

Program ANAELU on its way to a 2D Rietveld code

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The ANAELU program is part of the current trend towards 2D diffraction patterns processing. ANAELU is open source, distributed under MPL license. In its initial version this program was basically oriented to the characterization of axial textures by means of the qualitative comparison between modeled and observed 2D patterns. The basic conception of the program is that the user proposes the crystalline structure of the phase under study and the inverse pole figure of the considered texture. With this data, using the tools of mathematical texture analysis, the program simulates and graphically represents the 2D-XRD pattern of the model sample. An important feature of the considered patterns is the distribution of intensities along the Debye rings. The visual comparison between observed and calculated patterns is the criterion of correctness of the proposed model. The program has been successfully used in the characterization of minerals, alloys and functional ceramics. Some limitations that have been detected in the use of ANAELU are the limited number of input formats that it is able to read, the program relative slowness, the non-consideration of the diffraction background, the poor portability, the non-consideration of crystalline imperfections and its qualitative criterion of fitness.

The present update consists in the improvement of the raised aspects. ANAELU-2.0 presents the following innovations.

- A new GUI has been created, in WxPython, associated with a system for reading experimental patterns through the FABIO library. The current system reads patterns in the most internationally used formats
- The calculation of diffraction patterns, from the generation of the unit cell to the diffracted intensities, has been translated to FORTRAN 2003 with systematic use of the CRYSFML library. This change reduces the running time by one order.
- Various routines (Laplacian softening, spherical harmonics) have been introduced to model the two-dimensional background.
- The current version, ANAELU2.0, can be distributed by means of stable executable packages in Windows, LINUX and IOS wrapped by MiniConda.
- ANAELU-2.0 includes routines for the modeling of the reciprocal space associated with imperfect crystals and their projection in two-dimensional diffraction-scattering patterns.

With the achieved improvements ANAELU is now able to perform the 2D quantitative evaluation of observed-calculated adjustment and in this manner it is approaching the idea of a two-dimensional Rietveld code.

Fuentes-Montero, L., M. Elena Montero-Cabrera, and L. Fuentes-Cobas, 2011, The software package ANAELU for X-ray diffraction analysis using two-dimensional patterns: Journal of Applied Crystallography, v. 44, p. 241-246.

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