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

http://mpod.cimav.edu.mx

OUTLINE

Contents of MPOD. Data files.
Coupling properties.
Piezoelectricity in MPOD.
Implications of crystal symmetry (matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle).
Magnetic coupling.
MPOD and polycrystals' properties.

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

http://mpod.cimav.edu.mx

OUTLINE

Contents of MPOD. Data files.

Coupling properties.

Piezoelectricity in MPOD.

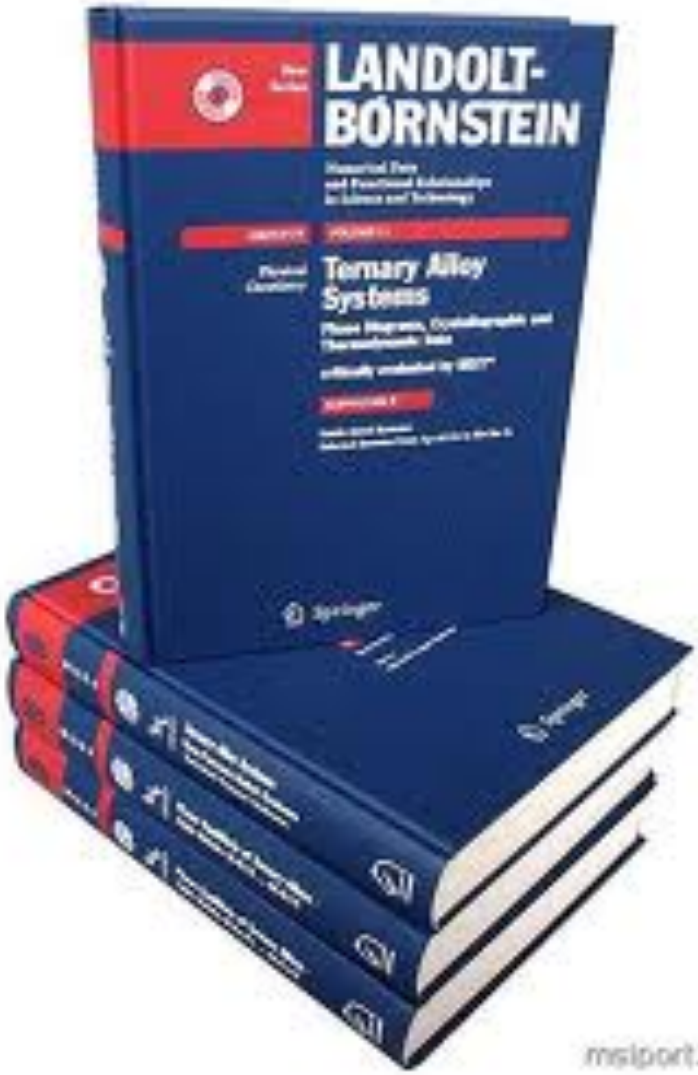
Daniel

Saulius

Giancarlo

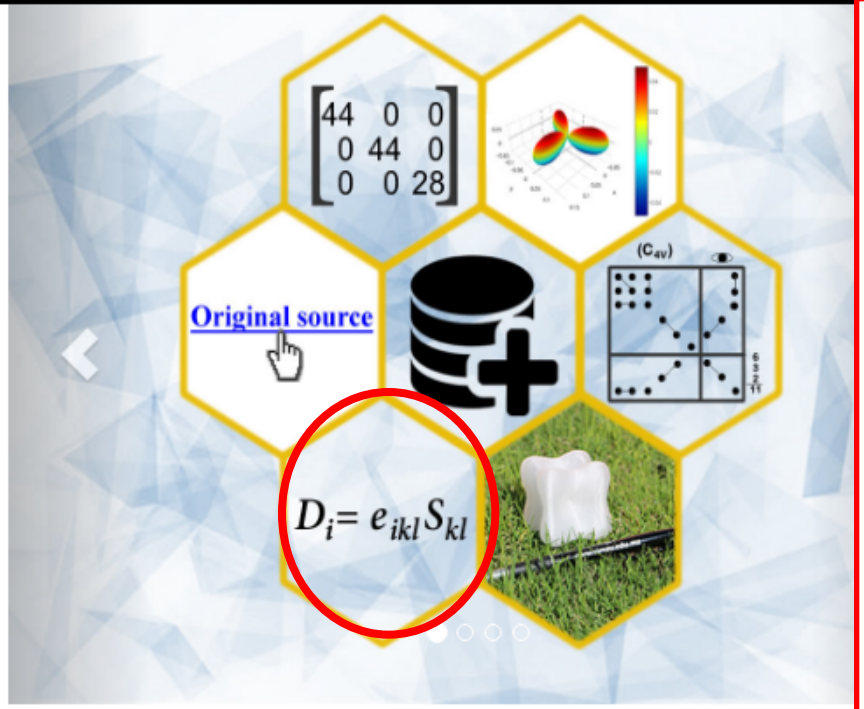
A selection of material properties databases and representation tools:

- The classical: Landolt-Börnstein (http://materials.springer.com/)
- The materials project. UC Berkeley (https://www.materialsproject.org/)
- WinTensor. Univ. Washington (http://cad4.cpac.washington.edu/wintensorhome/wintensor.htm)
- MPOD. UniCaen, CIMAV *et al* (http://mpod.cimav.edu.mx)



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

http://mpod.cimav.edu.mx



OUTLINE

Contents of MPOD. Data files.
Coupling properties.
Piezoelectricity in MPOD.
Implications of crystal symmetry (matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle).
Magnetic coupling.
MPOD and polycrystals' properties.

mpod Material Properties Open Database

Search by Property

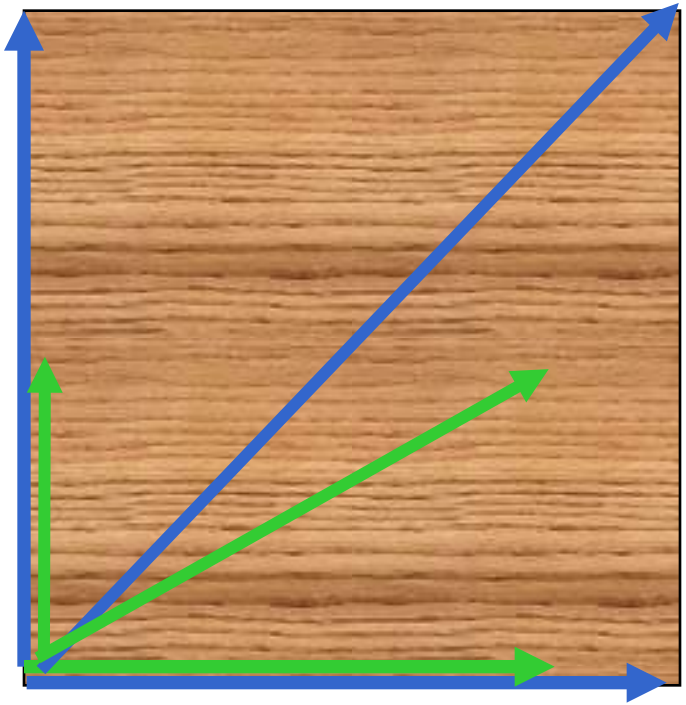
Here a list of all the properties present in the database is given. Following the link associated to the property name you can view the properties details and the set of datafiles associated with the property.

name	tensor dimensions	units	units detail
dielectric permittivity relative epsrij	3,3	1	pure number
dielectric permittivity relative epsrijS	3,3	1	pure number
dielectric permittivity relative epsrijT	3,3	1	pure number
dielectric stiffness relative betrijS	3,3	10^-4	pure number
dielectric stiffness relative betrijT	3,3	10^-4	pure number
elastic TOEC stiffness cijk	6,6,6	GPa	giga Pascal
elastic compliance sij	6,6	10^-12.Pa^-1	pico Pascal^-1
elastic compliance sijD	6,6	10^-12.Pa^-1	pico Pascal^-1
elastic compliance sijE	6,6	10^-12.Pa^-1	pico Pascal^-1
elastic stiffness cij	6,6	GPa	giga Pascal
elastic stiffness cijD	6,6	GPa	giga Pascal
elastic stiffness cijE	6,6	GPa	giga Pascal
elastic stiffness cijS	6,6	GPa	giga Pascal

Tensor nature of physical properties
(an example)

$$\mathbf{P} = \varepsilon_o \chi^P \cdot \mathbf{E}$$

P, *E*



P, *E*

χ^P is a 2nd rank tensor.

Properties are associated with constitutive equations:

Y = K · X

(K = Y / X)

Tensor ranks:

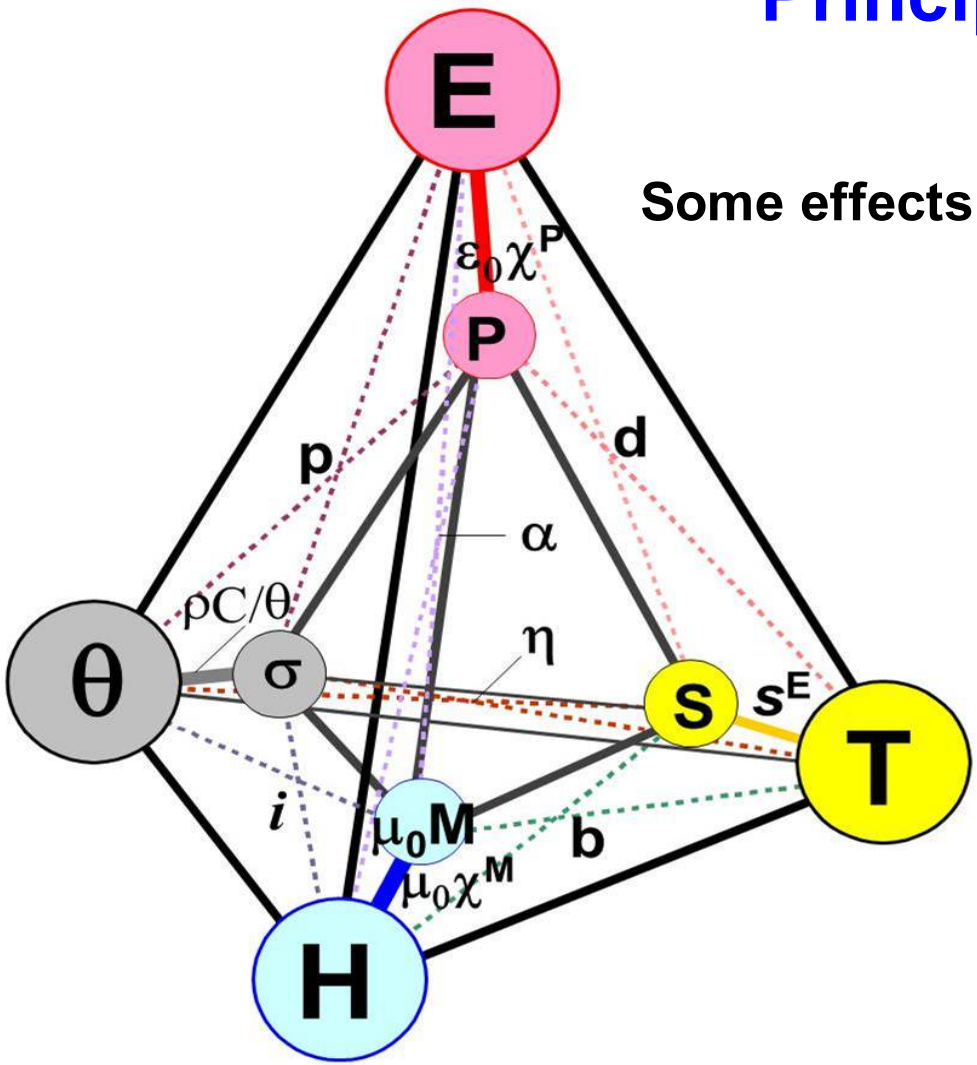
m, n, m+n

THERMO-ELASTO-ELECTRO-MAGNETIC EQUILIBRIUM PROPERTIES

Property	Related magnitudes	Tensor
Heat capacity C	Entropy (P0) / Temperature (P0)	P0
Elasticity s	Strain (P2) / Stress (P2)	P4
Electr. susceptibility χ^P	Polarization (P1) / Elec. Intensity (P1)	P2
Magn. susceptibility χ^M	Magnetization (A1) / Magn. Intensity (A1)	P2
Thermal expansion η	Strain (P2) / Temperature (P0)	P2
Pyroelectricity p	Polarization (P1) / Temperature (P0)	P1
Pyromagnetism i	Magnetization (A1) / Temperature (P0)	A1
Piezoelectricity d	Polarization (P1) / Stress (P2)	P3
Piezomagnetism b	Magnetization (A1) / Stress (P2)	A3
Magnetoelectricity α	Magnetization (A1) / Elec. Intensity (P1)	A2

P→ POLAR; A→ AXIAL; $\boldsymbol{r}$ = Tensor rank

Physical properties: "Principal" and "Coupling" Interactions.



Some effects and their constitutive equations:

Paraelectricity: $P = \varepsilon_0 \chi^P \cdot E$

Paramagnetism: $\mu_0 M = \mu_0 \chi^M \cdot H$

Elasticity: $S = s \cdot T$

Thermal expansion $S = \eta \cdot \Delta\theta$

Piezoelectricity: $P = d \cdot T$

$S = d \cdot E$

Magnetoelectricity: $P = \alpha \cdot H$

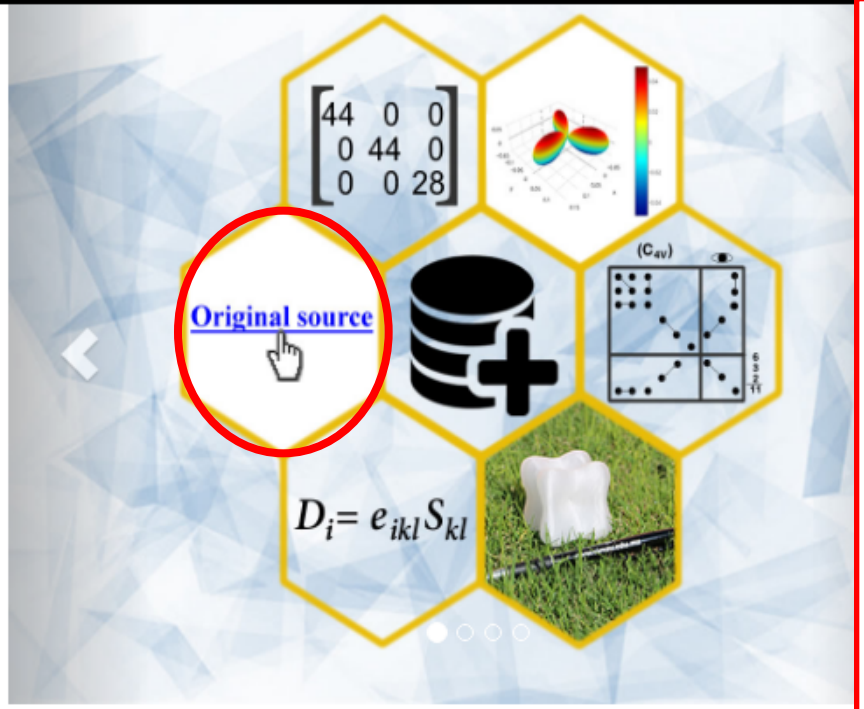
$\mu_0 M = \alpha \cdot E$

Textures and Microstructures **30**: 167-189 (1998).

magnetic antiferromagnetic ordering temperature Neel	0	K	kelvin
magnetic paramagnetic critical temperature Neel	0	K	kelvin
magnetic paramagnetic critical temperature Neel transitionwidth	0	K	kelvin
optical index extraordinary ne	0	1	pure number
optical index ordinary no	0	1	pure number
optical index principal Ni	0	1	pure number
photoelastic pij	6,6	1	pure number
photoelastic pijE	0	1	pure number
piezoelectric dij	3,6	m.V^-1	meter per volt
piezoelectric eij	3,6	C.N^-1	coulomb per newton
piezoelectric gij	3,6	C.m^-2	coulomb oer square metre
piezoelectric hij	3,6	V.m.N^-1	volt metre per newton
piezooptic pij	6,6	MPa^-1	one over mega Pascal
residual resistivity ratio	0	1	pure number
residual resistivity ratio high temperature	0	K	kelvin
residual resistivity ratio low temperature	0	K	kelvin
superconducting coherence length ksii	3	nm	nanometre
superconducting critical field1 Hc1i	3	T	tesla
superconducting critical field2 Hc2i	3	T	tesla
superconducting critical temperature mid 50	0	K	kelvin
superconducting critical temperature offset 10	0	K	kelvin
superconducting critical temperature onset	0	K	kelvin
superconducting critical temperature onset 90	0	K	kelvin

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

http://mpod.cimav.edu.mx



OUTLINE

Contents of MPOD. Data files.
Coupling properties.
Piezoelectricity in MPOD.
Implications of crystal symmetry (matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle).
Magnetic coupling.
MPOD and polycrystals' properties.

1000048	1000048.mpod	None	PMN-PT	Pb(Mg1/3Nb2/3)O3-PbTiO3(0.33)	Pb Nb0.447 Mg0.223 Ti0.33 O3	27
1000049	1000049.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.045)	Pb Nb0.637 Zn0.318 Ti0.07 O3	28
1000050	1000050.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.07)	Pb Nb0.62 Zn0.31 Ti0.07 O3	28
1000051	1000051.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.07)	Pb Nb0.62 Zn0.31 Ti0.07 O3	29
1000052	1000052.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.08)	Pb Nb0.613 Zn0.307 Ti0.08 O3	28
1000069	1000069.mpod	1010458	None	KDP, Mn-doped potassium dihydrogen phosphate	K H2 P O4 Mn0.009	38
1000070	1000070.mpod	1010458	None	KDP, potassium dihydrogen phosphate	K H2 P O4	38
1000094	1000094.mpod	9008860	None	Aluminum nitride	Al N	55
1000095	1000095.mpod	None	PIN-PMN-PT	Pb(In1/2Nb1/2)O3(0.33)-Pb(Mg1/3Nb2/3)O3(0.35)-PbTiO3(0.32)	Pb In0.165 Nb0.398 Mg0.167 Ti0.32 O3	56
1000096	1000096.mpod	None	PIN-PMN-PT	Pb(In1/2Nb1/2)O3(0.26)-Pb(Mg1/3Nb2/3)O3(0.46)-PbTiO3(0.28)	Pb In0.13 Nb0.436 Mg0.153 Ti0.28 O3	56
1000119	1000119.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.08)	Pb Nb0.613 Zn0.307 Ti0.08 O3	74
1000276	1000276.mpod	None	None	SBNN 70	Sr1.4 Ba0.6 Na Nb5 O15	128
1000277	1000277.mpod	None	None	SBNN 30	Sr0.6 Ba1.4 Na Nb5 O15	128
1000278	1000278.mpod	None	None	PIN-PMN-PT	Pb In0.135 Nb0.402 Mg0.133 Ti0.33 O3	129
1000279	1000279.mpod	None	None	PMN-PT	Pb Nb0.387 Mg0.193 Ti0.42 O3	130
1000281	1000281.mpod	None	None	BNTK	Bi0.5 Na0.25 K0.25 Ti1 O3	132
1000282	1000282.mpod	None	None	PZN-PT	Pb Nb0.613 Zn0.307 Ti0.08 O3	133
1000283	1000283.mpod	None	None	PZN-PT	Pb Nb0.613 Zn0.307 Ti0.08 O3	133
1000294	1000294.mpod	9011192	None	PbTiO3	Pb0.99 Ti1 O3	143
1000296	1000296.mpod	4500649	None	CTM	Cs2 Te1 Mo3 O12	145
1000304	1000304.mpod	2100858	None	barium titanate	Ba1 Ti1 O3	150
1000307	1000307.mpod	1508402	None	Lithium hydrogen selenide	Li1 H3 Se2 O6	152

Centro de Investigación en Materiales Avanzados, S.C.

mpod Material Properties Open Database

HOME | SEARCH BY | DOCUMENTATION | ABOUT MPOD

View Article

Publication details	
title	Elastic and piezoelectric coefficients of single-crystal barium titanate
authors	Berlincourt, Don; Jaffe,Hans
journal	Physical Review
year	1958
volume	111
issue	1
first page	143
last page	148
reference	None
pages number	None

code	filename	cod code	phase generic	phase name	chemical formula	publication
1000304	1000304.mpod	2100858	None	barium titanate	Ba1 Ti1 O3	150
1000305	1000305.mpod	2100862	None	barium titanate	Ba1 Ti1 O3	150

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

http://mpod.cimav.edu.mx

OUTLINE

Contents of MPOD. Data files.
Coupling properties.
Piezoelectricity in MPOD.
Implications of crystal symmetry (matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle).
Magnetic coupling.
MPOD and polycrystals' properties.

1000048	1000048.mpod	None	PMN-PT	Pb(Mg1/3Nb2/3)O3-PbTiO3(0.33)	Pb Nb0.447 Mg0.223 Ti0.33 O3	27
1000049	1000049.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.045)	Pb Nb0.637 Zn0.318 Ti0.07 O3	28
1000050	1000050.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.07)	Pb Nb0.62 Zn0.31 Ti0.07 O3	28
1000051	1000051.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.07)	Pb Nb0.62 Zn0.31 Ti0.07 O3	29
1000052	1000052.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.08)	Pb Nb0.613 Zn0.307 Ti0.08 O3	28
1000069	1000069.mpod	1010458	None	KDP, Mn-doped potassium dihydrogen phosphate	K H2 P O4 Mn0.009	38
1000070	1000070.mpod	1010458	None	KDP, potassium dihydrogen phosphate	K H2 P O4	38
1000094	1000094.mpod	9008860	None	Aluminum nitride	Al N	55
1000095	1000095.mpod	None	PIN-PMN-PT	Pb(In1/2Nb1/2)O3(0.33)-Pb(Mg1/3Nb2/3)O3(0.35)-PbTiO3(0.32)	Pb In0.165 Nb0.398 Mg0.167 Ti0.32 O3	56
1000096	1000096.mpod	None	PIN-PMN-PT	Pb(In1/2Nb1/2)O3(0.26)-Pb(Mg1/3Nb2/3)O3(0.46)-PbTiO3(0.28)	Pb In0.13 Nb0.436 Mg0.153 Ti0.28 O3	56
1000119	1000119.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.08)	Pb Nb0.613 Zn0.307 Ti0.08 O3	74
1000276	1000276.mpod	None	None	SBNN 70	Sr1.4 Ba0.6 Na Nb5 O15	128
1000277	1000277.mpod	None	None	SBNN 30	Sr0.6 Ba1.4 Na Nb5 O15	128
1000278	1000278.mpod	None	None	PIN-PMN-PT	Pb In0.135 Nb0.402 Mg0.133 Ti0.33 O3	129
1000279	1000279.mpod	None	None	PMN-PT	Pb Nb0.387 Mg0.193 Ti0.42 O3	130
1000281	1000281.mpod	None	None	BNTK	Bi0.5 Na0.25 K0.25 Ti1 O3	132
1000282	1000282.mpod	None	None	PZN-PT	Pb Nb0.613 Zn0.307 Ti0.08 O3	133
1000283	1000283.mpod	None	None	PZN-PT	Pb Nb0.613 Zn0.307 Ti0.08 O3	133
1000294	1000294.mpod	9011192	None	PbTiO3	Pb0.99 Ti1 O3	143
1000296	1000296.mpod	4500649	None	CTM	Cs2 Te1 Mo3 O12	145
1000304	1000304.mpod	2100858	None	barium titanate	Ba1 Ti1 O3	150
1000307	1000307.mpod	1508402	None	Lithium hydrogen selenide	Li1 H3 Se2 O6	152

View Datafile

Datafile info

code	:	1000304
filename	:	1000304.mpod
cod code	:	2100858
phase generic	:	None
phase name	:	barium titanate
chemical formula	:	Ba1 Ti1 O3
publication	:	150

General experimental conditions/parameters

measurement method		:	RT
conditions temperature	[K]	:	298

Properties' values

piezoelectric dij [m.V^-1]

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

dielectric permittivity relative epsrijT

2920	-	-
-	2920	-
-	-	168

Jet ▾ Graph

elastic compliance sijD [10^-12.Pa^-1]

7.25	-3.15	-3.26	-	-	-
-	7.25	-3.26	-	-	-
-	-	10.8	-	-	-
-	-	-	12.4	-	-
-	-	-	-	12.4	-
-	-	-	-	-	8.84

Jet ▾ Graph

elastic compliance sijE [10^-12.Pa^-1]

8.05	-2.35	-5.24	-	-	-
-	8.05	-5.24	-	-	-
-	-	15.7	-	-	-
-	-	-	18.4	-	-
-	-	-	-	18.4	-
-	-	-	-	-	8.84

1000048	1000048.mpod	None	PMN-PT	Pb(Mg1/3Nb2/3)O3-PbTiO3(0.33)	Pb Nb0.447 Mg0.223 Ti0.33 O3	27
1000049	1000049.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.045)	Pb Nb0.637 Zn0.318 Ti0.07 O3	28
1000050	1000050.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.07)	Pb Nb0.62 Zn0.31 Ti0.07 O3	28
1000051	1000051.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.07)	Pb Nb0.62 Zn0.31 Ti0.07 O3	29
1000052	1000052.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.08)	Pb Nb0.613 Zn0.307 Ti0.08 O3	28
1000069	1000069.mpod	1010458	None	KDP, Mn-doped potassium dihydrogen phosphate	K H2 P O4 Mn0.009	38
1000070	1000070.mpod	1010458	None	KDP, potassium dihydrogen phosphate	K H2 P O4	38
1000094	1000094.mpod	9008860	None	Aluminum nitride	Al N	55
1000095	1000095.mpod	None	PIN-PMN-PT	Pb(In1/2Nb1/2)O3(0.33)-Pb(Mg1/3Nb2/3)O3(0.35)-PbTiO3(0.32)	Pb In0.165 Nb0.398 Mg0.167 Ti0.32 O3	56
1000096	1000096.mpod	None	PIN-PMN-PT	Pb(In1/2Nb1/2)O3(0.26)-Pb(Mg1/3Nb2/3)O3(0.46)-PbTiO3(0.28)	Pb In0.13 Nb0.436 Mg0.153 Ti0.28 O3	56
1000119	1000119.mpod	None	PZN-PT	Pb(Zn1/3Nb2/3)O3-PbTiO3(0.08)	Pb Nb0.613 Zn0.307 Ti0.08 O3	74
1000276	1000276.mpod	None	None	SBNN 70	Sr1.4 Ba0.6 Na Nb5 O15	128
1000277	1000277.mpod	None	None	SBNN 30	Sr0.6 Ba1.4 Na Nb5 O15	128
1000278	1000278.mpod	None	None	PIN-PMN-PT	Pb In0.135 Nb0.402 Mg0.133 Ti0.33 O3	129
1000279	1000279.mpod	None	None	PMN-PT	Pb Nb0.387 Mg0.193 Ti0.42 O3	130
1000281	1000281.mpod	None	None	BNTK	Bi0.5 Na0.25 K0.25 Ti1 O3	132
1000282	1000282.mpod	None	None	PZN-PT	Pb Nb0.613 Zn0.307 Ti0.08 O3	133
1000283	1000283.mpod	None	None	PZN-PT	Pb Nb0.613 Zn0.307 Ti0.08 O3	133
1000294	1000294.mpod	9011192	None	PbTiO3	Pb0.99 Ti1 O3	143
1000296	1000296.mpod	4500649	None	CTM	Cs2 Te1 Mo3 O12	145
1000304	1000304.mpod	2100858	None	barium titanate	Ba1 Ti1 O3	150
1000307	1000307.mpod	1508402	None	Lithium hydrogen selenide	Li1 H3 Se2 O6	152

CIF format

```
#------------------------------------------------------------------------------
#$Date: 2012-11-25 18:49:00 +0000 $
#$Revision: 001 $ Daniel Chateigner
#------------------------------------------------------------------------------
#
# This file is available in the Material Properties Open Database (MPOD),
# http://www.mpod.net/
#
# The file may be used within the scientific community so long as
# proper attribution is given to the journal article from which the
# data were obtained.
#
data_1000304
_cod_database_code 2100858
_structure_refined 'no'
_phase_name 'barium titanate'
_phase_formula 'BaTiO3'
_chemical_formula_sum 'Ba1 Ti1 O3'
_symmetry_point_group_name_H-M '4 m m'
_cell_length_a  3.9998
_cell_length_b  3.9998
_cell_length_c   4.018
_cell_angle_alpha  90
_cell_angle_beta   90
_cell_angle_gamma  90

loop_
_publ_author_name
'Berlincourt, Don'
'Jaffe,Hans'
_publ_section_title
;
 Elastic and piezoelectric coefficients of single-crystal barium titanate
;
_journal_name_full               'Physical Review'
_journal_volume                  111
_journal_issue                   1
_journal_page_first              143
_journal_page_last               148
_journal_year                    1958

_prop_measurement_method 'RT'
_prop_dielectric_permittivity_relative_epsrijS 'epsrijS'
_prop_dielectric_permittivity_relative_epsrijT 'epsrijT'
 prop elastic compliance sijD 'sijD'
```

```
_prop_elastic_compliance_sijE 'sijE'
_prop_electromechanical_coupling_kij 'kij'
_prop_piezoelectric_dij 'dij'
_prop_piezoelectric_gij 'gij'
_prop_conditions_temperature 298

loop_
_prop_data_label
_prop_data_tensorial_index
_prop_data_value
epsrijT 11 2920
epsrijT 22 2920
epsrijT 33 168
epsrijS 11 1970
epsrijS 22 1970
epsrijS 33 109
sijD 11 7.25
sijD 12 -3.15
sijD 13 -3.26
sijD 22 7.25
sijD 23 -3.26
sijD 33 10.8
sijD 44 12.4
sijD 55 12.4
sijD 66 8.84
sijE 11 8.05
sijE 12 -2.35
sijE 13 -5.24
sijE 22 8.05
sijE 23 -5.24
sijE 33 15.7
sijE 44 18.4
sijE 55 18.4
sijE 66 8.84
kij 15 0.570
kij 24 0.570
kij 31 0.315
kij 32 0.315
kij 33 0.560
dij 15 392
dij 24 392
dij 31 -34.5
dij 32 -34.5
dij 33 85.6
```

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

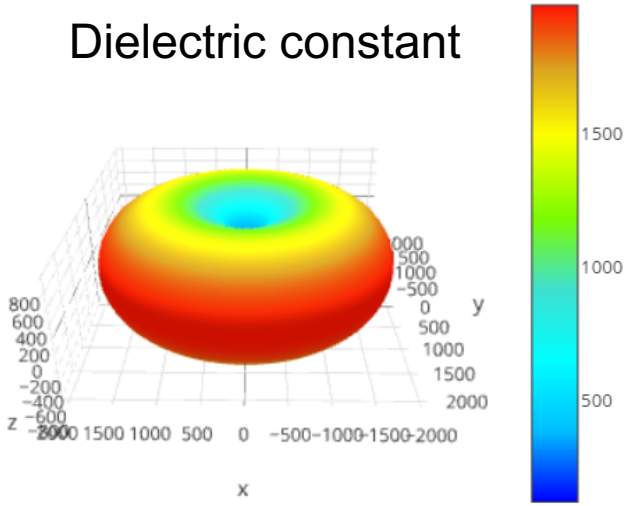
http://mpod.cimav.edu.mx

OUTLINE

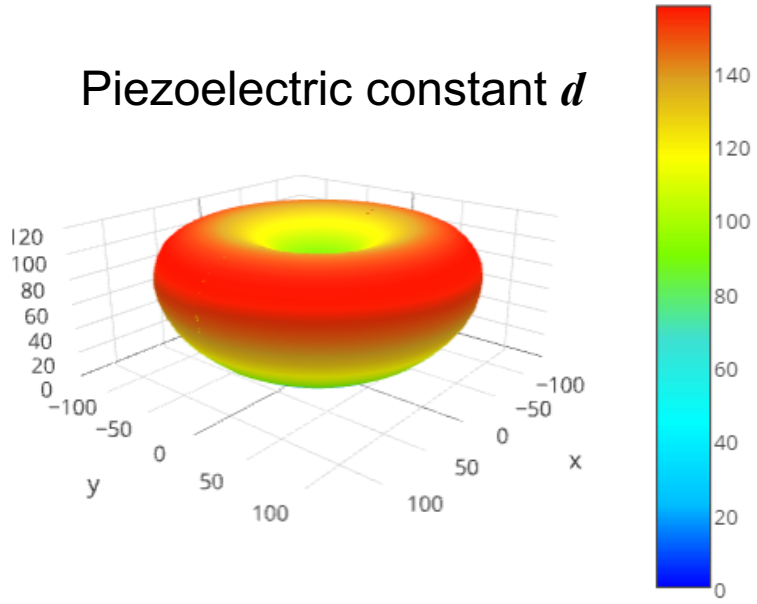
Contents of MPOD. Data files.
Coupling properties.
Piezoelectricity in MPOD.
Implications of crystal symmetry (matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle).
Magnetic coupling.
MPOD and polycrystals' properties.

$BaTiO_3$ *4mm*

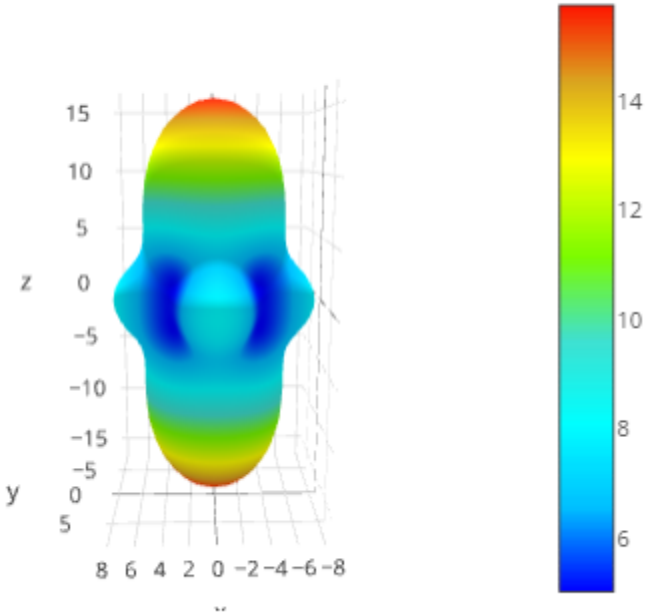
Dielectric constant



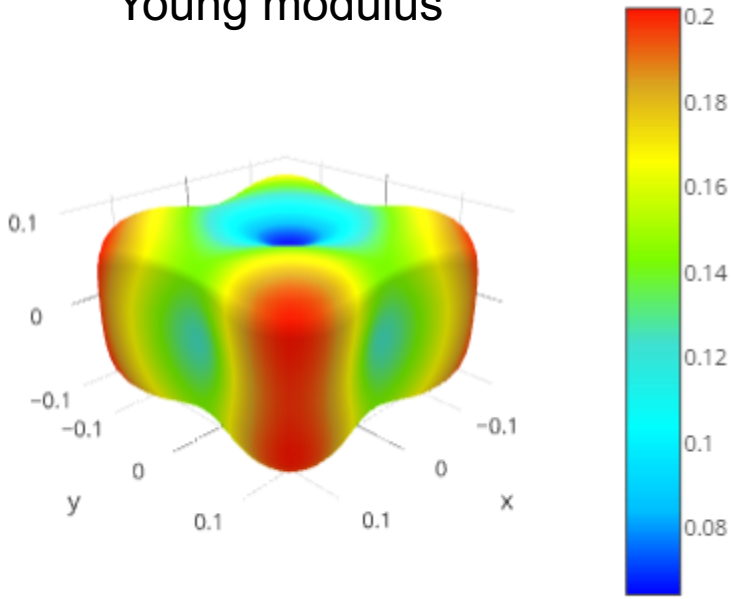
Piezoelectric constant *d*



Elastic compliance *s*



Young modulus



Structure-properties relationships: The role of Symmetry

THE NEUMANN PRINCIPLE

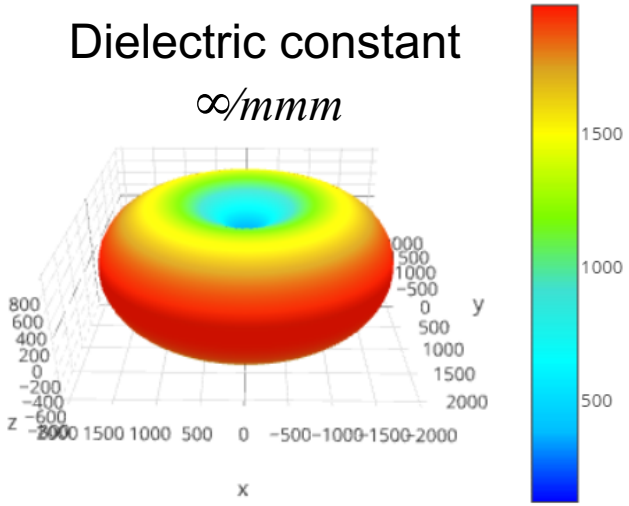
- Effect's symmetry is always -at least- equal to cause's symmetry

	Cause	Effect
Electromagnetic theory	Charges and currents	E and B fields
Crystal Physics	Structure	Properties

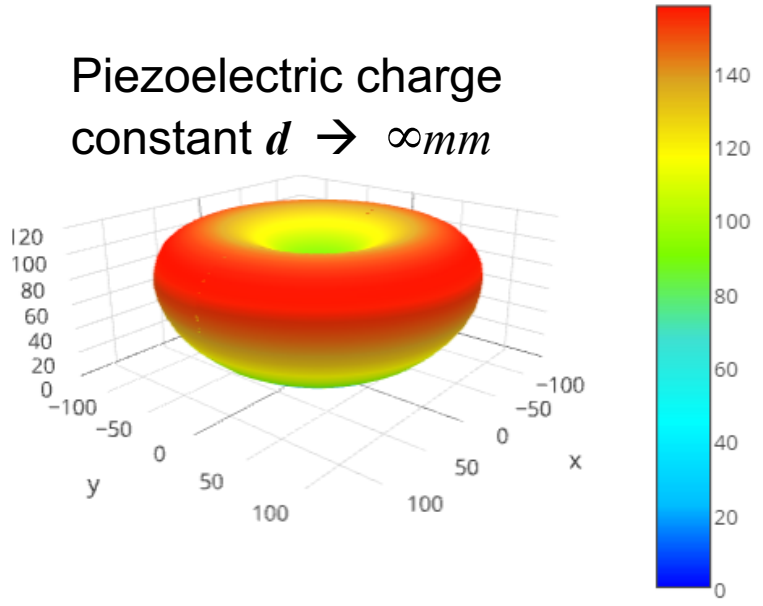
$BaTiO_3$ *4mm*

Dielectric constant

∞/mmm

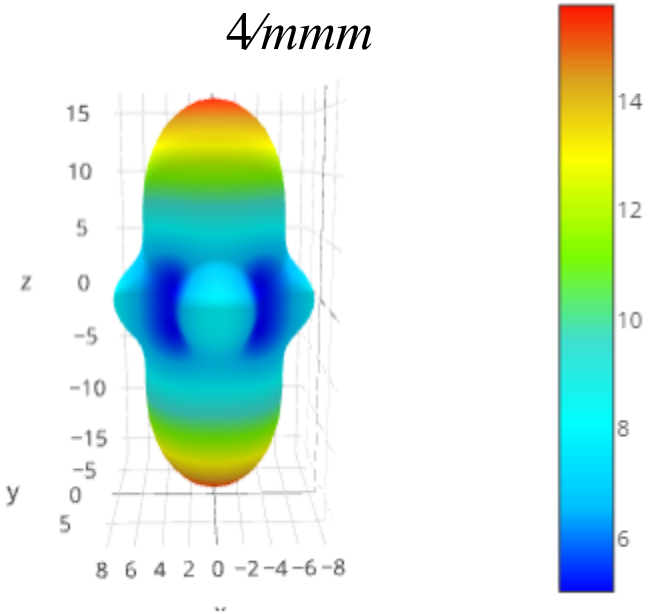


Piezoelectric charge constant ***d*** → *∞mm*



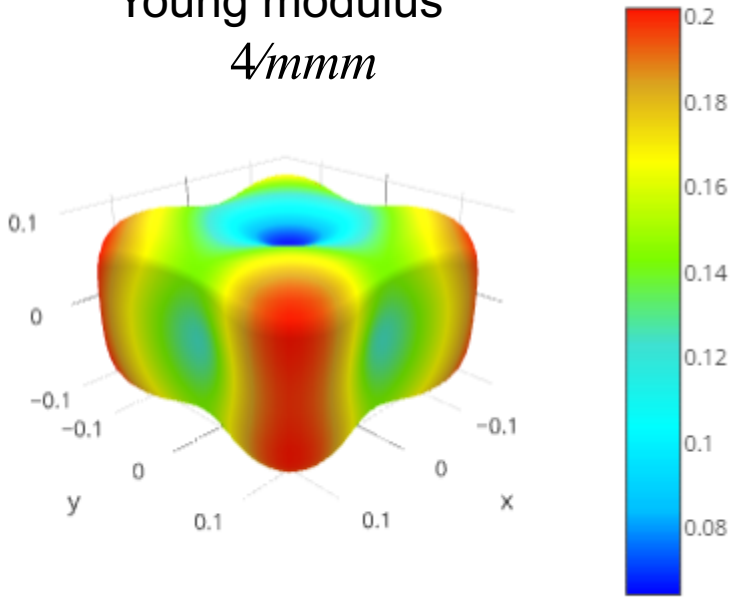
Elastic compliance ***s***

4/mmm



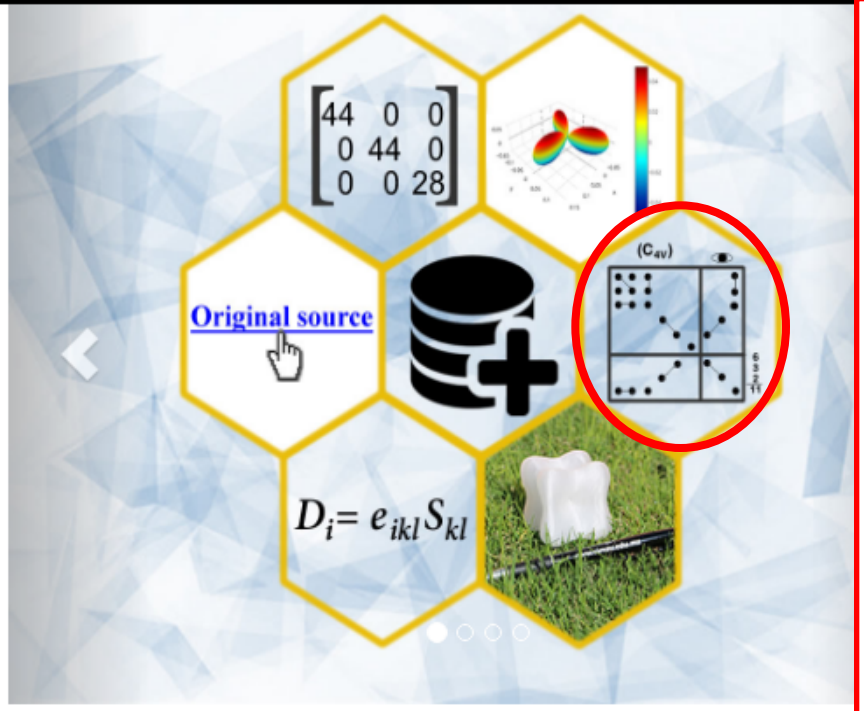
Young modulus

4/mmm



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

http://mpod.cimav.edu.mx



OUTLINE

Contents of MPOD. Data files.
Coupling properties.
Piezoelectricity in MPOD.
Implications of crystal symmetry (matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle).
Magnetic coupling.
MPOD and polycrystals' properties.

MATRIX NOTATION

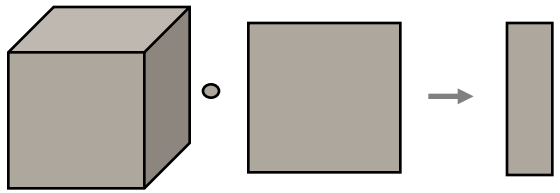
$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ \cdot & A_{22} & A_{23} \\ \cdot & \cdot & A_{33} \end{bmatrix} \Rightarrow \begin{bmatrix} \bullet & \times & \Leftarrow \\ & \searrow & \Uparrow \\ & & \Uparrow \end{bmatrix} \Rightarrow \begin{bmatrix} A_{11} \\ A_{22} \\ A_{33} \\ A_{23} \\ A_{13} \\ A_{12} \end{bmatrix} \Rightarrow \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \\ A_6 \end{bmatrix}$$

3X3 MATRIX

HYPERVECTOR

A_{ij} (for example): strain or sress tensor

PIEZOELECTRICITY



$$d \cdot T = P$$

or

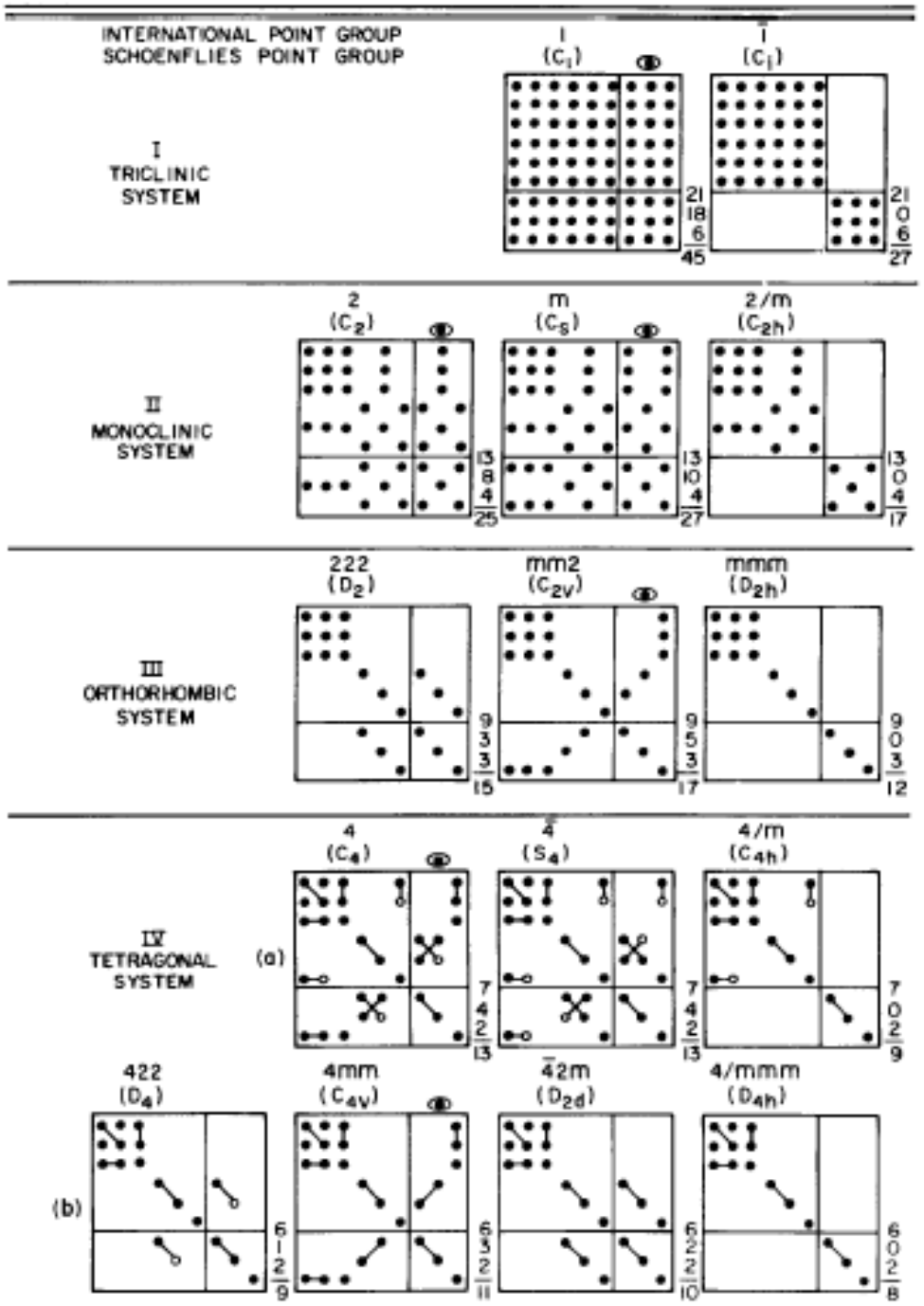
$$\begin{bmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{bmatrix} \bullet \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} = \begin{bmatrix} P_1 \\ P_2 \\ P_3 \end{bmatrix}$$

ELASTO-PIEZO-DIELECTRIC MATRIX

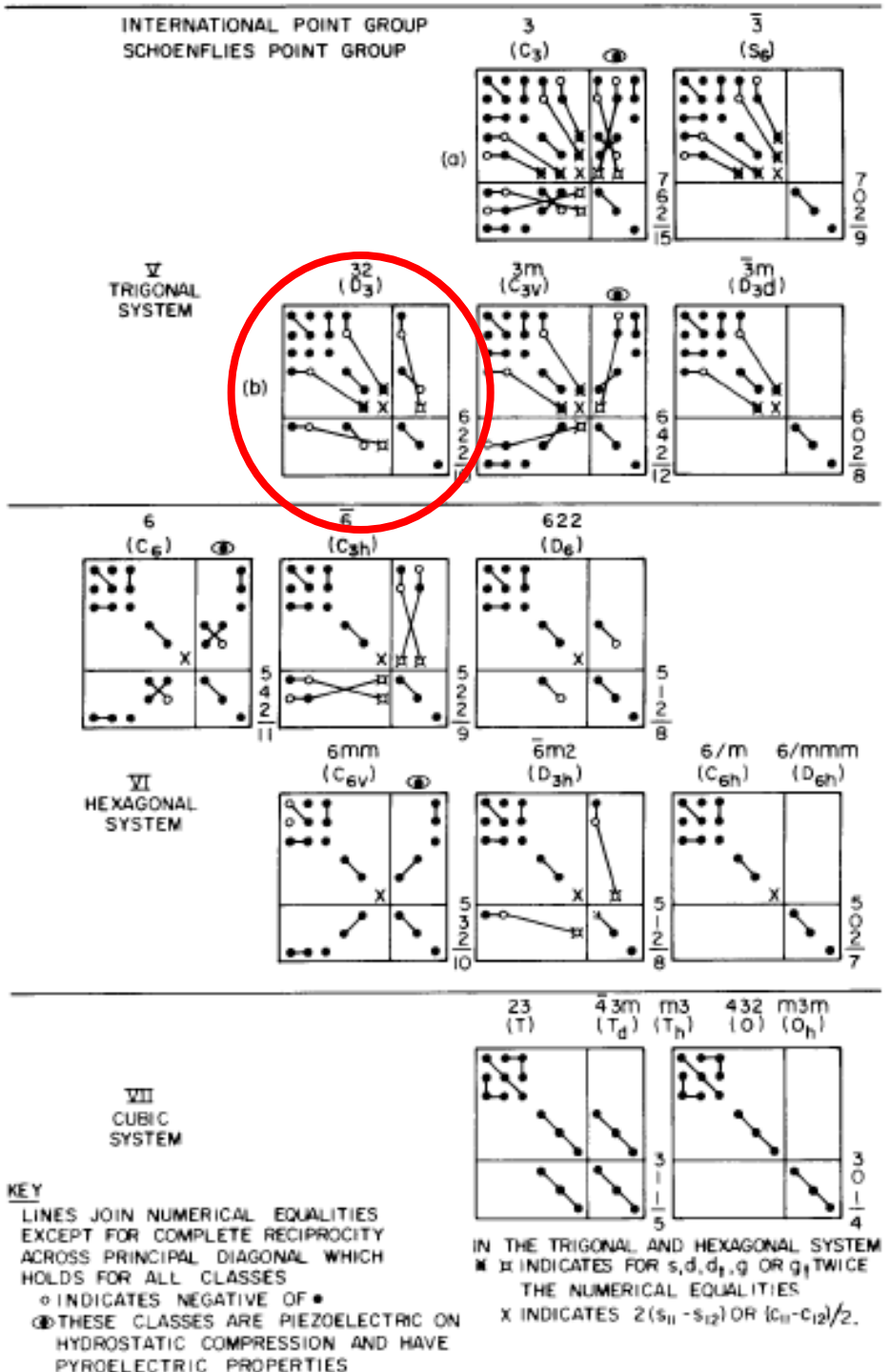
$$S = s \cdot T + d \cdot E \qquad D\ (\approx P) = d \cdot T + \varepsilon \cdot E$$

$$\begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \\ S_6 \\ D_1 \\ D_2 \\ D_3 \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} & s_{13} & s_{14} & s_{15} & s_{16} & d_{11} & d_{12} & d_{13} \\ s_{21} & s_{22} & s_{23} & s_{24} & s_{25} & s_{26} & d_{21} & d_{22} & d_{23} \\ s_{31} & s_{32} & s_{33} & s_{34} & s_{35} & s_{36} & d_{31} & d_{32} & d_{33} \\ s_{41} & s_{42} & s_{43} & s_{44} & s_{45} & s_{46} & d_{41} & d_{42} & d_{43} \\ s_{51} & s_{62} & s_{53} & s_{54} & s_{55} & s_{56} & d_{51} & d_{52} & d_{53} \\ s_{61} & s_{62} & s_{63} & s_{64} & s_{65} & s_{66} & d_{61} & d_{62} & d_{63} \\ d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} & \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} & \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} & \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ E_1 \\ E_2 \\ E_3 \end{bmatrix}$$

CRYSTALLOGRAPHIC ELASTO-PIEZO-DIELECTRIC MATRICES, IEEE



CRYSTALLOGRAPHIC ELASTO-PIEZO-DIELECTRIC MATRICES, IEEE



View Datafile

Datafile info

code	:	1000175
filename	:	1000175.mpod
cod code	:	5000035
phase generic	:	None
phase name	:	alpha-Quartz
chemical formula	:	Si O2
publication	:	98

General experimental conditions/parameters

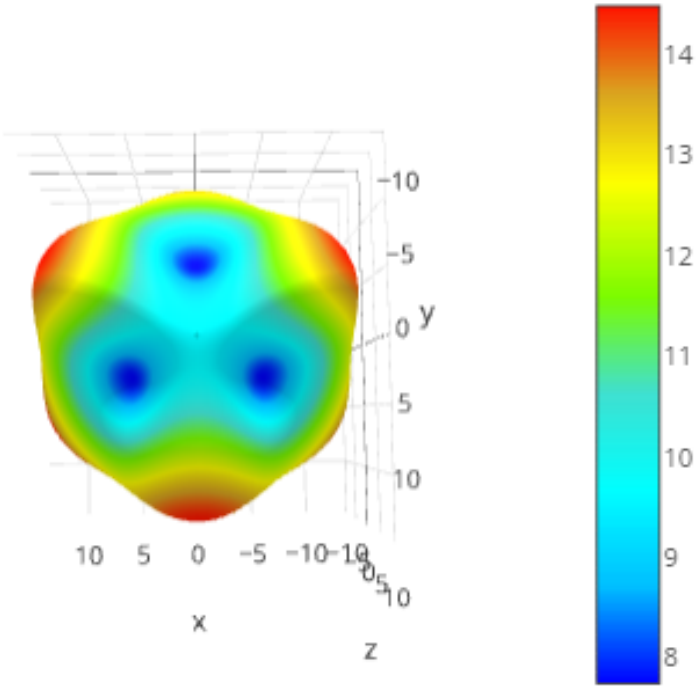
measurement method		:	?
conditions temperature	[K]	:	?

Properties' values

elastic compliance sij [10^-12 Pa^-1]

12.79	-1.53	-1.10	-4.46	-	-
-	12.79	-1.10	4.46	-	-
-	-	9.56	-	-	-
-	-	-	19.78	-	-
-	-	-	-	19.78	-8.92
-	-	-	-	-	28.62

4th Rank Tensor - Compliance



View Datafile

Datafile info

code	:	1000240
filename	:	1000240.mpod
cod code	:	5000035
phase generic	:	None
phase name	:	alpha-Quartz
chemical formula	:	Si O2
publication	:	119

General experimental conditions/parameters

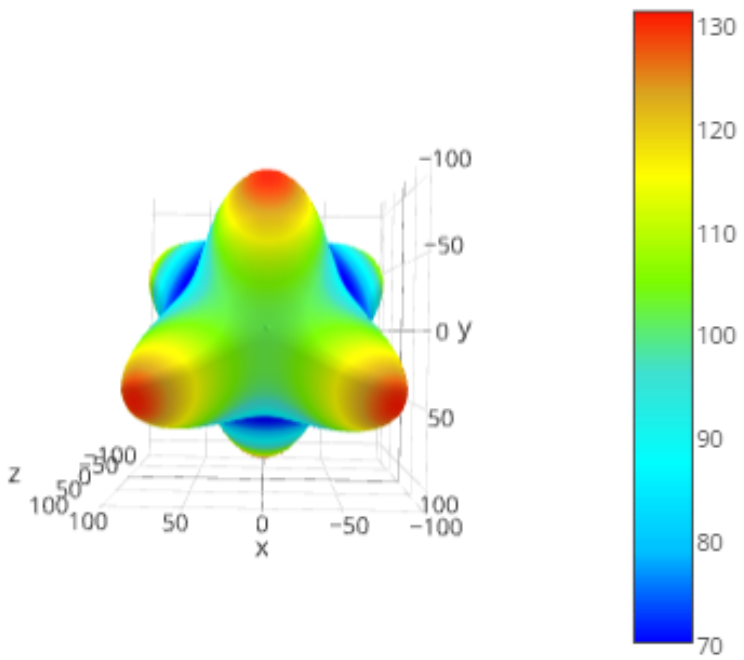
measurement method		:	COM
conditions temperature	[K]	:	?

Properties' values

elastic stiffness cij [GPa]

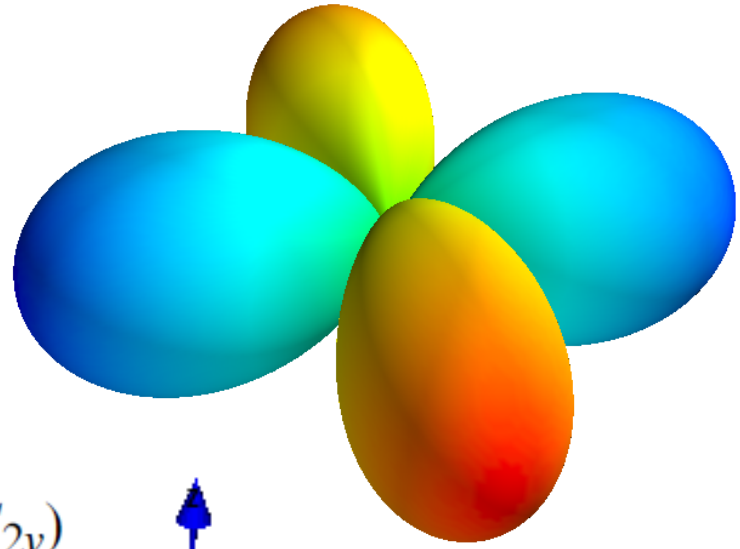
86.9	6.9	15.6	17.4	-	-
-	86.9	15.6	-17.4	-	-
-	-	106.8	-	-	-
-	-	-	57.6	-	-
-	-	-	-	57.6	17.4
-	-	-	-	-	40

Young Modulus, Single-crystal



Magnetic coupling: Magnetoelectricity

$$\begin{bmatrix} P_1 \\ P_2 \\ P_3 \end{bmatrix} = \begin{bmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} \cdot \begin{bmatrix} H_1 \\ H_2 \\ H_3 \end{bmatrix}$$



$LiCoPO_4$

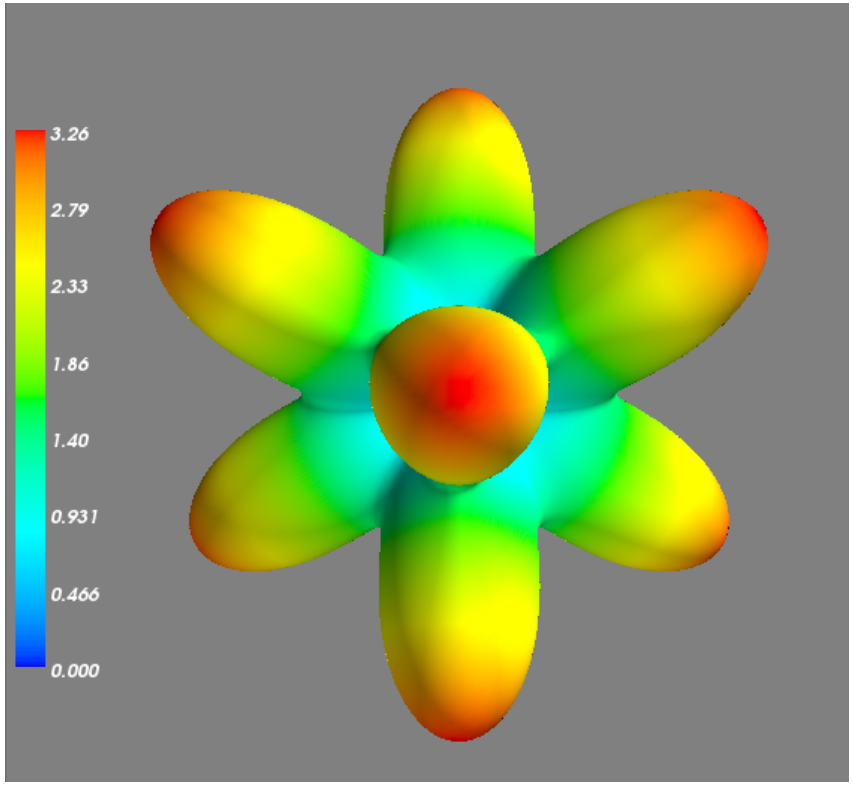
magnetic point group mmm′ (D_{2h}:C_{2v})

$$\propto = \begin{bmatrix} 0 & 18.4 & 0 \\ 30.6 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \text{ps/m} \quad (\text{LiCoPO}_4, \ T = 4.2 \ \text{K})$$

Rivera, Ferroelectrics **161**, 147 (1994)

Terfenol-D

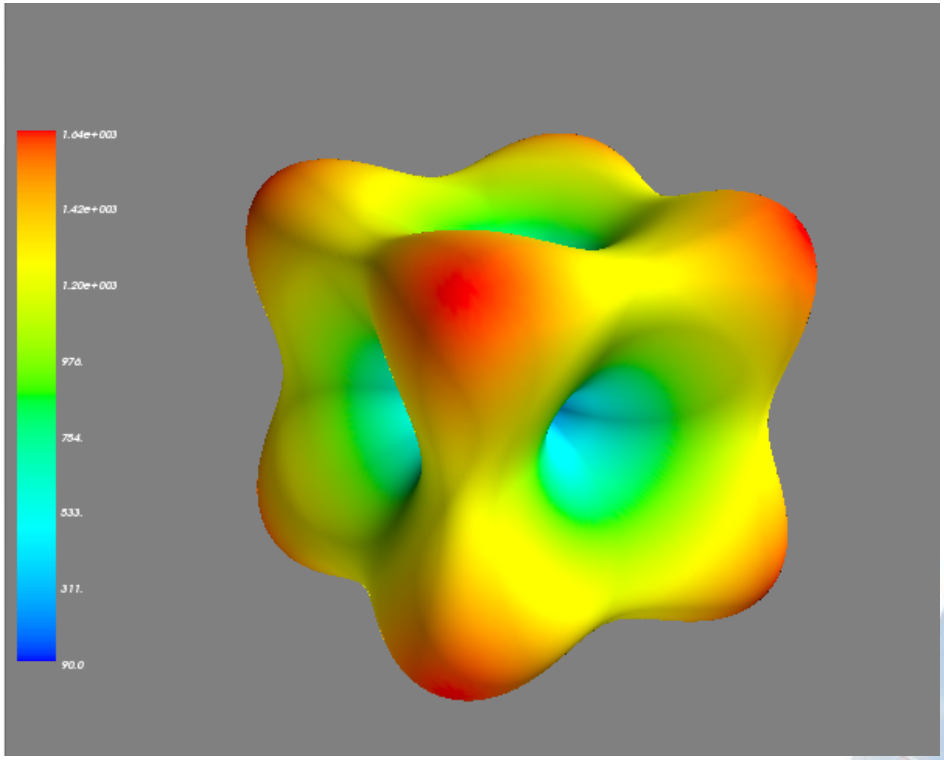
Magnetocrystalline anisotropy



$$E = K_0 + K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) + K_2(\alpha_1^2\alpha_2^2\alpha_3^2)$$

K_1 = -6.0; K_2 = -34

Magnetostriction

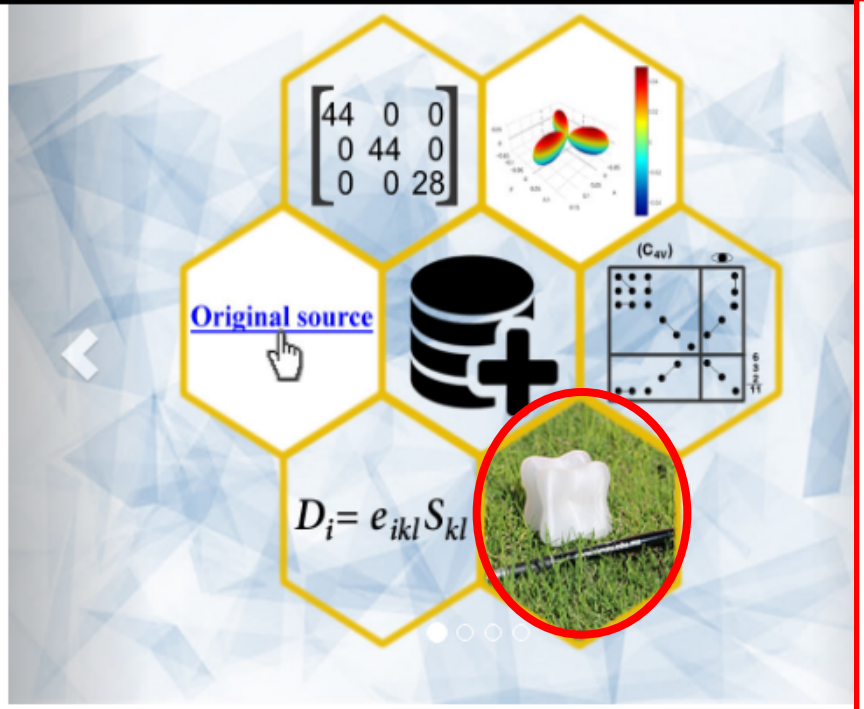


$$\lambda_{si} = \lambda_{100} + 3(\lambda_{111} - \lambda_{100})(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2).$$

λ_{100} = 90.0; λ_{111} = 1640.0

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

http://mpod.cimav.edu.mx



OUTLINE

Contents of MPOD. Data files.
Coupling properties.
Piezoelectricity in MPOD.
Implications of crystal symmetry (matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle).
Magnetic coupling.
MPOD and polycrystals' properties.

Materials **2013**, *6*, 4967-4984; doi:10.3390/ma6114967

OPEN ACCESS

materials

ISSN 1996-1944

www.mdpi.com/journal/materials

Article

Predicting the Coupling Properties of Axially-Textured Materials

Luis E. Fuentes-Cobas [1,*], Alejandro Muñoz-Romero [2], María E. Montero-Cabrera [1], Luis Fuentes-Montero [3] and María E. Fuentes-Montero [4]

1 Centro de Investigación en Materiales Avanzados, Miguel de Cervantes 120, Chihuahua, Chih 31109, Mexico; E-Mail: elena.montero@cimav.edu.mx

2 Delphi Automotive Systems, The Mexico Technical Center, Av Hermanos Escobar No 5756, Ciudad Juarez, Chih 32310, Mexico; E-Mail: alejandro.munoz07@gmail.com

3 Diamond Light Source Ltd., Diamond House, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK; E-Mail: luis.fuentes-montero@diamond.ac.uk

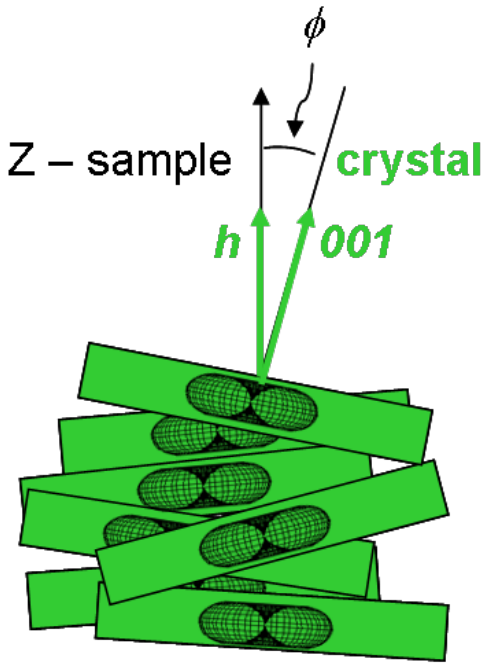
4 Facultad de Ciencia Químicas, Universidad Autónoma de Chihuahua, Nuevo Campus Universitario, Circuito Universitario Chihuahua, Chih 31125, Mexico; E-Mail: mfuentes@uach.mx

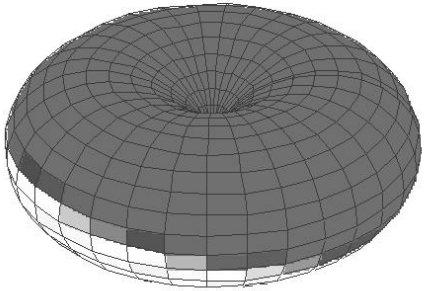
The effect of texture on the physical properties of polycrystals (work in progress)

DIELECTRIC CONSTANT. TEXTURED AURIVILLIUS CERAMICS

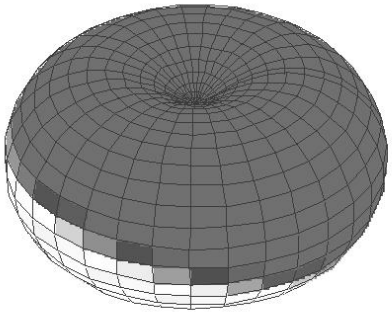
Inverse pole figure:

$$R(h) = R_0 e^{-\left(\frac{\phi}{\Omega}\right)^2}$$

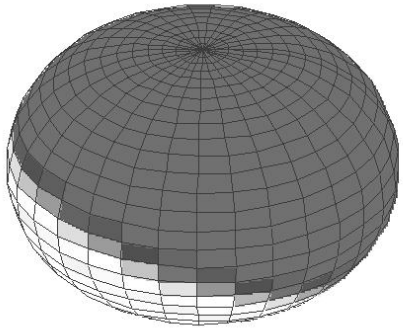




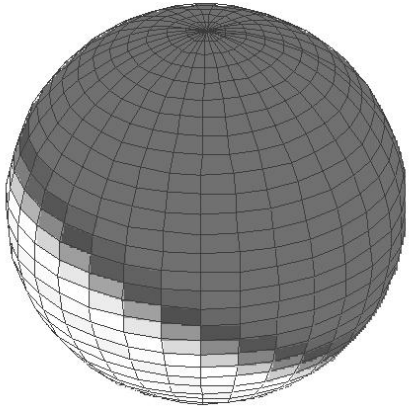
Single crystal



Polycrystal Ω = 30°



Polycrystal Ω = 60°



Random polycrystal

$PbBi_4Ti_4O_{15}$. Single crystal dielectric constant: $\varepsilon_{11} = \varepsilon_{22} = 18300$; $\varepsilon_{33} = 426$

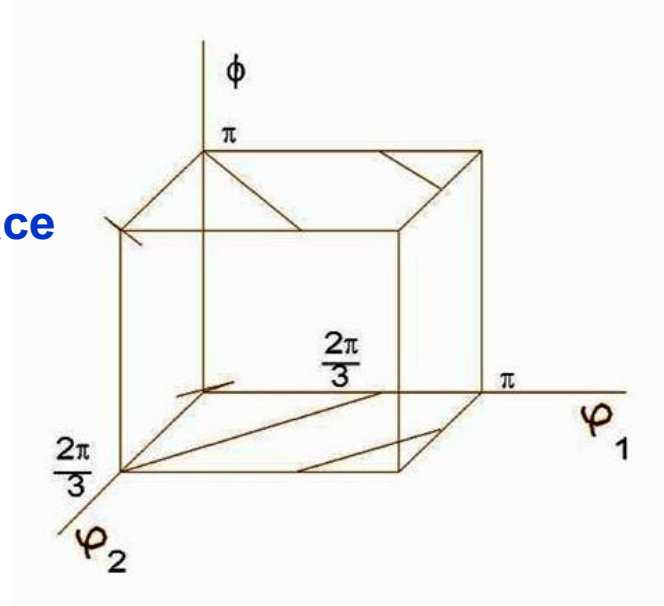
Longitudinal piezoelectric module. Quartz polycrystals

Tridimensional texture. ODF:

$$f(g) = f_0 \sum_j e^{-(\Omega_j/\Omega_0)^2}$$

$$\cos\Omega_1 = \frac{1}{2}[(1+\cos\phi)\cos(\varphi_1+\varphi_2)+\cos\phi - 1]$$

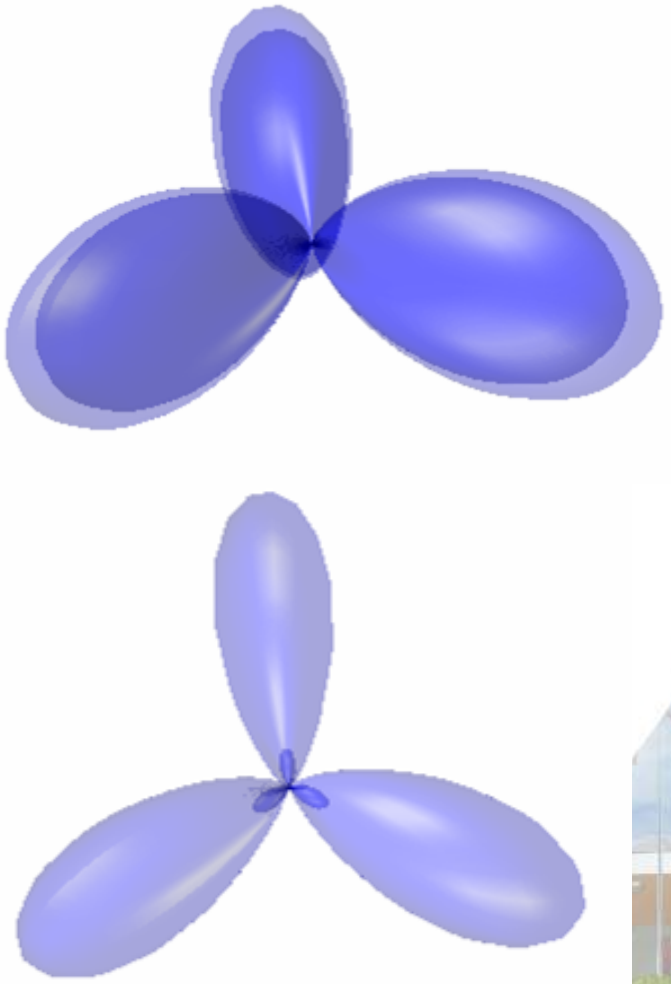
Euler space



Ω(°)

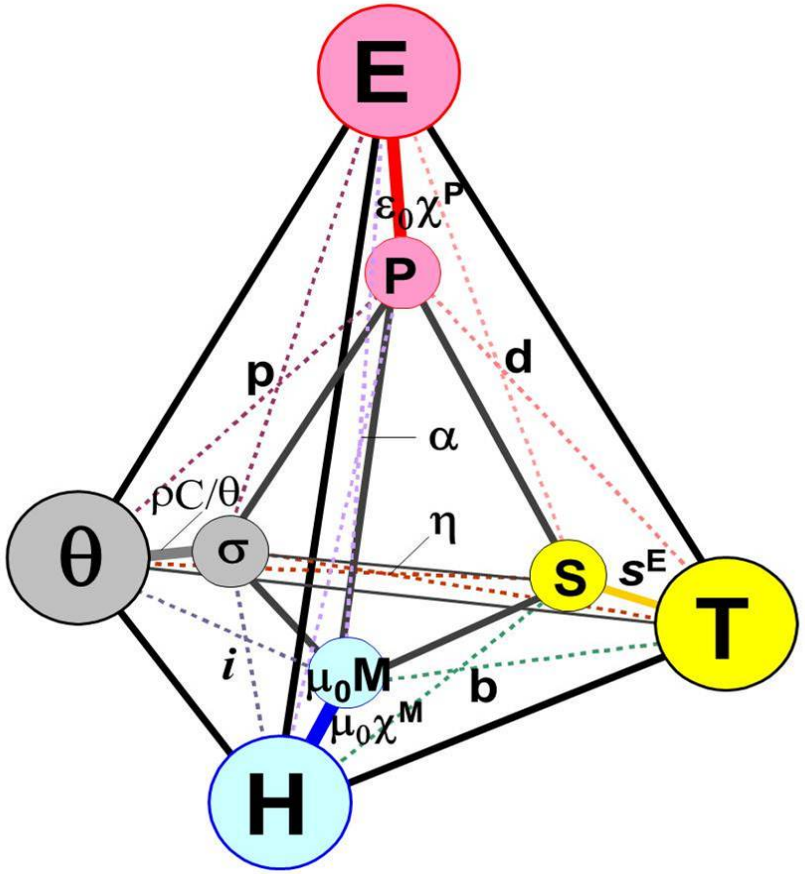
10 →

30 →



CONCLUSIONS

- MPOD (http://mpod.cimav.edu.mx) is an open database that delivers measured materials properties in matrix, surface and 3D printing descriptions.
- Crystal thermo - electro – magneto – elastic couplings exhibit a wide spectrum of anisotropic responses, linked with structural and magnetic symmetry, polar and axial nature of magnitudes and tensor ranks.
- Polycrystals' properties are derived from single-crystal ones, with texture as a modulating agent.



THANKS FOR YOUR ATTENTION! luis.fuentes@cimav.edu.mx

References:

- G. Pepponi, S. Grazulis, D. Chateigner: ***MPOD: A Material Property Open Database linked to structural information***. Nuclear Instruments and Methods in Physics Research (2012), **B284**, 10–14.
- L. Fuentes-Cobas, D. Chateigner, G. Pepponi et al: ***Implementing graphic outputs for the Material Properties Open Database (MPOD)***. Acta Cryst. (2014), **A70**, C1039.
- P. Moeck, W. Kaminsky, L. Fuentes-Cobas, J. C. Baloche, D. Chateigner: ***3D printed models of materials tensor representations and the crystal morphology of alpha quartz***. Symmetry, Culture and Science (2016), **27**, 319-330.
- L. 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).
- L. Fuentes, J. Matutes, Ma. E. Fuentes: ***Magnetoelectricity***. Ch. 3, **Vol. 19** (2011) & Ch.3 **Vol. 24** (2015), “Handbook of Magnetic Materials”. Ed: K.H.J. Buschow. Elsevier.