Simulated X-ray diffractograms for analysis of crystalline microstructure

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The principal phenomenon exploited to investigating internal structure of crystalline materials is X-ray diffraction. The description of crystals are generally split into recognising their structure (perfect crystalline lattice with periodic order of constituent atoms) and determining their microstructure (imperfections with respect to perfect order). The characterisation of real materials, being monocrystals (usually more or less defected) or polycrystals (bulk or powders) is based on exploiting the dependence of X-ray diffractograms (especially of positions and shapes of X-ray diffraction line profiles) on both structure or microstructure [1-7]. Both basic inverse problems of X-ray crystallography may be solved separately since crystalline structure influences mainly positions and intensities of diffraction peaks, while crystalline microstructure, being defined by imperfections with respect to perfect atom order, influences mainly peak shapes (line profiles). Mathematical models of microstructure have been being developed [1,2,3] since the discovery of X-ray diffraction, generally with taking into account different goals: description of defects in crystalline materials and possibility of solving corresponding inverse problems. Now, when fast computers are used to approximate solution of inverse problems, a new insight is necessary: construction of adequate mathematical models accounting for all important properties of studied materials on one side [4-7] and construction of effective method and algorithms for solving corresponding inverse problems on the other side [5-9].
Effective mathematical models of microstructure should include principal parameters enabling statistical characterisation of real materials, sufficient for further investigating their relation with macroscopic properties and formation processes. A polycrystalline material may be regarded as set of crystallites, separated by both small-angle or large-angle boundaries, being domains scattering X-rays coherently and independently each other. The line profiles in X-ray diffractograms may be simulated under some reasonable simplification. Especially a quite useful model is a polydisperse set of crystallites with the same shape described by a shape function and of sizes dispersed with a volume-weighted crystallite size distribution, with a second-order crystalline lattice strain distribution. Small-angle and large-angle boundaries separating crystallites are regarded amorphous. The crystallite shape is considered as cuboid or ellipsoid or cylinder or hexagonal prism with aspect ratios to be determined flexibly [6-11]. Such modelling provides variety of numerical X-ray diffractograms consisted of pure line profile produced by an ideal parallel monochromatic X-ray beam. The separate question is the construction of instrumental function to describing instrumental contribution to approximating and simulating experimental data. The goal of this work is a study of the dependence of X-ray diffractograms on microstructural material characteristics (prevalent crystallite shape parameters, volume-weighted crystallite size distribution and second-order crystalline lattice strain distribution), via numerical simulations, and observation the basic regularities and correlations.

[1] A.J.C. Wilson, The Mathematical Theory of X-ray Powder Diffractometry (1963). Eindhoven: Philips Technical Library.
[2] B.E. Warren, X-Ray Diffraction (1969). Reading, Massachusetts: Addison-Wesley.
[3] M.A. Krivoglaz, X-ray and neutron diffraction in nonideal crystals (1996). Berlin: Springer-Verlag.
[4] J.I. Langford, D. Louër, P. Scardi, J. Appl. Crystallogr. (2000). 33, 964-974.
[5] P. Scardi, M. Leoni, Diffraction Analysis of the Microstructure of Materials (2004). Berlin: Springer. pp. 51-91
[6] M.A. Kojdecki, Mater. Sci. Forum (2004). 443-444, 107-110.
[7] M.A. Kojdecki, J. Bastida, P. Pardo, P. Amorós, J. Appl. Crystallogr. (2005). 38, 888-899.
[8] M.A. Kojdecki, E. Ruiz de Sola, F.J. Serrano, E. Delgado-Pinar, M.M. Reventós, V.J. Esteve, J.M. Amigó, J. Alarcón, J. Appl. Crystallogr. 40 (2007), 260-276.
[9] M.A. Kojdecki, E. Ruiz de Sola, F.J. Serrano, J.M. Amigó, J. Alarcón, J. Appl. Crystallogr. (2009). 42, 198-210.
[10] P. Pardo, M.A. Kojdecki, J.M. Calatayud , J.M. Amigó, J. Alarcón, Powder Diffraction, (2017). 32 (S1) S87-S98.
[11] S. Odrzywolski, M.A. Kojdecki, S. Złotnik, Ł. Kubiszyn, J. Wróbel, Metrol. Meas. Syst. (2024). 31, 231-257.

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