FAULTS, AN ACCESSIBLE PROGRAM FOR REFINING POWDER DIFFRACTION PATTERNS OF LAYERED STRUCTURES

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Layered systems include a large number of mineral families and synthetic compounds of great technological importance with, for instance, applications in the field of electrochemical energy storage. Their physical-chemical properties being directly related to their structural features, the microstructural characterization of these materials is of high importance and includes the determination of different kinds of defects, their amount and their locations.

So far, a widely used tool to interpret the diffraction data of one-dimensionally disordered systems was the program DIFFaX [1], which permits to simulate X-ray and Neutron powder diffraction patterns. In order to overtake the limitations of simple simulations, we have developed the FAULTS program [2-3], based on the DIFFaX code, which enables to refine experimental XRD and NPD patterns of crystal systems with any type of planar defects, such as twins and stacking faults. An improved version of this program, more performant and with additional features is now available within the FullProf suite of programs [4] or as an independent program [5].

FAULTS can read experimental XRD and NPD data from many different formats. Refinable parameters are provided by the user in a free-format input data file, in which the structure is described in terms of layers of atoms which are interconnected *via* stacking operations that occur with a certain probability. Refinements of all the parameters involved in the calculation of the diffracted intensities is carried out using the Levenberg-Marquard optimization algorithm, implemented in the Crystallographic Fortran Modules Library (CrysFML) [6].

Another major feature of FAULTS with respect to DIFFaX is the implementation of a more adequate isotropic size broadening treatment which takes into account the Gaussian (H_G) and Lorentzian (H_L) contributions to the FWHM in addition to the consideration of a finite number of layers per crystallite already present in DIFFaX. As these are refinable parameters, this treatment allows a successful description of the separate contributions to line broadening of instrumental features, the finite crystallite size and planar defects.

Our presentation will show the structure and operation of the program FAULTS, and some examples will be given.

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