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Recent Improvements to the ANAELU-MPOD Polycrystal Characterization System

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Abstract. The CIMAV Crystal Physics Group, with international collaboration, has been working in the creation of a computer-aided system for the approximate prediction of textured polycrystals' physical properties. The input for the developed application is formed by: a) the investigated polycrystal 2D-XRD pattern and b) the considered single-crystal properties' tensors, accessible through the Material Properties Open Database (MPOD). Recent developments of the mentioned system consist on a) significative approximarions to quantitative fitting of calculated 2D-XRD patterns to observed ones and b) the inclusion of textured polycrystals properties in MPOD.

Key words: 2D-XRD texture analysis, polycrystal properties, material properties open database ((MPOD)

Recent enhancements to the ANAELU-MPOD software system for the prediction of textured polycrystal tensor proeprties starting from the measured two-dimensional x-ray diffraction pattern (2D-XRD) and single-crystal properties data in the Material Properties Open database (MPOD) are described.

Version 2.0 of program ANAELU [1] allows the determination of the fiber axis inverse pole figure (the ODF of axially symmetric samples) by a Rietved-style procedure. Recent improvements in this code include background modelling and semiautomatic scale fitting by quantitative point-by-point comparison of observed-calculated differences. Heavy crystallographic calculations are performed by use of the Institute Laue-Langevin CrysFML Fortran95 library [2] and the Graphic User Interface was programed in Python language. Mixed Fortran-Python programming has been facilitated by application of the F2PY platform [3]

A valid approximate prediction of polycrystal properties is that of averaging single-crystal properties tensors, usually in compact matrix notation, with the orientation distribution function (ODF) as weight factor. This treatment, with application of the Voigt, Reuss and Hill approximations, requires particular precaucions when dealing with so-called coupling properties (piezoelectricity, magnetostriction, magnetoelectricity). Tensors averaging via ODF, particular cases and limitations are discued in references [4, 5].

In the current work a closed system of programs that performs the mentioned tasks for fiber textured materials is presented. Reported experimentally-obtained single-crystals' properties matrices are accessible through the Material Properties Open Database MPOD [6] (http://mpod.cimav.edu.mx). The developed program system combines MPOD matrices with ANAELU inverse pole figures to calculate several polycrystal physical properties.

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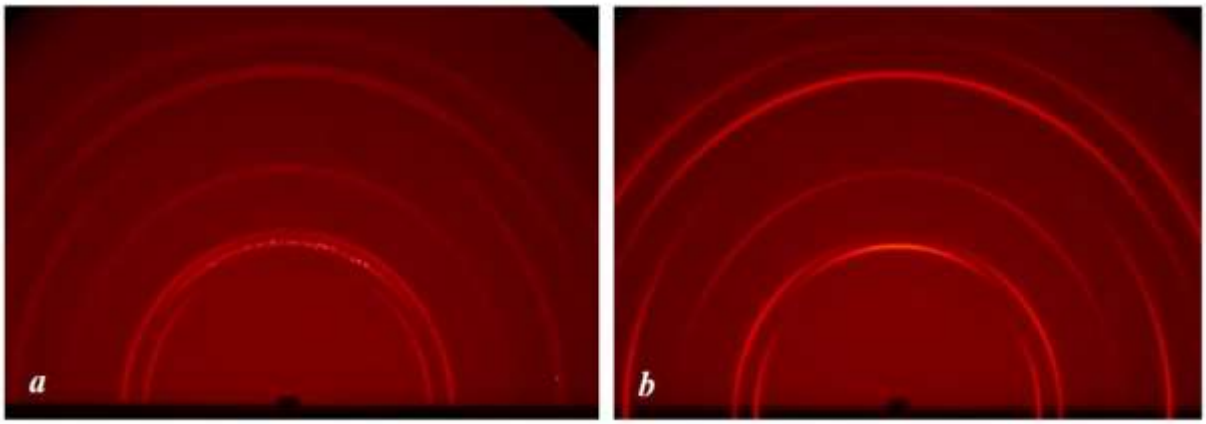

Figure 1: *a*) Observed and *b*) calculated 2D-XRD patterns of a textured platinum sample.

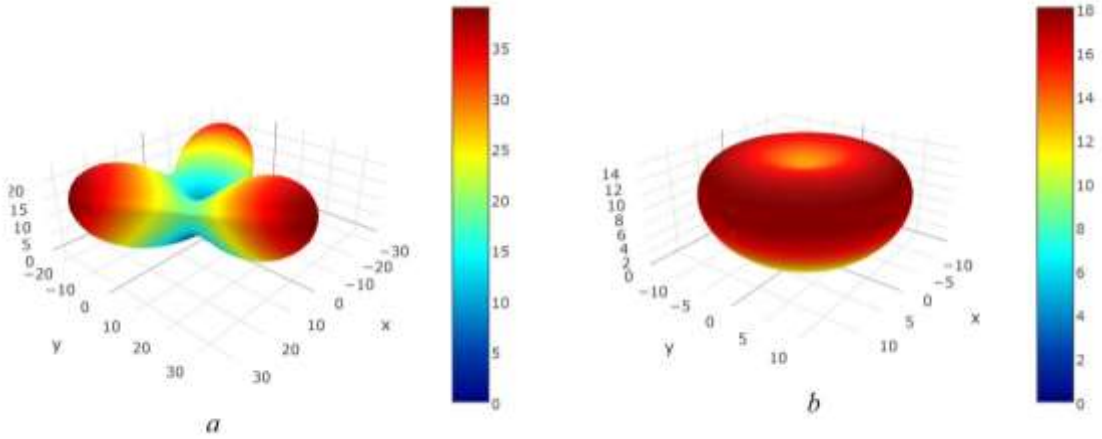

Figure 2: Longitudinal piezoelectric surfaces of *a*) single crystal and *b*) axially textured polycrystal of LiNbO3. Single crystal point group: *3m*. Fiber texture symmetry: ∞m.

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