SMCr. First International Meeting on Diffraction
V Mexican Meeting on Diffraction
Meeting of Synchrotron Light Users
21ST to 26TH October 2017, Mérida, Yucatán, México

From 2D-XRD to Polycrystals' Properties

L. E. Fuentes-Cobas[1*], L. Fuentes-Montero[2], D. Burciaga-Valencia[1], E. E. Villalobos-Portillo[1], J. A. Marín-Romero[3], M. E. Montero-Cabrera[1], A. Muñoz-Romero[4], J. A. Cardona-Vasquez[5], V. L. Barrera-Colín[1]

[1] Centro de Investigación en Materiales Avanzados, Chihuahua, México
[2] Diamond Light Source Ltd., Didcot, UK
[3] Centro de Investigación y de Estudios Avanzados, Mérida, México
[4] Shepherd Controls, El Paso, TX, USA
[5] Universidad Nacional de Colombia, Bogotá, Colombia
*e-mail: luis.fuentes@cimav.edu.mx

Abstract. A system of methods and programs for crystal physics calculations is described. Program ANAELU allows the characterization of axially-symmetric textures from 2D-XRD patterns. The Material Properties Open Database MPOD provides numerical values of single-crystal properties' tensors and SAMZ code combines texture and single crystal data to estimate polycrystal properties under various approximations. The mathematical foundations and computational tools of the project are presented. Representative case studies are explained.

Key words: Two-dimensional XRD, polycrystal properties, ANAELU-MPOD-SAMZ software package

The characterization-prediction route here proposed starts with texture evaluation by means of program ANAELU [1, 2]. This code is part of the current trend towards 2D diffraction patterns processing. ANAELU is open source, distributed under MPL license. 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 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.

The experimentally determined values of several physical properties are been collected and are available at the Material Properties Open Database MPOD [3] (http://mpod.cimav.edu.mx). In MPOD, properties are presented as matrices according to their corresponding tensor ranks. Crystal structure symmetry and polar-axial nature of properties are taken into account. Properties' longitudinal representations and 3D printing are among the features of MPOD. The maths underlying the properties representations are briefly reviewed.

Starting with the (MPOD) single-crystal properties and making use the (ANAELU) texture information, polycrystals' properties are estimated by means of the so-called Voigt, Reuss and Hill approximations. Program SAMZ [4] performs the calculations. The user selects the property of interest, enters the considered polycrystal inverse pole figure parameters (preferred orientation direction and distribution width) and the program calculates the polycrystal effective property according to the mentioned treatments. The symmetrized spherical harmonics representation of single- and polycrystal properties is used thoroughly.

The presentation includes real-life examples of the proposed methodology. Figure 1 simulates the effect of texture on the 2D-XRD pattern of a $PbTiO_3$ ceramic. Figure 2 models the dielectric constants of sharp and broad $PbTiO_3$ textures.

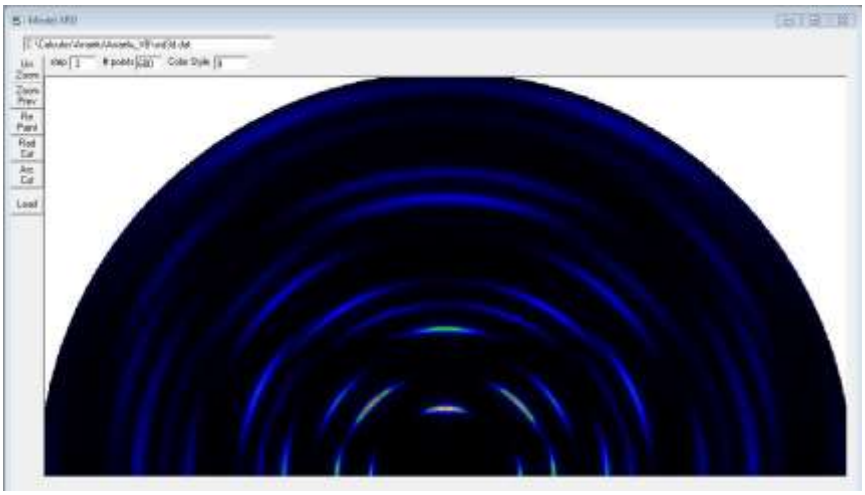

Figure 1: 2D-XRD pattern of a highly textured $PbTiO_3$ ceramic. The distribution of diffracted intensities along the Debye rings is modeled by the ANAELU program. Gaussian [0, 0, 1] inverse pole figure. Texture width: $\Omega = 10°$.

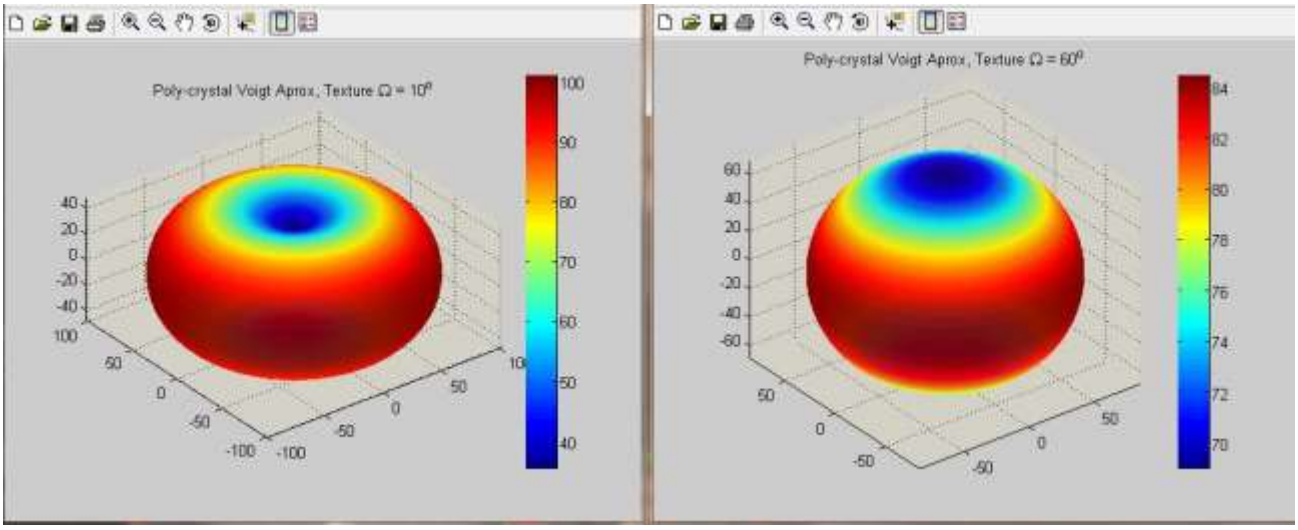

Figure 2: Modeled longitudinal dielectric constant surfaces of sharp ($\Omega = 10°$) and broad ($\Omega = 60°$) $PbTiO_3$ textures. Single crystal data from MPOD [3]. Polycrystal calculations via SAMZ program [4].

Acknowledgements. Support from CONACYT, Project 257912, is acknowledged. 2D-XRD experiments were performed at the Stanford Synchrotron Radiation Lightsource and Elettra Sincrotrone Trieste.

References

1. Fuentes-Montero, L., M. Elena Montero-Cabrera, and L. Fuentes-Cobas: *The software package ANAELU for X-ray diffraction analysis using two-dimensional patterns.* J. Appl. Crystallography, **44**, 241-246 (2011).
2. E. E. Villalobos-Portillo, D. C. Burciaga-Valencia, L. Fuentes-Montero, J.A. Marín-Romero, L. E. Fuentes-Cobas: *Program ANAELU on its way to a 2D Rietveld code*. 24th Congress & General Assembly of the International Union of Crystallography, poster # 1007. Hyderabad, India (2017).
3. L. E. Fuentes-Cobas, D. Chateigner, M. E. Fuentes-Montero et al: *The Representation of Coupling Interactions in the Material Properties Open Database (MPOD).* Advances in Applied Ceramics (2017). dx.doi.org/10.1080/17436753.2017.1343782
4. L. Fuentes-Cobas, A. Muñoz-Romero, M. E. Montero-Cabrera et al: *Predicting the Coupling Properties of Axially-Textured Materials.* Materials **6**, 4967 (2013).