PIELASZEK METHOD FOR FAST ESTIMATION OF CRYSTALLITE SIZE DISTRIBUTIONS IN FUNCTIONAL MATERIALS

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The FW15/45M method proposed by R. Pielaszek is a simple diffraction line-profile approach for estimating crystallite size distributions from broadened diffraction peaks. Unlike the classical Scherrer equation, which provides only an average crystallite size, this method uses peak widths measured at one-fifth and four-fifths of the peak maximum and makes it possible to estimate both the characteristic size and the dispersion of the distribution [1].

The method has already been used in different diffraction studies. One of the early examples is the synchrotron diffraction study of ferrofluids by Vorobiev et al. at SNBL, ESRF, where it was used to evaluate the mean particle size and size dispersion of colloidal nanoparticles [2]. It was also applied to other crystalline materials, including nanocrystalline MgO xerogel [3], Tb-doped $CaWO_4$ phosphor materials [4], and nanodiamond systems [5]. These examples show that the method can be used with diffraction data obtained from both laboratory X-ray sources and synchrotron radiation.

In the present work, the Pielaszek method was applied to several classes of functional materials, including Ni-rich cathode materials for Li-ion batteries, deposited coatings, and Fe-based alloys [6]. The approach was adapted for both X-ray diffraction data containing the $K\alpha_1/K\alpha_2$ doublet and neutron diffraction data. In addition, a dedicated software application was developed to automate the analysis and to process not only individual diffraction patterns, but also continuous arrays of related datasets, which is especially useful for systematic studies and large experimental series.

The main advantages of the method are its simplicity, fast implementation, low computational cost, and the possibility to obtain information on crystallite size distribution rather than only on average crystallite size. This makes it convenient for rapid comparative analysis of large sets of similar diffraction patterns. At the same time, the method is most reliable when peak broadening is governed mainly by crystallite size effects and when instrumental broadening is properly taken into account. Contributions from microstrain, stacking faults, peak overlap, or unresolved wavelength splitting may affect the extracted distribution parameters and should be considered during data treatment [1,3].

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