A Route from 2D-XRD to Polycrystal Properties

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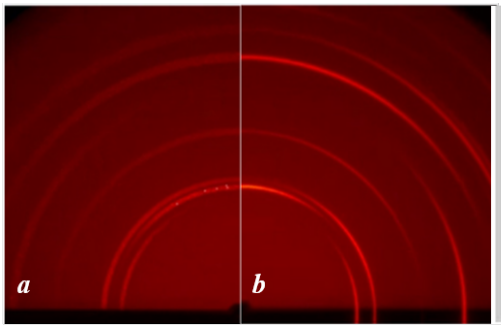
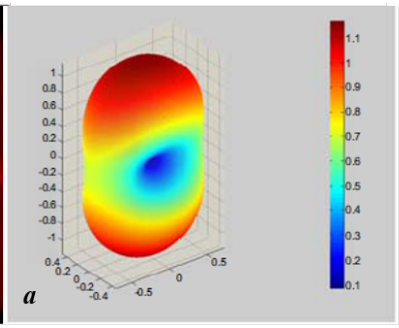
A computer-aided system for the approximate prediction of axially textured polycrystals' physical properties is presented. The input for the developed application is formed by: a) the investigated polycrystal 2D-XRD pattern and b) the considered single-crystal properties' tensors.

Program ANAELU [1] allows the determination of the fiber axis inverse pole figure (IPF) by means of a Rietved-style procedure. The user proposes the crystal structure, the texture preferred direction and the initial distribution width. Crystal diffraction calculations are performed by use of the CrysFML Fortran library and point-by-point comparison of observed-calculated differences leads to the texture model refinement. User Interface is programed in Python language and mixed Fortran-Python programming has been facilitated by application of the F2PY interface generator [3].

Published experimental single-crystal tensor properties are accessible through the Material Properties Open Database (MPOD, http://mpod.cimav.edu.mx) [2]. A valid estimation of polycrystal properties is that of averaging single-crystal properties tensors, with the orientation distribution function (the IPF, in fiber textures) as weight factor. This treatment, with application of the Voigt, Reuss and Hill approximations, requires particular precaucions when dealing with so-called coupling properties (e.g. piezoelectricity, magnetostriction, magnetoelectricity).

In the current work a closed system of programs that performs the mentioned tasks for fiber textured materials is described. The developed program package combines MPOD single-crystal matrices with ANAELU inverse pole figures to calculate several polycrystal physical properties. Figure 1 shows the experimental and calculated 2D-XRD patterns for a textured ZnO sample. Figure 2 represents the comparison between the longitudinal magnetoelectric surfaces of a single crystal and a virtual axially textured polycrystal of ($K_2[FeCl_5(H_2O)]$).





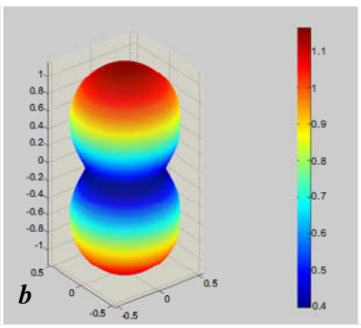


Figure 1: a) Observed and b) calculated 2D-XRD. Figure 2: a) Single- and b) polycrystal magnetoelectric surfaces.

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References

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