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ANAELU, a 2D-Rietveld-type refinement program.

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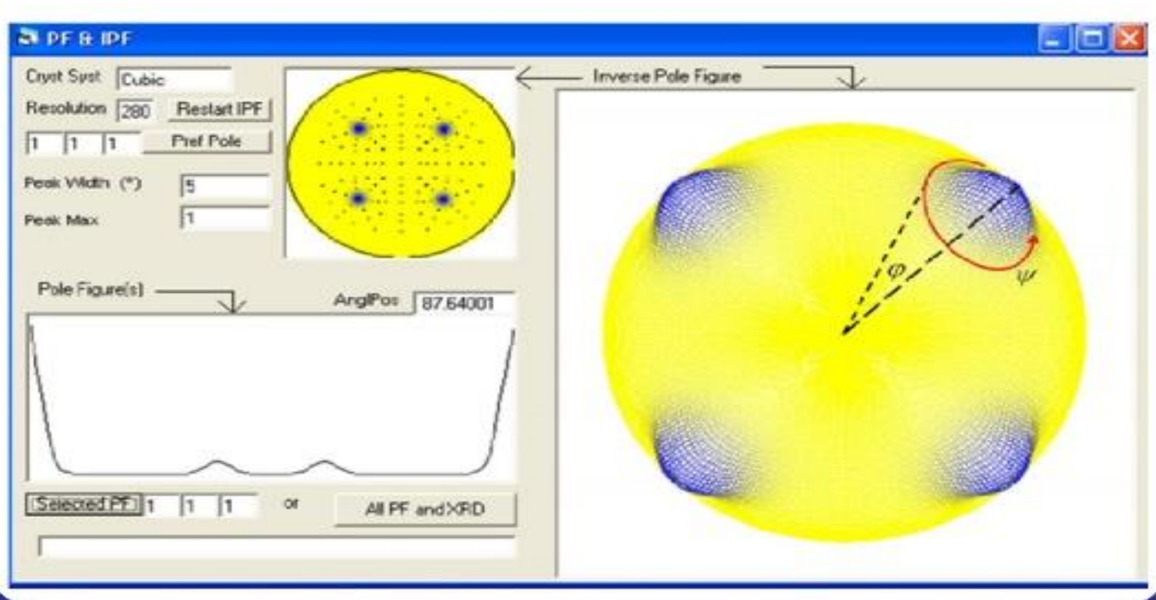
Abstract

The recent improvement in the electronics of two-dimensional X-ray detectors and the availability of this type of detectors in synchrotron light sources has created the demand for fast and reliable tools for 2D-XRD patterns interpretation. Answering this need our group introduces: The ANAELU program (ANAlytical Emulator Laue Utility) [1,2] wich allows the diffractometric determination of the fiber axis inverse pole (IPF) by means of a Rietvled-style procedure. The User proposes the initial crystal structure, de texture preferred direction and a starting distribution width (Ω). Then the program models the intensities distribution along the Debye rings, represents the diffractogram background using a smooth surface, compares the calculated and experimental patterns quantitatively, calculates descriptors of goodness of fit and allows variations of textural parameters in the search of an optimal fit. Crystallographic calculations are performed by using the CrysFML Fortran library [3]. The computer-user interface is programmed using the wrapper wxPython [4] and the Fortran-Python mixed programming is achieved through the F2PY binding module [5].

Introduction

The current version of ANAELU approximates a 2D-Rietveld refinement program, which offers a graphic representation of 2-D XRD patterns, based on the crystal structure and a inverse pole figure (IPF) proposed by the user.

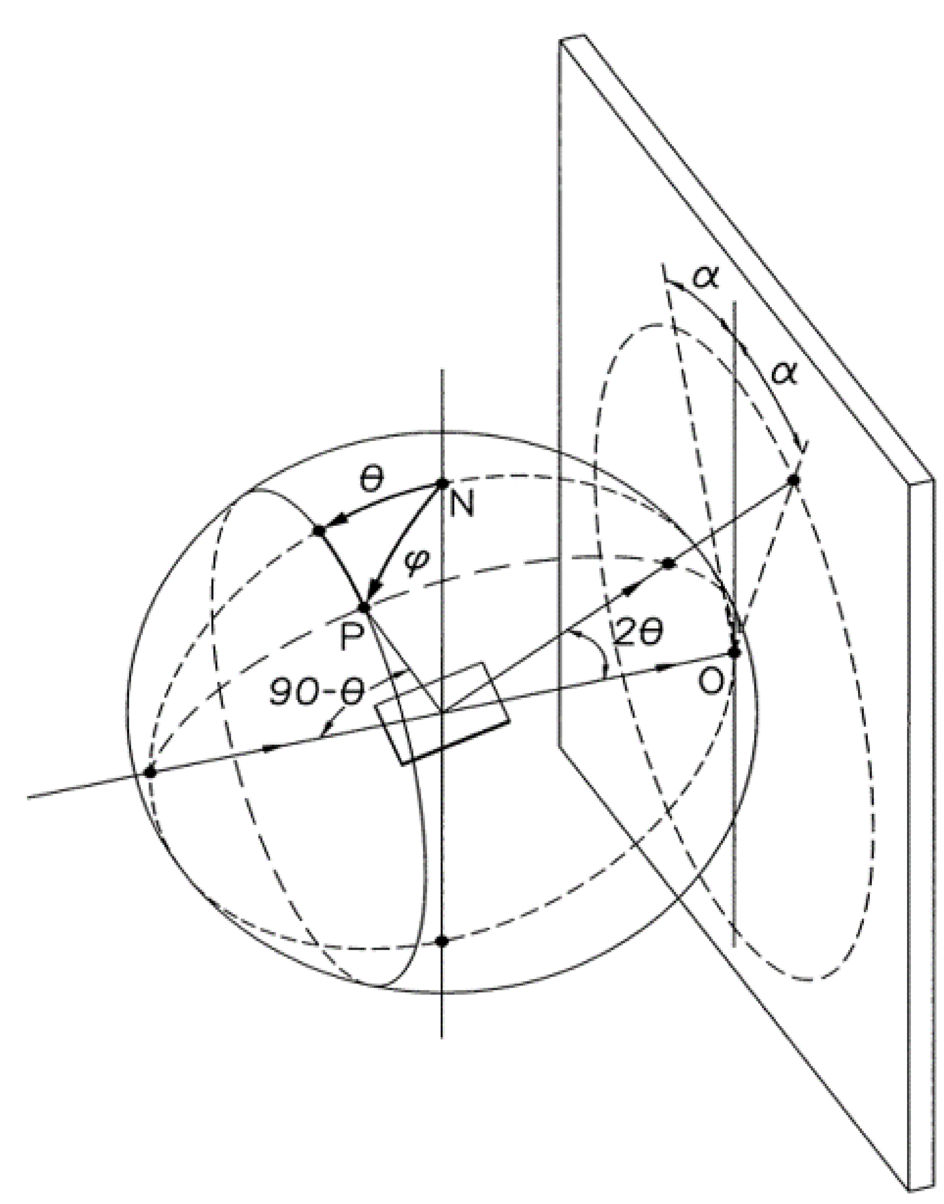


Format Adaptability

ANAELU is capable of working with most data formats obtained directly from synchrotron detectors. The following table shows the data formats it can read.

Detector/format	Extension	Detector/format	Extension
ADSC quantum	.img	General Electric	–
Bruker	.sfrm	Hamamatsu CCD	.tiff
Gatan digital micrograph	.dm3	MarCCD/mar165	Mccd
ESRF	.edf	Mar345 image plate	.mar3450
EDNA	.xml	Oxford diffraction	.img
CIF binary files	.cbf	Dectris Pilatus tiff	.tiff
Nonius KappaCCD	.kccd	Portable aNy map	.pnm
Fit2D	.msk, .spr	Tagged image file format	.tiff

Mathematical background



The pole figure $P_h(\theta)$, associated with the reciprocal vector h = [h, k, l], modulates the intensities distribution along the Debye ring associated with the reflection h in the 2D diffractogram. Mathematically:

$$I_h^{textured}(2\theta, \alpha) = I_h^{random} P_h\left[\varphi(\theta, \alpha)\right]$$

The relationship between the angles of the figure is represented by:

$$\cos\varphi = \cos\theta\cos\alpha$$

The pole figures $P_h(\theta)$ corresponding to the IPF considered are calculated by applying the fiber textures fundamental equation:

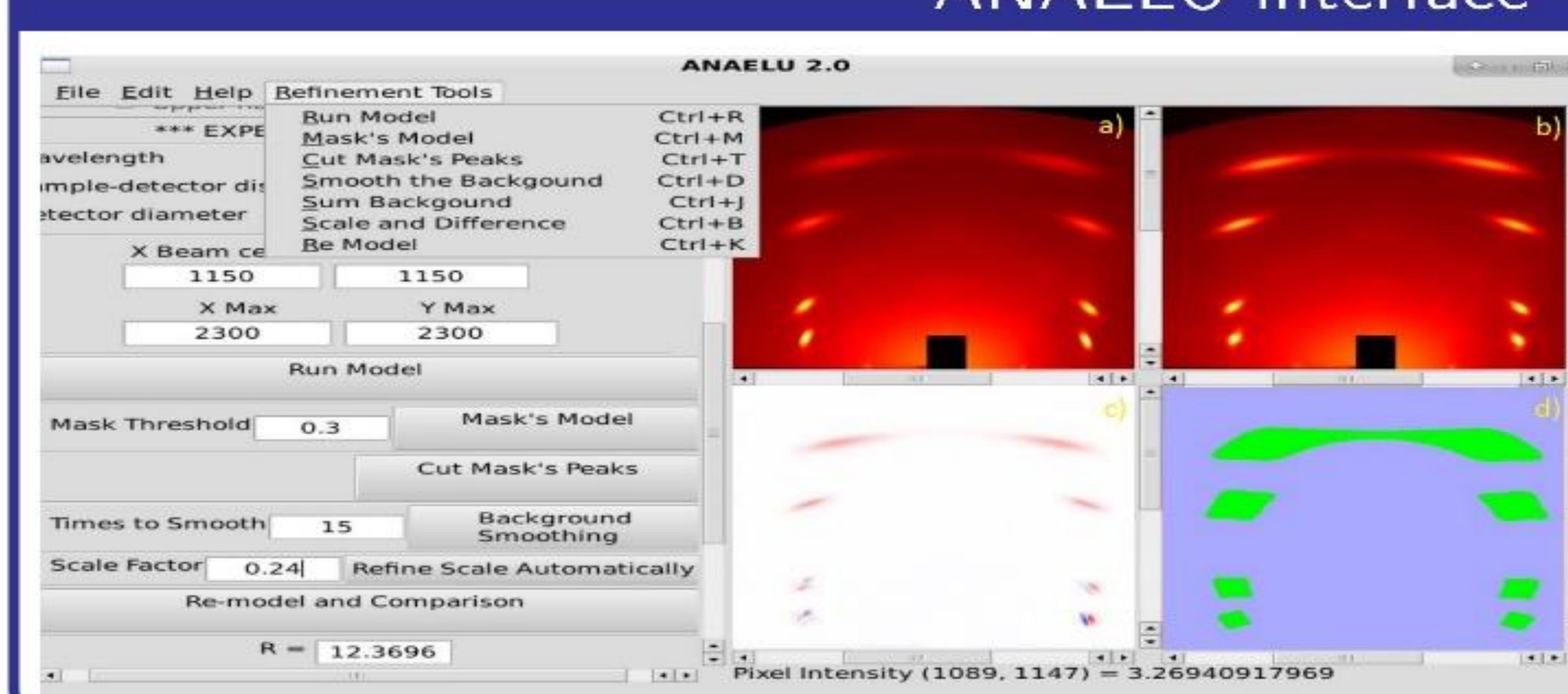
$$P_h(\varphi) = \frac{1}{2\pi}\int_0^{2\pi} R_z(\varphi, \psi) d\psi$$

In ANAELU, IPFs are represented by Gaussian distributions:

$$R_{y_o}(h) = R_o e^{-[\phi(h)/\Omega]^2}$$

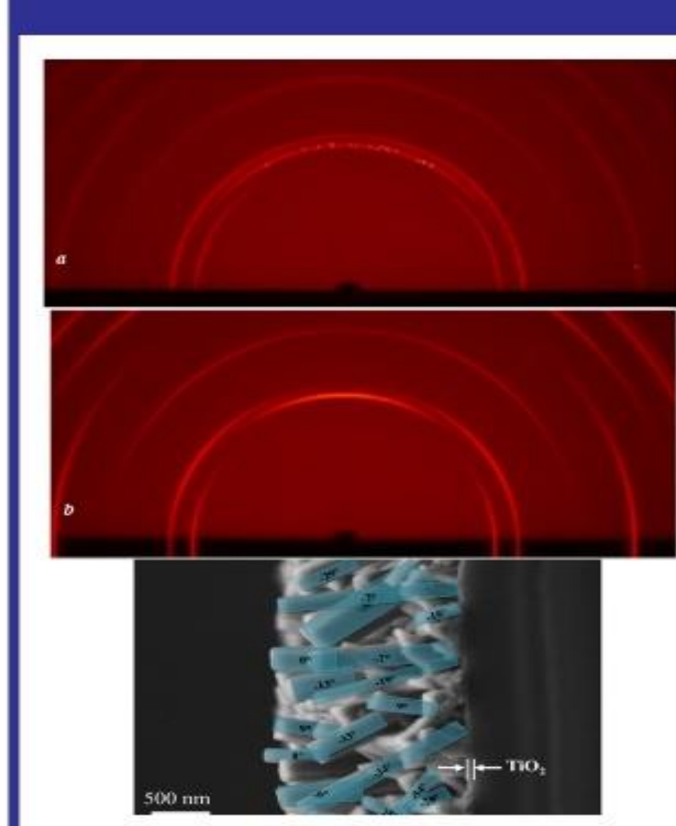
R_o is a scale factor. (Ω) characterizes the orientation distribution width.

ANAELU interface



Screenshot of ANAELU's graphic user interface. The left window displays the input data needed. The four right hand images go as following: a) Experimental 2D-XRD pattern of Platinum b) Final diffractogram modeled by ANAELU . c) Difference image. d)Background mask.

A case of study



Thin film of ZnO nanorods grows with a tendency that their crystallographic c axes, are oriented perpendicular to the glass substrate [6]. image a) shows a 2-D diffractogram obtained in grazing incidence geometry, in Stanford synchrotrons channel 11-3. Image b) shows the diffractogram modeled by ANAELU under the hypothesis of one fiber texture component, with [001] directions aligned with the sample plane normal and a distribution width Ω = 20°.
The image at the bottom shows a TEM image in which it can be confirmed that the average distribution width is the same as that predicted by ANAELU.

References

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