ADVANCES IN THE MATERIAL PROPERTIES OPEN DATABASE

L. E. Fuentes-Cobas[1], D. Chateigner[2], E. E. Villalobos[1], V. Barrera[1], R. Domínguez[1], A. Ledezma[1], A. Ramos[1], L. Fuentes-Montero[3], J. A. Cardona[4]

[1] Centro de Investigación en Materiales Avanzados, S.C. Chihuahua, México. [2] Normandie Université, Université de Caen Normandie, CRISMAT-CNRS, France. [3] Diamond Light Source Ltd, Software Development Team, Didcot OX11 0DE, England. [4] Universidad Nacional de Colombia, Colombia

The Material Properties Open Database (MPOD, http://mpod.cimav.edu.mx) is a functional element of the web-based *open databases* system linked with Crystallography. MPOD delivers single-crystal tensor properties in several representations, ranging from numerical matrices to 3D printing. Longitudinal moduli surfaces are expressed as symmetrized spherical harmonics expansions and displayed in computer displays as well as in smart cell phones. Properties are stored as ".mpod" files. IUCr formatting standards (CIF) are followed. The original paper containing the data is cited. Structural and experimental information is also registered and linked. The MPOD system includes a physical properties dictionary with pertinent constitutive equations according to Vol. D of the International Tables of Crystallography. "Coupling properties", e.g. piezo-effects, represent interactions linking different subsystems in a material. The implications of crystal symmetry in physical properties are systematically taken into account. Matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle.

The representation of magnetic coupling properties, e.g. magnetoelectricity, and their link with magnetic symmetry concepts represent newly added features of MPOD. Color-symmetry and time-inversion considerations add complexity and interest to the task of systematizing the reception, validation and representation of this family of properties.

Starting with registered single-crystal properties, textured polycrystals' properties are estimated by MPOD. The user selects the crystal and 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 Voigt, Reuss and Hill considerations. The symmetrized spherical harmonics treatment introduced in the characterization of single-crystal properties is extended to the calculation of textured polycrystals properties.

The MPOD presentation includes a real-time demonstration of the database possibilities. Funding from Project CONACYT 257912 is acknowledged.

Keywords: Crystal physical properties, Open database, Polycrystal effective properties

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Presenting author's email: luis.fuentes@cimav.edu.mx