JORNADAS ACADÉMICAS 2019

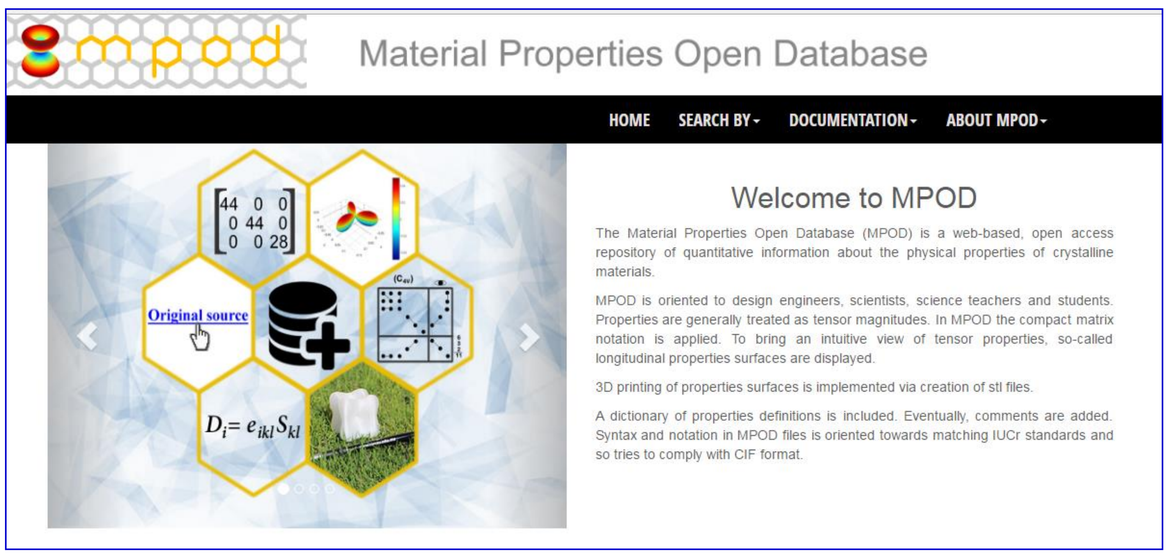
Advances in the Material Properties Open Data base MPOD

E. Villalobos-Portillo[1*], B. Batista-Fierro[2], A. Ramos-Palomino[1], R. Dominguez-Garcia[1], L. Fuentes-Cobas[1]
[1] Centro de Investigación en Materiales Avanzados (CIMAV), Chihuahua 31136, Mexico
[2] Universidad Autonoma de Chihuahua (UACH), Chihuahua 31125, Mexico
*e-mail: edgar.villalobos@cimav.edu.mx

A complete web based system for material physical properties representation sand predictions is presented. The work consists in two complementary parts, a single-crystal properties data base (MPOD) and a polycrystal physical properties predicting routine (GISELLE).

MPOD (Material Properties Open Database)

The Material Properties Open Database (MPOD) [1] http://mpod.cimav.edu.mx is a collection of published experimental single-crystal tensor properties. Matrix, surface and 3D printing representations are available. Structure-properties symmetry relationships (the Neumann Principle) are intuitively shown.



GISELLE (Global Integration System for Estimating Longitudinal and Lateral Effects).

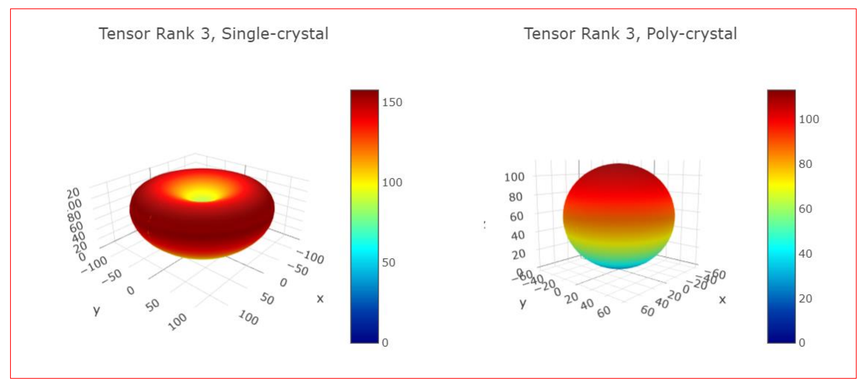
Averaging single-crystal properties tensors, with the orientation distribution function (the IPF, in fiber textures) as weight factor is a valid estimation of polycrystal properties [2].

$$\tilde{K} = \frac{1}{V}\int K dV = \int K(g)\cdot f(g) dg$$

$$\bar{d}_{ijk} = \frac{1}{8\pi^2}\iiint \sum_{m=1}^{3}\sum_{n=1}^{3}\sum_{o=1}^{3} a_{im}\, a_{jn}\, a_{ko}\, d_{mno} f(\varphi_1,\phi,\varphi_2)\, sin\,\phi\, d\phi\, d\varphi_1\, d\varphi_2$$

$$\mathbf{A} = \begin{bmatrix} \cos\varphi_2\cos\varphi_1 - \cos\phi\sin\varphi_1\sin\varphi_2 & \cos\varphi_2\sin\varphi_1 + \cos\phi\cos\varphi_1\sin\varphi_2 & \sin\varphi_2\sin\phi \\ -\cos\varphi_1\sin\varphi_2 - \cos\phi\sin\varphi_1\cos\varphi_2 & -\sin\varphi_1\sin\varphi_2 + \cos\phi\cos\varphi_1\cos\varphi_2 & \sin\phi\cos\varphi_2 \\ \sin\phi\sin\varphi_1 & -\sin\phi\cos\varphi_1 & \cos\phi \end{bmatrix}$$

The Voigt, Reuss and Hill approximations require particular precautions when dealing with so-called coupling properties (e.g. piezoelectricity, magnetostriction, magnetoelectricity).



phase name	:	barium titanate
chemical formula	:	Ba1 Ti1 O3
publication	:	150
symmetry point group name H-M	:	4 m m

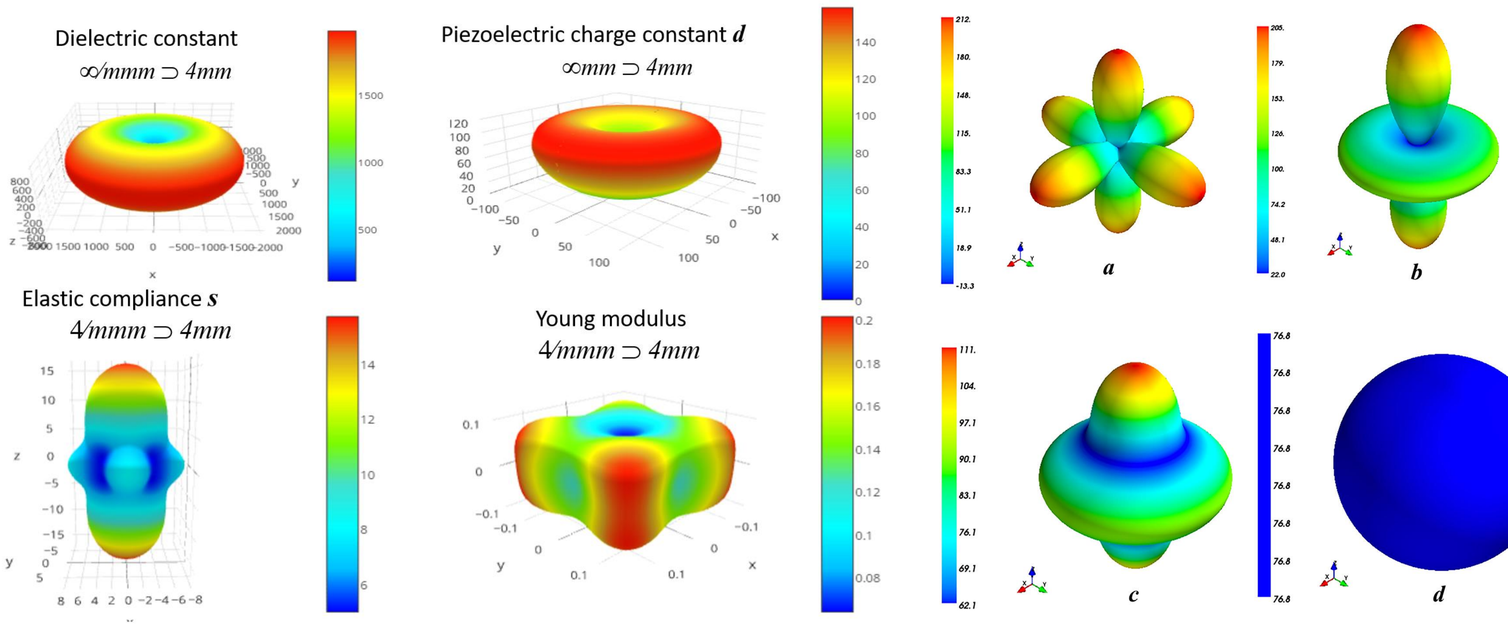
Properties' values

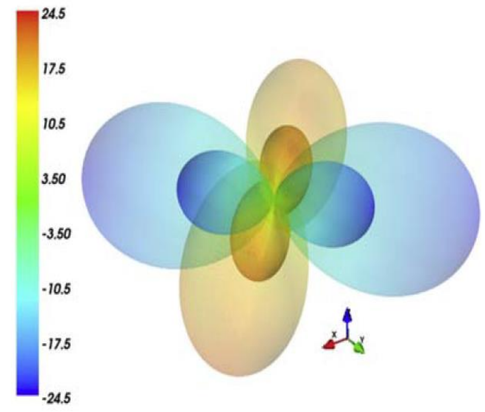
piezoelectric dij [m.V^-1]

0	0	0	0	392	0
0	0	0	392	0	0
-34.5	-34.5	85.6	0	0	0

H: 0 K: 0 L: 1 Omega: 60 Apply Texture

0.0	-0.0	-0.0	0.0	178.04	0.0
-0.0	0.0	-0.0	178.04	0.0	0.0
-51.48	-51.48	113.07	0.0	0.0	0.0





Single- and polycrystal longitudinal magnetoelectric surfaces for $LiCoPO_4$. The external surface corresponds to the single crystal. The considered ODF is composed by a Gaussian component at the origin of the Euler space, with an FWHM of 30°.

Single- and polycrystal longitudinal magnetoelectric surfaces for LiCoPO4. The external surface corresponds to the single crystal. The considered ODF is composed by a Gaussian component at the origin of the Euler space, with an FWHM of 30.

Single- and polycrystal longitudinal magnetostriction surfaces for Galfenol. Modelled texture evolves from single-crystal to random distribution of orientations.

References

[1] Luis E. Fuentes-Cobas, Daniel Chateigner, María E. Fuentes-Montero, Giancarlo Pepponi & Saulius Grazulis “The representation of coupling interactions in the Material Properties Open Database (MPOD)”. Advances in Applied Ceramics (2017).
[2] Edgar E. Villalobos-Portillo, Luis Fuentes-Montero, María E. Montero Cabrera, Diana C. Burciaga-Valencia, Luis E. Fuentes-Cobas: “Polycrystal piezoelectricity: revisiting the Voigt-Reuss-Hill approximation”. Materials Research Express (2019).