinement using the dynamic theory of X-ray diffraction

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The Rietveld structure refinement is used to analyze X-ray powder diffraction data, at the end the calculation the output parameters can be used to calculate the crystallite size, microstrain, and others. The least squares method is implemented in the program to adjust the structural and instrumental parameters in order to minimize the difference in the calculated and observed intensity of diffractogram. In all Rietveld refinement programs the integrated intensities are calculated using the kinematic theory of X-ray diffraction, which neglects X-ray interactions inside the crystallite, for instance, absorption effect. X-ray diffraction line profiles are adjusted by analytical functions distribution. The crystallite size is calculated with the Scherrer equation, which is limited to hundreds of nanometers. As an alternative way to apply the Rietveld refinement for thick samples with high absorption coefficient will be present in this work. Rietveld refinement software was developed in the C++ language, where the intensity is calculated by the dynamic theory of X-ray diffraction. Dynamic theory describes the X-ray interactions inside the crystallite and its effects on intensity and line profile is considered. The line profile was calculated taking into account the crystallite size distribution and the instrumental parameters. The software was initially applied in the refinement of the LaB6 (SRM 660b) and the instrumental profile of the Beamline 11-BM of the Argonne National Laboratory.