

Advances in the Material Properties Open Data base MPOD

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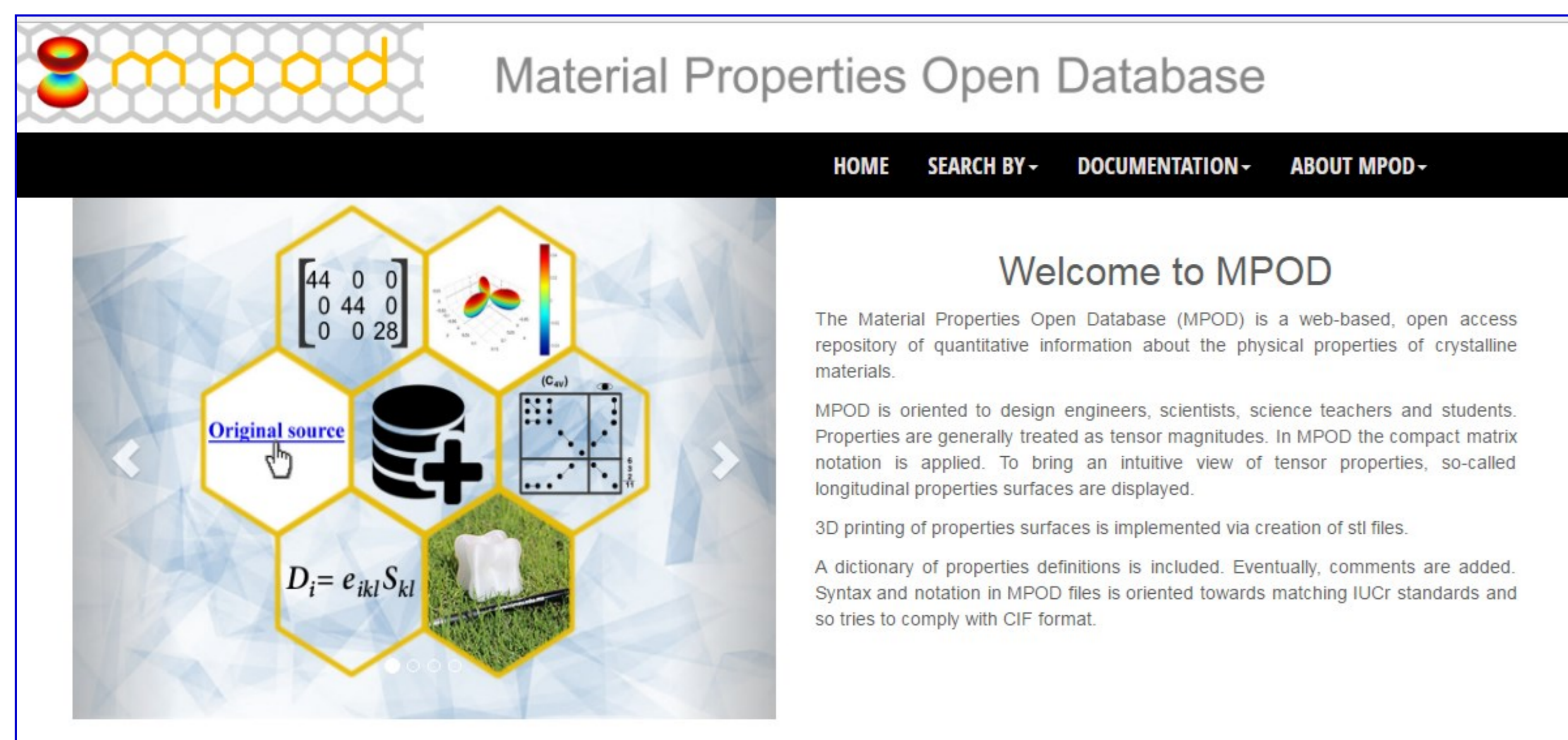
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A complete web based system for material physical properties representation and predictions is presented. The work consists in two complementary parts, a single-crystal properties data base (MPOD) and a polycrystal physical properties predicting routine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



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

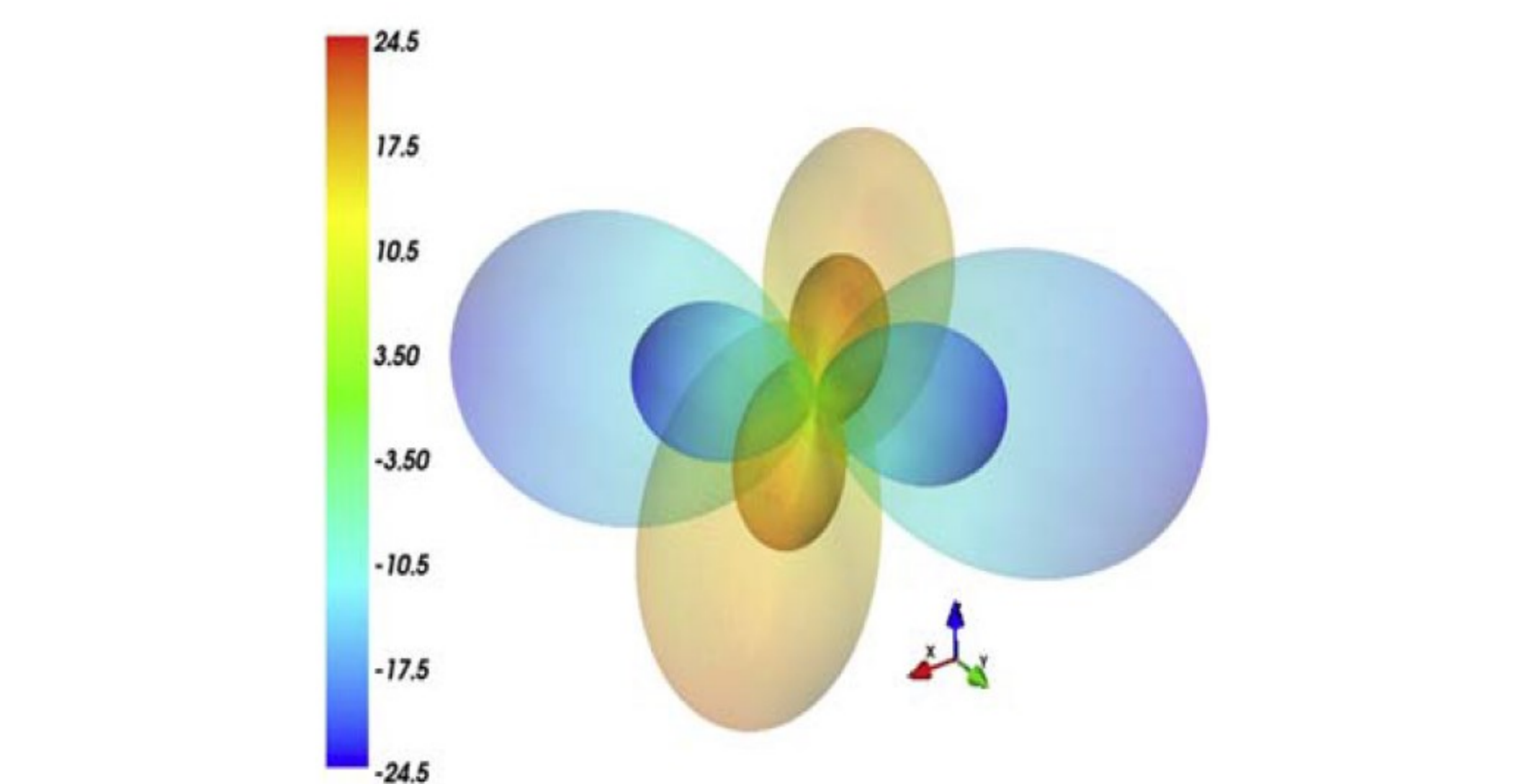
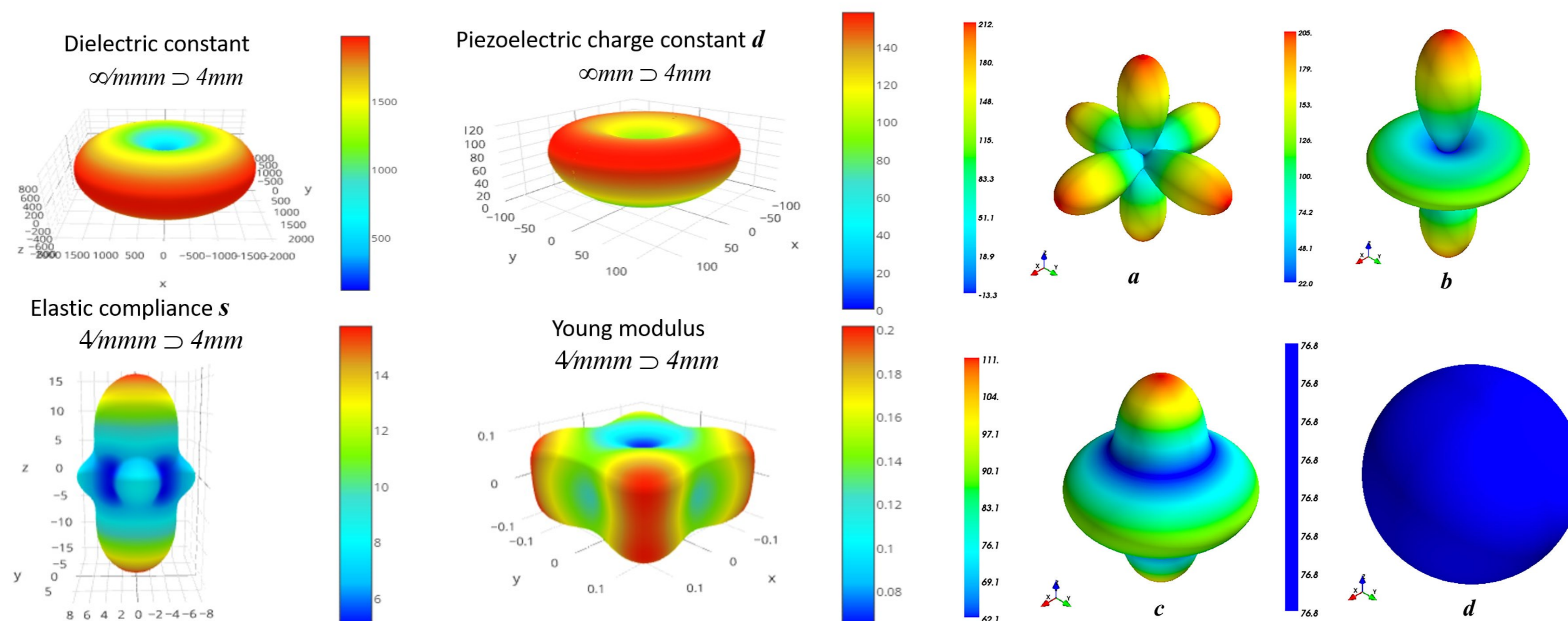
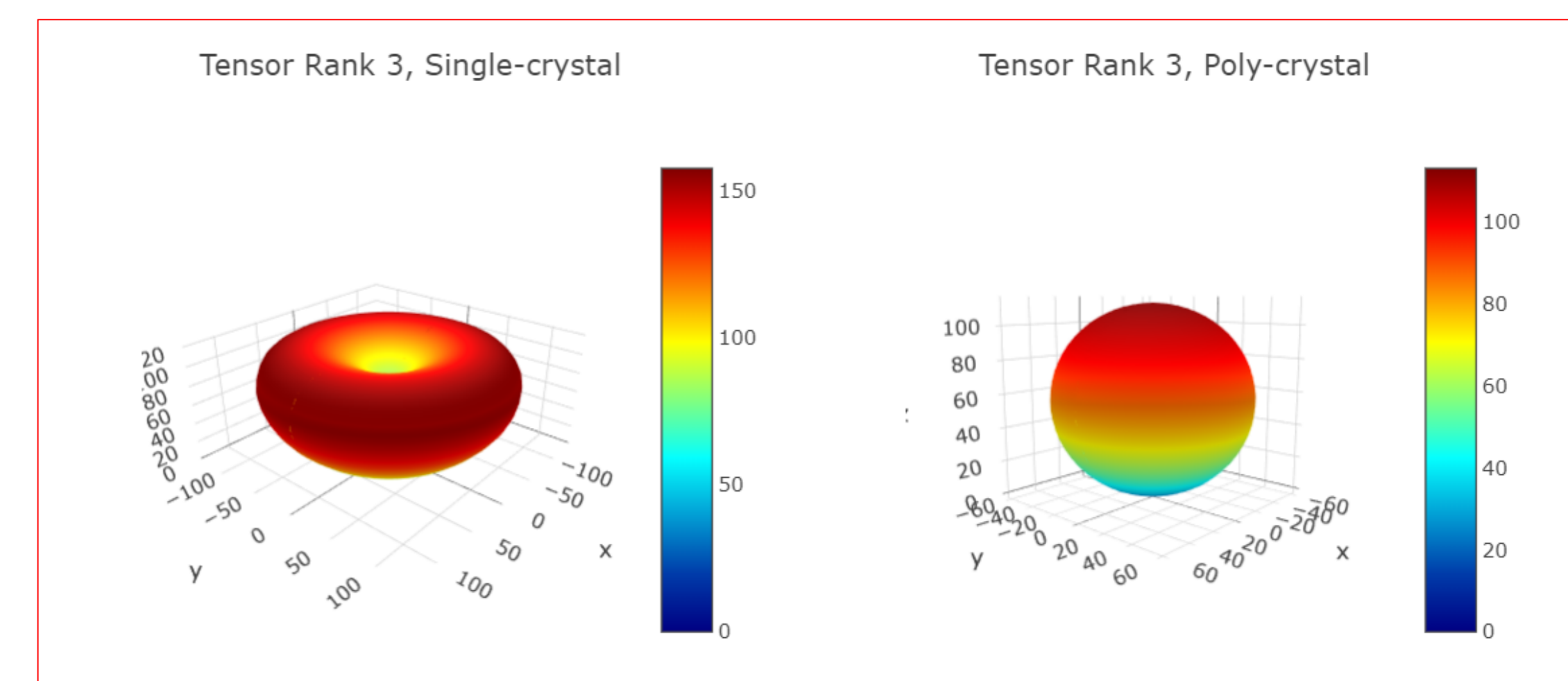
Averaging single-crystal properties tensors, with the orientation distribution function (the IPF, in fiber textures) as weight factor is a valid estimation of polycrystal properties [2].

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

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

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

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



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 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).