# IMPLEMENTING GRAPHIC OUTPUTS FOR THE MATERIAL PROPERTIES OPEN DATABASE (MPOD)

## http://mpod.cimav.edu.mx


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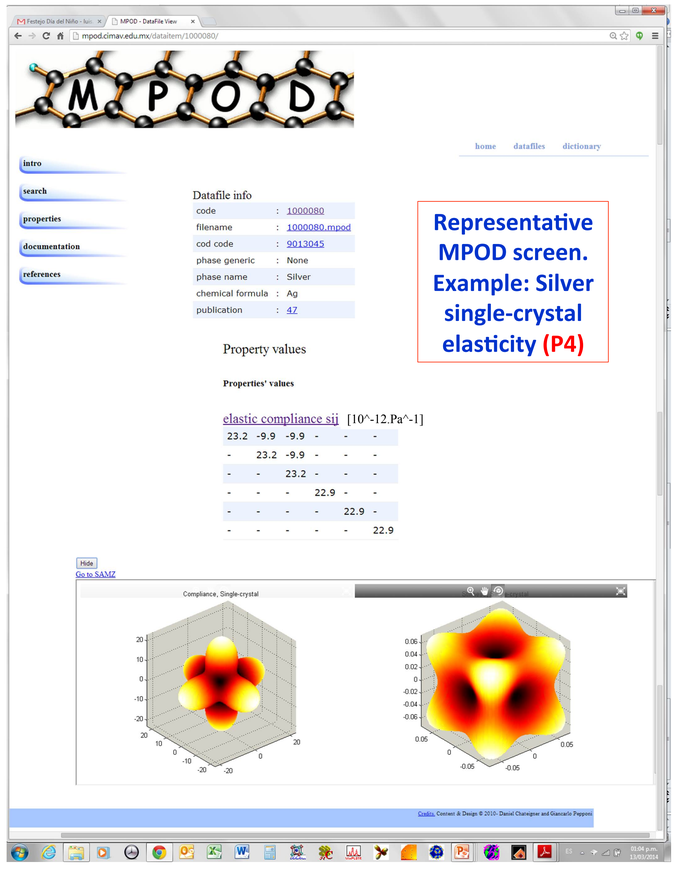
### ABSTRACT

The tensor nature of single- and polycrystalline materials' physical properties highlights both the diversity of possible technological applications and the difficulties of assimilation for those new to the subject. The Material Properties Open Database (MPOD) is a useful tool that provides access to a wide spectrum of properties tensors for an extensive selection of materials. The Material Properties Open Database was initiated by Daniel Chateigner in July 2010. The MPOD was inspired by the Crystallography Open Database. (Grazulis et al, 2009). Here an extension of the MPOD system is reported. The introduced innovation is the output, in the form of a graphical representation, of registered second, third and fourth rank tensors. The objective, as an educational project, is to provide the crystallographic community a friendly means to help the intuitive understanding of crystalline anisotropy. The given graphical output is the so-called *longitudinal surface representation*. Figures in the present poster show examples of the MPOD graphical output. Displayed surfaces represent physical properties described by polar tensors of ranks 2 to 4 and axial tensors of second rank. The MPOD websites continue under development. The international MPOD group systematically adds new published data. Modeling and representing textured polycrystals' properties is on target.

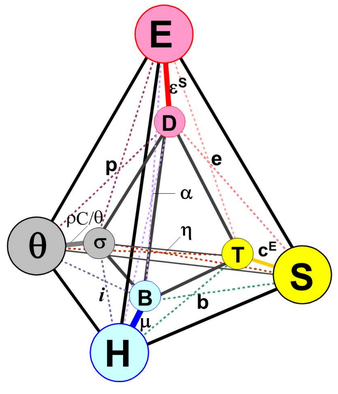




**Representative MPOD screen. Example: Silver single-crystal elasticity (P4)**

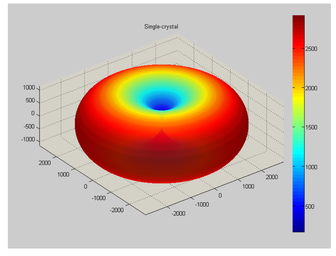
| Property **K** | Related magnitudes **K = Y / X** | Tensor |
|---|---|---|
| Heat capacity $C$ | σ = Entropy (P0) / θ = Temperature (P0) | P0 |
| Stiffness $\mathbf{c}^E$ | T = Stress (P2) / S = Strain (P2) | **P4** |
| Permittivity $\boldsymbol{\varepsilon}^S$ | Elec. Displacement (P1) / Elec. Intensity (P1) | **P2** |
| Permeability **μ** | Magn. Induction (A1) / Magn. Intensity (A1) | P2 |
| Thermal expansion $\boldsymbol{\eta}$ | Stress (P2) / Temperature (P0) | P2 |
| Pyroelectricity **p** | Elec. Displacement (P1) / Temperature (P0) | P1 |
| Pyromagnetism ***i*** | Magn. Induction (A1) / Temperature (P0) | A1 |
| Piezoelectricity **e** | Elec. Displacement (P1) / Strain (P2) | **P3** |
| Piezomagnetism **b** | Magn. Induction (A1) / Strain (P2) | A3 |
| Magnetoelectricity **α** | Magn. Induction (A1) / Elec. Intensity (P1) | **A2** |

P = Polar A = Axial # = Tensor rank

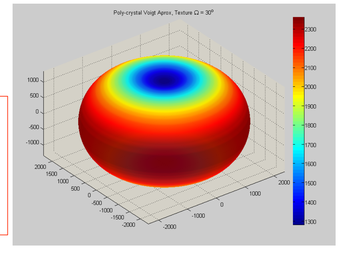
**Schematic representation of "principal" and "coupling" thermo-elasto-electro-magnetic equilibrium properties**




**$BaTiO_3$ dielectric constant (P2)**

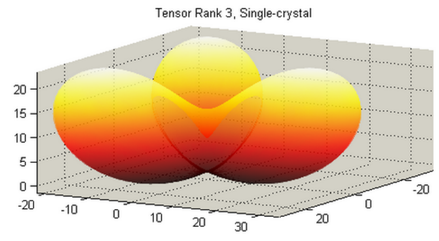



**↑ Single-crystal**
**↓ Textured polycrystal**

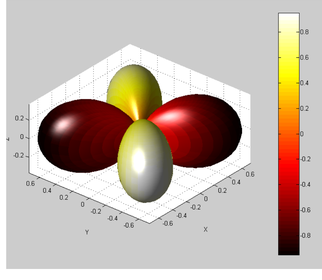



Comment: Texture affects differently even- and odd-rank properties

**$LiNbO_3$ single-crystal piezoelectricity (P3)**

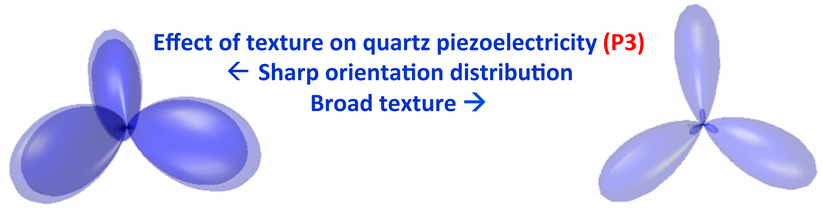



**$LiNiPO_4$ single-crystal magnetoelectricity (A2)**



Comment: Symmetry affects differently polar and axial properties

**Effect of texture on quartz piezoelectricity (P3)**
**← Sharp orientation distribution**
**Broad texture →**




**References:**

Giancarlo Pepponi, Saulius Gražulis, Daniel Chateigner. MPOD: A Material Property Open Database linked to structural information. Nuclear Instruments and Methods in Physics Research **B 284** 10–14 (2012).

Grazulis et al: Crystallography Open Database (http://www.crystallography.net/)

L. E. Fuentes-Cobas, A. Muñoz-Romero, M. E. Montero-Cabrera, L. Fuentes-Montero, M. E. Fuentes-Montero: Predicting the Coupling Properties of Axially-Textured Materials. Materials **6** (11), 4967-4984 (2013).