Checking tensor properties to crystal point group coherence in MPOD

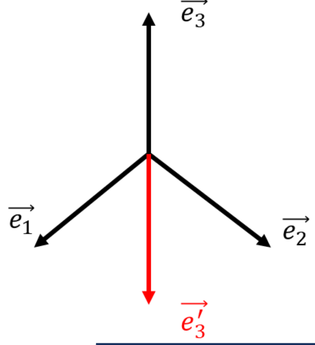
N. Lailler[1], B. Maëstracci [2], D. Chateigner [2], L. E. Fuentes-Cobas[3] , C. Eveno[1]
[1]CESI Ecole d'Ingénieurs – Rouen (France), [2]Université Caen Normandie - Caen (France), [3]University Of Habana - Chihuahua (Mexico)

Introduction

A community of researchers has launched the Cristallography Open Database (http://www.crystallography.net/cod/) in 2003. In just one year and thanks to many contributors, the database has reached more than 13.000 entries. The quick development of COD allowed the emergence of four databases, one of them being the Material Properties Open Database (http://mpod.cimav.edu.mx/).
The aim of this work is to provide a Python code to check the coherence of property tensor components with point group symmetry for the property selected. Some improvements are proposed.

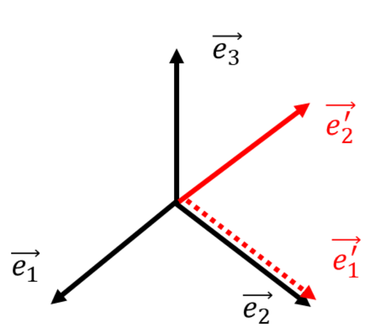
Two examples of tensors' reduction due to point-group symmetry

The crystal point-group symmetry operators can significantly reduce the number of property tensor components. For instance (Figure 1) a mirror plane reduces the number of non-zero 2nd-order tensor components to 5 instead of 9. Also, tensor components can be equalized due to some symmetry operators, like in a 2nd-order tensor submitted to a symmetry axis 4 (Figure 2). Consequently, in the MPOD database, the coherence between the symmetry elements of the crystal point group and the tensor components has to be checked.



$$T = \begin{vmatrix} T_{11} & T_{12} & 0 \\ T_{21} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{vmatrix}$$

Figure 1: *2nd-order tensor submitted to a mirror plane parallel to $\vec{e_1}$ and $\vec{e_2}$:*



$$T = \begin{vmatrix} T_{11} & T_{12} & 0 \\ -T_{12} & T_{11} & 0 \\ 0 & 0 & T_{33} \end{vmatrix}$$

Figure 2: *2nd-order tensor submitted to a symmetry axis 4 aligned with $\vec{e_3}$*

Code organisation

The main concern is to produce a code that respects crystal symmetry relationships. All point groups are considered, and the user is guided when adding a given property values (Figure 3).

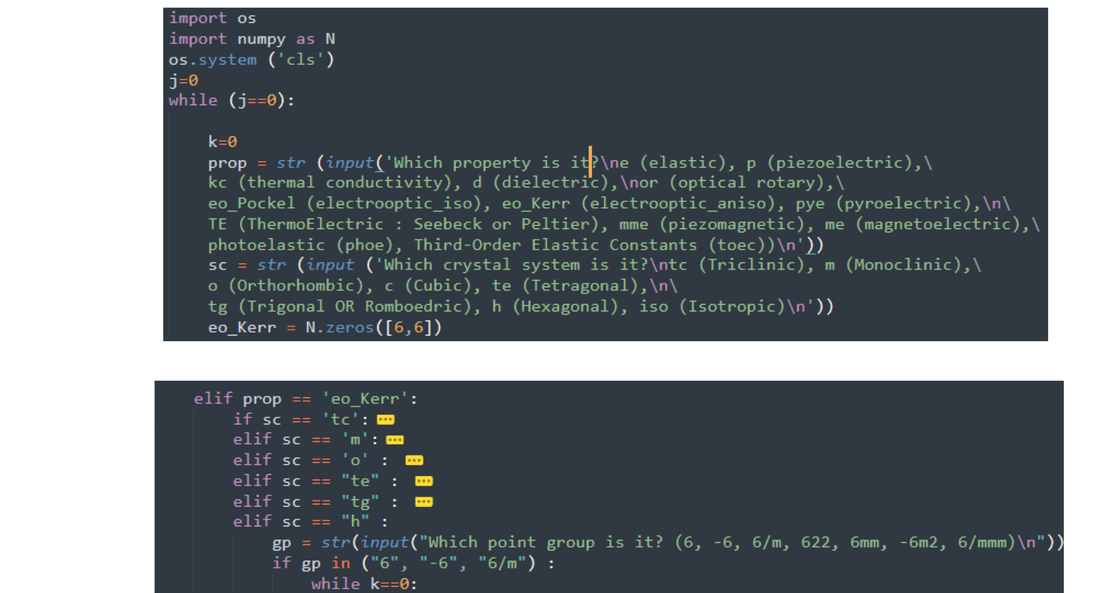


Figure 3: *Global Code Structure*

Code section

We wrote a code in Python to help checking tensor coherences for several properties. An example of code is shown in Figure 5 for the hexagonal crystal system, specifically in 6, $\bar{6}$ and 6/m point groups

```
import os
import numpy as N
os.system ('cls')
j=0
while (j==0):

    k=0
    prop = str (input('Which property is it?\ne (elastic), p (piezoelectric),\
    kc (thermal conductivity), d (dielectric),\nor (optical rotary),\
    eo_Pockel (electrooptic_iso), eo_Kerr (electrooptic_aniso), pye (pyroelectric),\n\
    TE (ThermoElectric : Seebeck or Peltier), mme (piezomagnetic), me (magnetoelectric),\
    photoelastic (phoe), Third-Order Elastic Constants (toec))\n'))
    sc = str (input ('Which crystal system is it?\ntc (Triclinic), m (Monoclinic),\
    o (Orthorhombic), c (Cubic), te (Tetragonal),\n\
    tg (Trigonal OR Romboedric), h (Hexagonal), iso (Isotropic)\n'))
    eo_Kerr = N.zeros([6,6])
```

```
elif prop == 'eo_Kerr':
    if sc == 'tc': ...
    elif sc == 'm': ...
    elif sc == 'o' : ...
    elif sc == "te" : ...
    elif sc == "tg" : ...
    elif sc == "h" :
        gp = str(input("Which point group is it? (6, -6, 6/m, 622, 6mm, -6m2, 6/mmm)\n"))
        if gp in ("6", "-6", "6/m") :
            while k==0:
                try:
                    k=1
                    eo_Kerr[0,0] = eo_Kerr[1,1] = float (input ('eo_Kerr11 = '))
                    eo_Kerr[0,1] = eo_Kerr[1,0] = float (input ('eo_Kerr12 = '))
                    eo_Kerr[0,2] = eo_Kerr[1,2] = float (input ('eo_Kerr13 = '))
                    eo_Kerr[2,0] = eo_Kerr[2,1] = float (input ('eo_Kerr31 = '))
                    eo_Kerr[2,2] = float (input ('eo_Kerr33 = '))
                    eo_Kerr[3,3] = eo_Kerr[4,4] = float (input ('eo_Kerr44 = '))
                    eo_Kerr[5,5] = (eo_Kerr[0,0] - eo_Kerr[0,1]) /2
                    eo_Kerr[0,5] = eo_Kerr[5,1] = float (input ('eo_Kerr16 = '))
                    eo_Kerr[1,5] = eo_Kerr[5,0] = - eo_Kerr[0,5]
                except :
                        k=0
                        print()
            print ('\n', eo_Kerr)
        elif gp in ("622", "6mm", "-6m2", "6/mmm") : ...
        else :
            print("point group does not exist")
    elif sc == "c" : ...
    elif sc == "iso" : ...
```

Figure 5: *Code extraction*

Tensors Notation

Nye introduced a schematic way to represent existing tensor components, and Voigt a simplified notation to reduce the number of tensor indices (Figure 4).

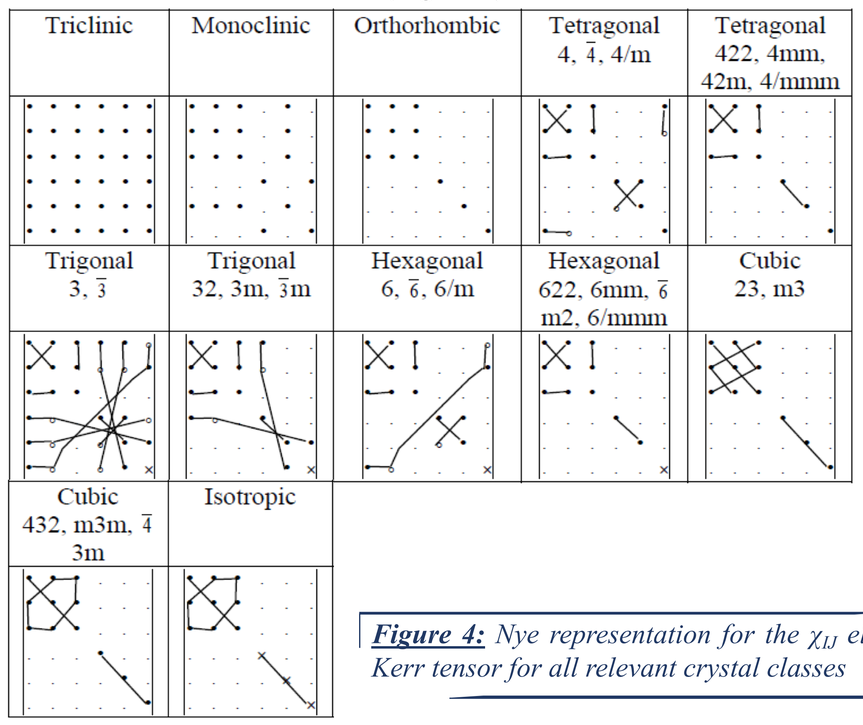


Figure 4: *Nye representation for the χ_{IJ} electrooptic Kerr tensor for all relevant crystal classes*

Conclusion

Figure 6 shows the implemented properties I could achieve during this training period, in Python.

Index for new entry rules		
Name	**Notation**	**Python name**
thermal conductivity	κij and Kij	kc
dielectric	χij	d
optical rotary	gij	or
linear electrooptic	χijk	eo_Pockel
quadratique electrooptic	χIJ	eo_Kerr
pyroelectric	pi	pye
thermoelectric seebeck/peltier	Seij and Peij	TE-> Se / Pe
piezomagnetic	bijk	mme
magnetoelectric	mij	me
photoelectric	pIJ	phoe
TOEC	cijk	toec

Figure 6: *Recap of added property rules*

Future MPOD development proposals :

- Configure new properties according to the STAR file syntax (data property tag with it's own components : index, label, units) on the database
- Update code for checking entry duplicates
- Indicate units to the user when creating new entries and/or propose data unit conversions
- Increase visibility and ergonomy of the website (particulary outdated error messages can demotivate users).

Références

- Pepponi, G., Gražulis, S., Chateigner, D. (2012). MPOD: A Material Property Open Database linked to structural information. *Nuclear Instruments and Methods in Physics Research, Section* ***B*** **284**, 10–14. https://doi.org/10.1016/j.nimb.2011.08.070
- Fuentes-Cobas, L. E., Chateigner, D., Fuentes-Montero, M. E., Pepponi, G., Grazulis, S. (2017). The representation of coupling interactions in the Material Properties Open Database (MPOD). *Advances in Applied Ceramics* **116(8)**, 428–433. https://doi.org/10.1080/17436753.2017.1343782
- D. Chateigner, Combined Analysis, Wiley-ISTE, 2010. p. 496.
- S. R. Hall, A. P. F. Cook, in: S. R. Hall, B. McMahon (Eds.), International Tables for Crystallography Volume G: Definition and Exchange of Crystallographic Data, International Union of Crystallography, 2006 (Chapter 2.5).
- S. Grazulis, D. Chateigner, R. T. Downs, A. F. T. Yokochi, M. Quiros, L. Lutterotti, E. Manakova, J. Butkus, P. Moeck, A. Le Bail. *J. Appl. Cryst.* **42** (2009) 726–729, 10.1107/S0021889809016690.
- S.R. Hall, F.H. Allen, I.D. Brown, *Acta Cryst.* **A47** (1991) 655–685.
- J.-F. Nye, Physical Properties of Crystals: Their Representation by Tensors and Matrices, Lavoisier Publishers, 1985. p. 330.
http://www.iucr.org/resources/cif/dictionaries/cif_core.