THE REPRESENTATION OF COUPLING INTERACTIONS IN THE MATERIAL PROPERTIES OPEN DATABASE (MPOD)

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The Material Properties Open Database (MPOD) is a functional element of the web-based *open databases* system linked with the International Union of Crystallography (IUCr). MPOD delivers single-crystal tensor properties in several representations, ranging from numerical matrices to 3D printing. Longitudinal moduli surfaces can be displayed in computers as well as in smart cell phones. MPOD was initiated by D. Chateigner in 2010. Properties are stored as ".mpod" files. IUCr formatting standards (CIF) are followed. The original published 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.

"Coupling properties", say piezo-effects and magnetoelectricity, represent interactions linking different subsystems in a material. Currently, piezoelectricity occupies a significant fraction of cases in MPOD. The implications of crystal symmetry in piezoelectricity are systematically taken into account. Matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle. Magnetoelectric axial tensors introduce exciting features into MPOD. Color-symmetry and time-inversion considerations add complexity and interest to the task of systematizing the reception, validation and representation of this remarkable coupling property. The representation of polycrystals' properties symbolizes a forthcoming challenge to the MPOD international group. The MPOD presentation includes a real-time demonstration of the database possibilities.

Keywords: Properties database, piezoelectric tensor, magnetoelectricity