MAELAS code

User manual v1.0

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- INSTALLATION
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WHAT IS MAELAS CODE?

- MAELAS code is a software to calculate spin-dependent magnetostriction coefficients and magnetoelastic constants up to second order.

- It generates required input files for VASP code to perform Density Functional Theory calculations, and it deduces the value of magnetostriction coefficients from the calculated energies given by VASP.

- If the elastic tensor is provided, then it can also calculate the magnetoelastic constants.

- MAELAS can also be used with other DFT codes instead of VASP, after file conversion to VASP format files.

INSTALLATION

MAELAS code is just one python3 file "maelas.py", so it only requires to have Python3 and imported python libraries. For example, in Ubuntu Linux machine you can check the installed version of python3 by opening a terminal and typing

python3 –version

In case you need to install it in your machine, you can type

sudo apt-get update
sudo apt-get install python3.8

In HPC facilities you may need to load the Python3 module. For example, in Centos 7 Linux you can check all installed Python modules by typing

ml avail Python

and load the last version of Python3 using command ml

ml Python/3.8.2-GCC-8.3.0-2.32-base

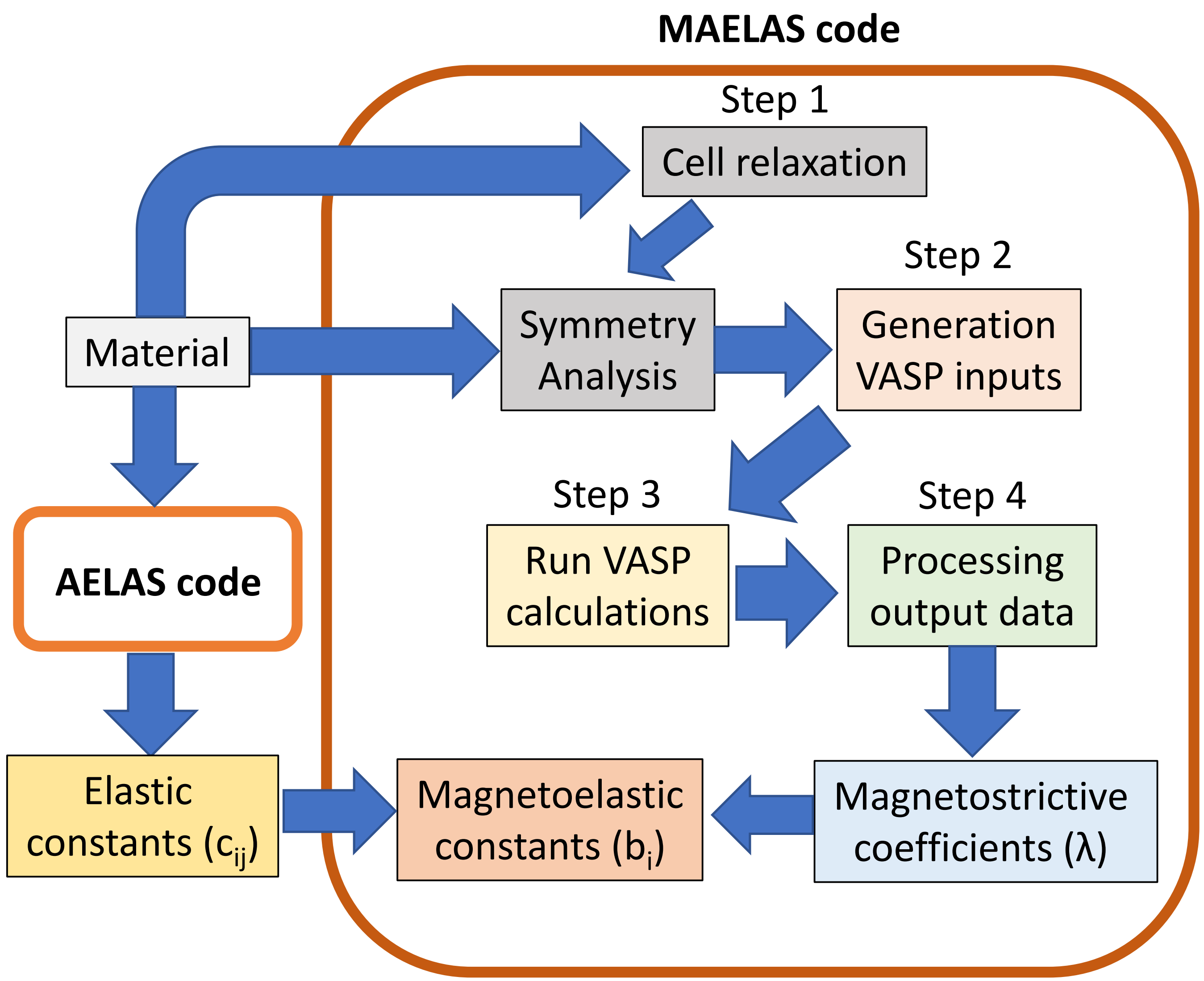
Additionally, MAELAS makes use of the following python libraries: pymatgen, scikit-learn, pyfiglet, argparse, numpy, matplotlib, scipy, math, os and stat. In case you need to install them, you can do it using pip3 as:

pip3 install library_name

where “library_name” is the name of the python library that you need to install. For example, you should type the following command to install numpy library:

pip3 install numpy

HOW TO USE MAELAS CODE



HOW TO USE MAELAS CODE

Step 1: Cell relaxation

If your initial POSCAR is not relaxed and you want to perform a cell relaxation before calculating the magentostriction coefficients, then you can use MAELAS code to generate INCAR and KPOINTS files to relax the structure with VASP. To do so, in the terminal you should copy your initial POSCAR and maelas.py files in the same folder where you want to generate the input files for VASP, and after going to this folder then type

python3 maelas.py -r -i POSCAR0 -k 40

where tag -r indicates that you want to generate VASP files for cell relaxation, -i POSCAR0 is the input non-relaxed POSCAR file (you can name it whatever you want) and -k 40 is the length parameter that determines a regular mesh of k-points. It will generate 4 files: POSCAR, INCAR, KPOINTS and vasp_jsub_rlx. Here, one still needs to copy manually the POTCAR file in this folder in order to have all required files for VASP run. The generated file vasp_jsub_rlx is a script to submit jobs in HPC facilities, one can specify some settings in this script by adding more tags in the command line. For instance,

python3 maelas.py -r -i POSCAR0 -k 40 -t 48 -c 24 -q qprod -a OPEN-00-00 -f /scratch/example_rlx

where -t 48 indicates that the number of maximum CPU hours for the VASP calculation is 48 hours,-c 24 means that the number of cores for the VASP calculation is 24, -q qprod set to production queuethe type of queue in HPC facilities, -a OPEN-00-00 is the project identification number for running jobs in HPC facilities and -f /scratch/example_rlx is the folder where you want to run VASP calculations. All these data are included in the vasp_jsub_rlx file, so one can submit this VASP job inmediately in HPC facilities by typing

qsub vasp_jsub_rlx

This procedure might be helpful for high-throughput routines. More options can be added in vasp_jsub_rlx file through the terminal command line, to see them just type

python3 maelas.py –h

Note that generated INCAR and KPOINTS files contain standard setting for cell relaxation. The user are free to change this setting either directly on the generated files or in the maelas.py. In case your structure is already relaxed or you do not want to perform a cell relaxation, then you can skip this step and move to step 2.

HOW TO USE MAELAS CODE

Step 2: Generation of VASP files for the calculation of spin-dependent magnetostriction coefficients

Copy the relaxed POSCAR, POTCAR and maelas.py files in the same folder where you want to generate the input files for VASP run. In the terminal, after going to this folder then type

python3 maelas.py -g -i POSCAR_rlx -k 70 -n 7 -s 0.1

where -g indicates that you want to generate input VASP files for the calculation of spin-dependent magnetostriction coefficients, -i POSCAR_rlx is the initial relaxed POSCAR file (you can name it whatever you want), -k 40 is the length parameter that determines a regular mesh of k-points, -n 7 means that it will generate 7 distorted states for each magentostriction mode and-s 0.1 is the maximum strain applied for distorting the structure. It will generate the following files:

POSCAR_A_B (volume-conserving distorted cell where A=magnetostriction mode, B=1,...,n distorted cell for each magentostriction mode)
INCAR_A_C (non-collinear calculation where A=magnetostriction mode, C=1,2 is the spin orientation case)
INCAR_std (collinear calculation to generate the WAVECAR and CHGCAR files to run non-collinear calculations)
KPOINTSvasp_maelas, vasp_jsub and vasp_0 (interconnected bash scripts to run VASP calculations automatically)
vasp_cp_oszicar (bash script to get calculated OSZICAR_A_B_C files after VASP calculation is finished)

The generated files vasp_maelas, vasp_jsub and vasp_0 are interconnected scripts to submit jobs in HPC facilities, one can specify some job settings in these scripts by adding more tags in the command line. For instance,

python3 maelas.py -g -i POSCAR_rlx -k 70 -n 7 -s 0.1 -t 48 -c 24 -q qprod -a OPEN-00-00 -f /scratch/example_mag

where -t 48 indicates that the number of maximum CPU hours for the VASP calculation is 48 hours,-c 24 means that the number of cores for the VASP calculation is 24, -q qprod set to production queuethe type of queue in HPC facilities, -a OPEN-00-00 is the project identification number for running jobs in HPC facilities and -f /scratch/example_mag is the folder where you want to run VASP calculations. This procedure might be helpful for high-throughput routines. More options can be added in these script files through the terminal command line, to see them just type

python3 maelas.py –h

HOW TO USE MAELAS CODE

Step 3: Run VASP calculations

For each generated POSCAR_A_B one should run first a collinear calculation using INCAR_std and use the generated WAVECAR and CHGCAR files to run non-collinear calculations for each INCAR_A_C (C=1,2) using the same POSCAR_A_B. This procedure can be automatically done in HPC facilities just by running the generated bash script

```
./vasp_maelas
```

This will launch independent jobs for each POSCAR_A_B. Each job will run 3 VASP calculations: a collinear one to generate WAVECAR and CHGCAR files, and two non-collinear for INCAR_A_1 and INCAR_A_2. The jobs will be executed in subfolders P_A_B inside the folder indicated by tag -f in the step 2.

Once all jobs are finished, then one can easily get calculated non-collinear OSZICAR files (needed in step 4), by running the bash script

```
./vasp_cp_oszicar
```

it will copy these OSZICAR files and name them as OSZICAR_A_B_C (C=1,2) in the same folder where this script is executed.

HOW TO USE MAELAS CODE

Step 4: Derivation of spin-dependent magnetostriction coefficients and magnetoelastic constants

Finally, to derive the spin-dependent magnetostriction coefficients one needs to have in the same folder the following files:

maelas.py
POSCAR_rlx (the relaxed POSCAR file used as input in step 2)
POSCAR_A_B (distorted POSCAR generated in step 2)
OSZICAR_A_B_C (non-collinear OSZICAR files calculated in step 3 for each POSCAR_A_B and INCAR_A_C)

Next, in the terminal go to this folder a type

python3 maelas.py -d -i POSCAR_rlx -n 7

where -d indicates that you want to derive the spin-dependent magnetostriction coefficients from the calculated OSZICAR files, -i POSCAR_rlx is the relaxed POSCAR file used as input in step 2 (you can name it whatever you want) and -n 7 is the number of distorted states for each magentostriction mode used in step 2.

It will derive and print the calculated spin-dependent magnetostriction coefficients in the terminal. If you want to print it in a file (for example, "results.out"), then you can type

python3 maelas.py -d -i POSCAR_rlx -n 7 > results.out

Additionally, the energy values extracted from OSZICAR_A_B_C files are shown in generated files ene_A_C.dat and fit_ene_A_C.png. The energy difference between the two spin configurations for each magnetostriction mode are shown in Fig. dE_A.png. If the elastic tensor is provided as input, then MAELAS can also calculate the magnetoelastic constants. To do so, one needs to add tags -b and -e with the name of the file containing the elastic tensor with the same format and units (GPa) as it is written by AELAS code (file ELADAT). Hence, you could type

python3 maelas.py -d -i POSCAR_rlx -n 7 -b -e ELADAT

Format of the elastic tensor file

```
Elastic tensor:

262.03  186.20  186.20    0.00    0.00    0.00
186.20  262.03  186.20    0.00    0.00    0.00
186.20  186.20  262.03    0.00    0.00    0.00
  0.00    0.00    0.00  116.63    0.00    0.00
  0.00    0.00    0.00    0.00  116.63    0.00
  0.00    0.00    0.00    0.00    0.00  116.63
```

where ELADAT is the name of the file (it could be whatever name you want) with the elastic tensor data.

HOW TO USE MAELAS CODE

Full list of arguments in MAELAS code

User can see all possible optional arguments by typing

python3 maelas.py -h

The optional arguments are the following:

-h, --help	Show this help message and exit
-i POS	Name of the initial non-distorted POSCAR file (default: POSCAR)
-n NDIST	Number of distorted states for each magnetostriction mode (default: 7)
-s STRAIN	Maximum strain to generate the distorted POSCAR files (default: 0.01)
-k KP	VASP automatic k-point mesh generation to create the KPOINTS file (default: 60)
-g	Generation of required VASP files for the calculation of magnetostriction coefficients.
-d	Derivation of magnetostriction coefficients from the energy written in the OSZICAR files.
-r	Generation of required VASP files for the cell relaxation
-b	Calculation of the magnetoelastic constants from the calculated magnetostriction coefficients and provided elastic tensor.
-e ELAS	File with the elastic tensor data in the same format and units (GPa) as it is written by ELAS code (file ELADAT).
-sp SYMPRE	Tolerance for symmetry finding (default: 0.01)
-sa SYMANG	Angle tolerance for symmetry finding (default: 5.0)
-c CORE	Number of cores for the VASP calculation (default: 24)
-t TIME	Number of maximum CPU hours for the VASP calculation (default: 48)
-f VASP_FOLD	Folder where you will run VASP calculations (default: /scratch)
-m MPI	Command for mpi run of VASP (default: mpiexec.hydra)
-a P_ID	Project id for running jobs in HPC facilities (default: OPEN-X-X)
-l LOAD_MODULE	Module of VASP that should be loaded (default: VASP/5.4.4-intel-2017c-mkl=cluster)
-q QUEUE	Type of queue to be used for VASP calculations in HPC facilities (default: qprod)

HOW TO USE MAELAS CODE

Summary: In a nutshell

Step 1: Cell relaxation

python3 maelas.py -r -i POSCAR0 -k 40

qsub vasp_jsub_rlx

Step 2: Generate VASP inputs for calculation of magnetostriction coefficients

python3 maelas.py -g -i POSCAR_rlx -k 70 -n 7 -s 0.1

Step 3: Run VASP calculations

./vasp_maelas

./vasp_cp_oszicar

Step 4: Derivation of spin-dependent magnetostriction coefficients

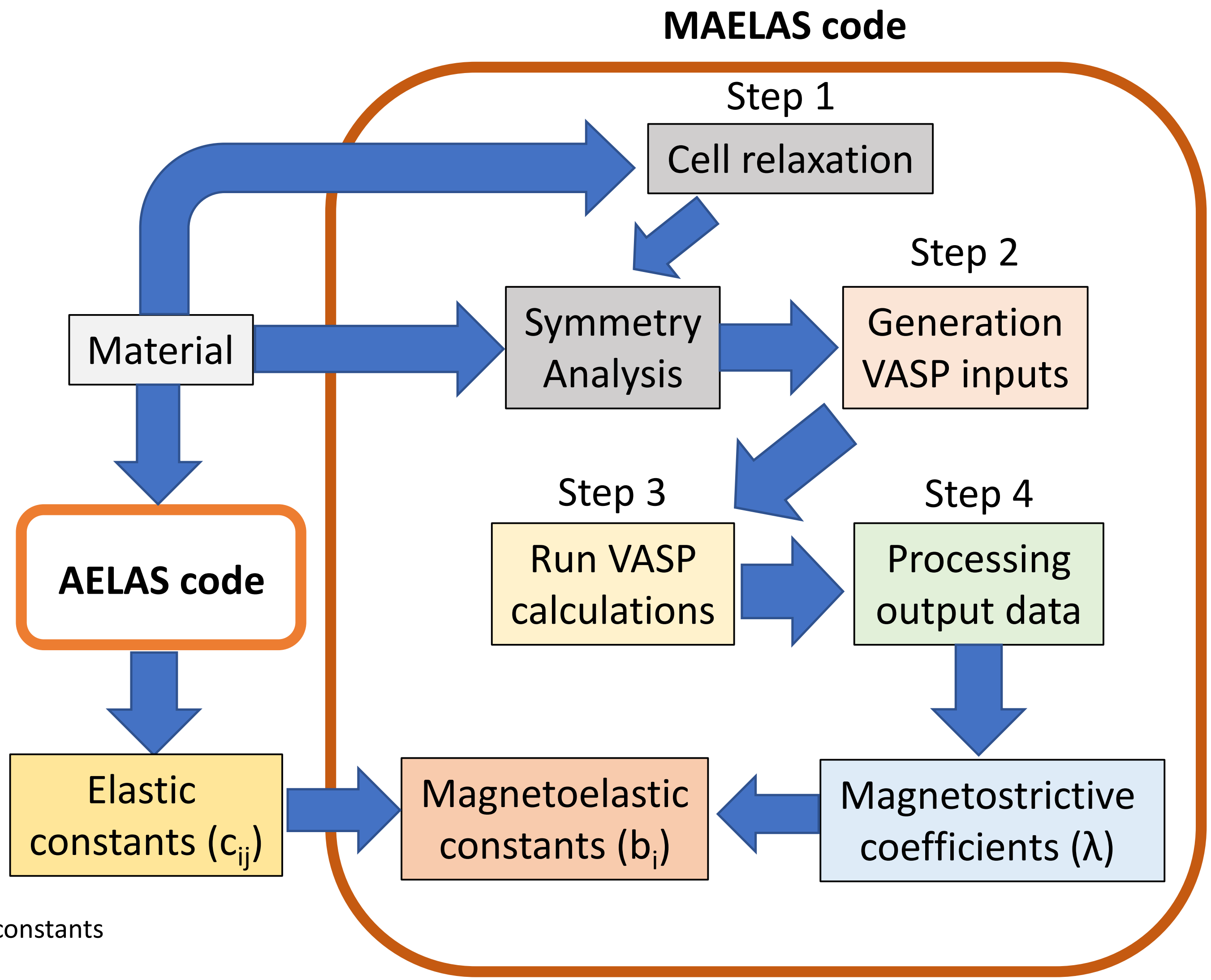
python3 maelas.py -d -i POSCAR_rlx -n 7

Step 4: Derivation of spin-dependent magnetostriction coefficients and magnetoelastic constants

python3 maelas.py -d -i POSCAR_rlx -n 7 -b -e ELADAT

See all optional arguments:

python3 maelas.py -h



Using MAELAS with other DFT codes instead of VASP

MAELAS has been designed to read and write files for VASP code automatically. However, it is possible to use MAELAS with other DFT codes instead of VASP, after file conversion to VASP format files. Although, this process might require some extra work for the user. Namely, converting initial and distorted POSCAR files into the other DFT code format, reading the spin direction of each state from INCAR_A_C files (variable SAXIS) and write the calculated energies in a OSZICAR-like file (called OSZICAR_A_B_C) on the penultimate line and third column with same format as in VASP (this is the place where MAELAS reads the energy value of each OSZICAR_A_B_C file). For instance, in the following OSZICAR file, one should write the energy value at "**Energy_DFT_code**":

```
       N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1    -0.219086777516E+02   -0.21909E+02    0.99185E+02******   0.709E+00
DAV:   2    -0.219092777733E+02   -0.60002E-03   -0.60002E-03******   0.452E-01
DAV:   3    -0.219092846144E+02   -0.68411E-05   -0.68405E-05******   0.485E-02
DAV:   4    -0.219092847670E+02   -0.15258E-06   -0.15274E-06******   0.641E-03
DAV:   5    -0.219092847725E+02   -0.55161E-08   -0.52995E-08******   0.117E-03
DAV:   6    **Energy_DFT_code**   -0.19827E-09   -0.11530E-09868760   0.143E-04
   1 F= -.21909285E+02 E0= -.21909330E+02  d E =0.135168E-03  mag=     0.0000     0.0000     2.5077
```

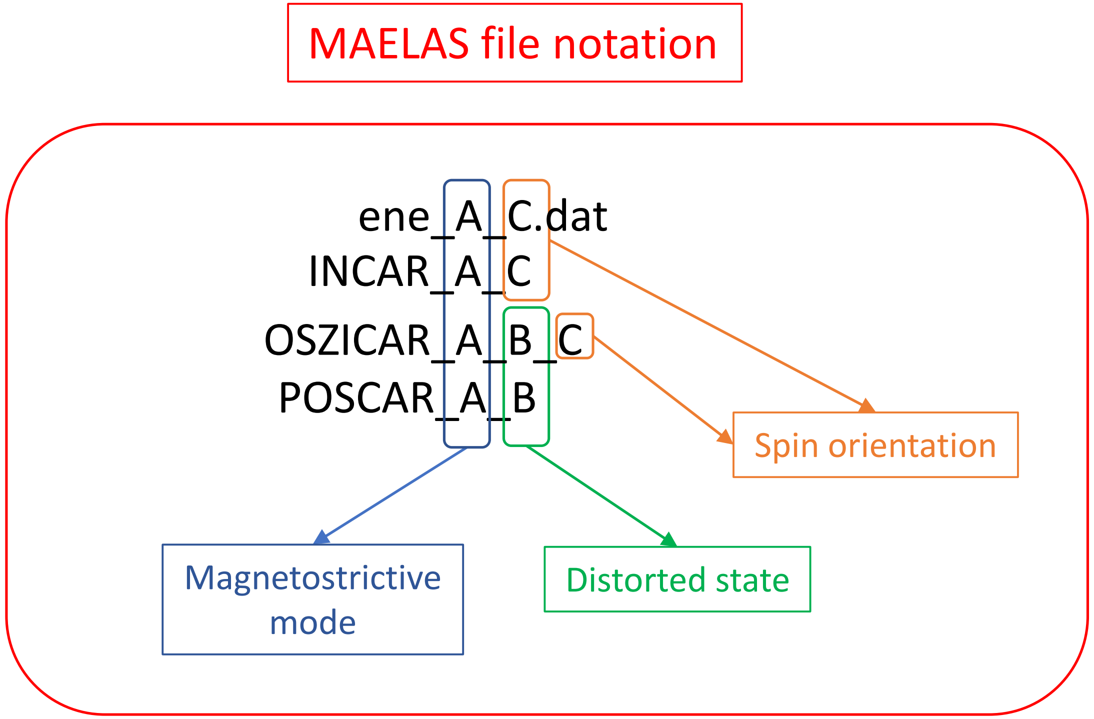
Crystal systems supported by MAELAS v1.0

Current version supports the following crystal systems:

- Cubic (I) (space groups 207-230)
- Cubic (II) (space groups 195-206)
- Hexagonal (I) (space groups 177-194)
- Hexagonal (II) point group 6/m (space groups 175-176)
- Trigonal (I) (space groups 149-167)
- Tetragonal (I) (space groups 89-142)
- Orthorhombic (space groups 16-74)

In the future, if the theoretical expressions of magnetostriction are derived for the remain crystal systems, then we will try to implement them in the new versions of the code.

HOW TO USE MAELAS CODE



Magnetostriction coefficients

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Not supported by MAELAS v1.0

System	Point groups	Basis functions[a]	Dimensionality of irreducible representation	Number of elastic constants		Number of one-ion magneto-elastic coupling constants		Number of two-ion magneto-elastic coupling constants (=number of macroscopic magneto-striction coefficients) for $l=0,2$	
Triclinic SG 1-2	$1,\bar{1}$	x^2,y^2,z^2,xy,yz,xz	1	21	21	30	30	36	36
Monoclinic SG 3-15	$2,m,2/m$	x^2,y^2,z^2,xy xz,yz	1 1	10 3	13	12 4	16	16 4	20
Orthorhombic SG 16-74	222, $mm2$, mmm	x^2,y^2,z^2 xy yz xz	1 1 1 1	6 1 1 1	9	6 1 1 1	9	9 1 1 1	12
Tetragonal SG 75-88	$4,\bar{4}$, $4/m$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $\frac{1}{2}(x^2-y^2)$, xy $\{yz,xz\}$	1 1 {1 complex {1 complex	3 3 1	7	3 4 2	9	4 4 2	10
SG 89-142	422, $4/mmm$, $4mm$, $\bar{4}2m$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $\frac{1}{2}(x^2-y^2)$ xy $[yz,xz]$	1 1 1 2	3 1 1 1	6	3 1 1 1	6	4 1 1 1	7
Trigonal SG 143-148	$3,\bar{3}$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $\{(x^2-y^2)/2,xy\}$, $\{yz,xz\}$	1 {1 complex {1 complex	3 4	7	3 8	11	4 8	12
SG 149-167	$32,3m$, $\bar{3}m$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $[(x^2-y^2)/2,xy]$, $[yz,xz]$	1 2	3 3	6	3 4	7	4 4	8
Hexagonal SG 168-174 SG 175-176	$6,\bar{6}$, $6/m$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $\{xy,xz\}$ $\{(x^2-y^2)/2,xy\}$	1 {1 complex {1 complex {1 complex {1 complex	3 1 1	5	3 2 2	7	4 2 2	8
SG 177-194	622, $6mm$, $\bar{6}m2$, $6/mmm$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $[yz,xz]$ $[(x^2-y^2)/2,xy]$	1 2 2	3 1 1	5	3 1 1	5	4 1 1	6
Cubic SG 195-206	23, $m3$	$x^2+y^2+z^2$ $\{(x^2-y^2)/2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)\}$ $[xy,yz,xz]$	1 {1 complex {1 complex 3	1 1 1	3	0 2 1	3	1 2 1	4
SG 207-230	432, $\bar{4}3m$, $m3m$	$x^2+y^2+z^2$ $(x^2-y^2)/2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $[xy,yz,xz]$	1 2 3	1 1 1	3	0 1 1	2	1 1 1	3

$$
\begin{aligned}
\lambda=&\lambda_1[\alpha_1^2\beta_1^2-\alpha_1\alpha_2\beta_1\beta_2-\alpha_1\alpha_3\beta_1\beta_3]\\
&+\lambda_2[\alpha_2^2\beta_1^2-\alpha_1\alpha_2\beta_1\beta_2]+\lambda_3[\alpha_1^2\beta_3^2-\alpha_1\alpha_2\beta_1\beta_2]\\
&+\lambda_4[\alpha_2^2\beta_2^2-\alpha_1\alpha_2\beta_1\beta_2-\alpha_2\alpha_3\beta_2\beta_3]+\lambda_5[\alpha_1^2\beta_3^2\\
&-\alpha_1\alpha_3\beta_1\beta_3]+\lambda_6[\alpha_2^2\beta_3^2-\alpha_2\alpha_3\beta_2\beta_3]+4\lambda_7(\alpha_1\alpha_2\beta_1\beta_2)\\
&+4\lambda_8\alpha_1\alpha_3\beta_1\beta_3+4\lambda_9\alpha_2\alpha_3\beta_2\beta_3,
\end{aligned}
$$

$$
\begin{aligned}
\left.\frac{\Delta l}{l}\right|_{\text{tetragonal}} =& \lambda^{\alpha 1,0}(\beta_x^2+\beta_y^2)+\lambda^{\alpha 2,0}\beta_z^2+\\
&+\lambda^{\alpha 1,2}(\alpha_z^2-1/3)(\beta_x^2+\beta_y^2)+\\
&+\lambda^{\alpha 2,2}(\alpha_z^2-1/3)\beta_z^2+\\
&+\tfrac{1}{2}\lambda^{\gamma,2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2)+\\
&+2\lambda^{\delta,2}\alpha_x\alpha_y\beta_x\beta_y+\\
&+2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z+\alpha_y\alpha_z\beta_y\beta_z) \qquad (16\text{-}34)
\end{aligned}
$$

$$
\begin{aligned}
\left.\frac{\Delta l}{l}\right|_{\text{trigonal}} =&\\
=&(\beta_x^2+\beta_y^2)\cdot[\lambda^{\alpha 1,0}+\lambda^{\alpha 1,2}(\alpha_z^2-1/3)]+\\
&+\beta_z^2[\lambda^{\alpha 2,0}+\lambda^{\alpha 2,2}(\alpha_z^2-1/3)]+\\
&+\lambda^{\gamma 1}[\tfrac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2)+2\alpha_x\alpha_y\beta_x\beta_y]+\\
&+\lambda^{\gamma 2}[\alpha_x\alpha_z\beta_x\beta_z+\alpha_y\alpha_z\beta_y\beta_z]+\\
&+\lambda_{12}[\tfrac{1}{2}\alpha_y\alpha_z(\beta_x^2-\beta_y^2)+\alpha_x\alpha_z\beta_x\beta_y]+\\
&+\lambda_{21}[\tfrac{1}{2}(\alpha_x^2-\alpha_y^2)\beta_y\beta_z+\alpha_x\alpha_y\beta_x\beta_z] \qquad (16\text{-}40)
\end{aligned}
$$

$$
\left.\frac{\Delta l}{l}\right|_{\text{b/m}}=\left.\frac{\Delta l}{l}\right|_{\text{Hex}}+\bar{\lambda}(\alpha_x\alpha_z\beta_y\beta_z-\alpha_y\alpha_z\beta_x\beta_z) \qquad (16\text{-}31)
$$

$$
\begin{aligned}
\Delta l/l|_{\text{hex}} =& \lambda^{\alpha 1,0}(\beta_x^2+\beta_y^2)+\lambda^{\alpha 2,0}\beta_z^2\\
&+\lambda^{\alpha 1,2}(\alpha_z^2-\tfrac{1}{3})(\beta_x^2+\beta_y^2)+\lambda^{\alpha 2,2}(\alpha_z^2-\tfrac{1}{3})\beta_z^2\\
&+\lambda^{\gamma,2}[\tfrac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2)+2\alpha_x\alpha_y\beta_x\beta_y]\\
&+2\lambda^{\epsilon,2}[\alpha_y\alpha_z\beta_y\beta_z+\alpha_z\alpha_x\beta_z\beta_x]
\end{aligned}
$$

$$
\begin{aligned}
\delta l/l=&\tfrac{1}{3}\lambda^{\alpha}+\tfrac{1}{2}\lambda_1^{\gamma}[3(\alpha_z^2-\tfrac{1}{3})(\beta_z^2-\tfrac{1}{3})+(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2)]\\
&+(\sqrt{3}/2)\lambda_2^{\gamma}[(\alpha_x^2-\alpha_y^2)(\beta_z^2-\tfrac{1}{3})-(\alpha_z^2-\tfrac{1}{3})(\beta_x^2-\beta_y^2)]\\
&+2\lambda^{\epsilon}[\alpha_x\alpha_y\beta_x\beta_y+\alpha_y\alpha_z\beta_y\beta_z+\alpha_x\alpha_z\beta_x\beta_z]
\end{aligned}
$$

$$
\begin{aligned}
\left.\frac{\Delta l}{l}\right|_{\text{cubic}} =&\lambda^{\alpha}+\frac{3}{2}\lambda_{100}\left(\alpha_x^2\beta_x^2+\alpha_y^2\beta_y^2+\alpha_z^2\beta_z^2-1/3\right)\\
&+3\lambda_{111}\left(\alpha_x\alpha_y\beta_x\beta_y+\alpha_y\alpha_z\beta_y\beta_z+\alpha_x\alpha_z\beta_x\beta_z\right)
\end{aligned}
$$

Elastic constants

Not supported by MAELAS v1.0

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	Crystal system	Laue class	Point groups	C_{ij}'s
SG 1-2	Triclinic	$\bar{1}$	$1, \bar{1}$	21
SG 3-15	Monoclinic	$2/m$	$2, m, 2/m$	13
SG 16-74	Orthorhombic	mmm	$222, 2mm, mmm$	9
SG 75-88	Tetragonal (II)	$4/m$	$4, \bar{4}, 4/m$	7
SG 89-142	Tetragonal (I)	$4/mmm$	$4mm, 422, \bar{4}2m, 4/mmm$	6
SG 143-148	Rhombohedral (II)	$\bar{3}$	$3, \bar{3}$	7
SG 149-167	Rhombohedral (I)	$\bar{3}m$	$32, 3m, \bar{3}m$	6
SG 168-176	Hexagonal (II)	$6/m$	$6, \bar{6}, 6/m$	5
SG 177-194	Hexagonal (I)	$6/mmm$	$6mm, 622, \bar{6}2m, 6/mmm$	5
SG 195-206	Cubic (II)	$m\bar{3}$	$23, m\bar{3}$	3
SG 207-230	Cubic (I)	$m\bar{3}m$	$432, \bar{4}3m, m\bar{3}m$	3

$$E = E_0 + \frac{1}{2} V_0 \sum_{i,j=1}^{6} C_{ij}\varepsilon_i\varepsilon_j + O(\varepsilon^3)$$

$$C_{tric} = \begin{vmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ & & c_{33} & c_{34} & c_{35} & c_{36} \\ & & & c_{44} & c_{45} & c_{46} \\ & & & & c_{55} & c_{56} \\ & & & & & c_{66} \end{vmatrix}$$

$$C_{mono} = \begin{vmatrix} c_{11} & c_{12} & c_{13} & 0 & c_{15} & 0 \\ & c_{22} & c_{23} & 0 & c_{25} & 0 \\ & & c_{33} & 0 & c_{35} & 0 \\ & & & c_{44} & 0 & c_{46} \\ & & & & c_{55} & 0 \\ & & & & & c_{66} \end{vmatrix}$$

$$C_{\mathrm{ortho}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & & & \\ \cdot & C_{22} & C_{23} & & & \\ \cdot & \cdot & C_{33} & & & \\ & & & C_{44} & & \\ & & & & C_{55} & \\ & & & & & C_{66} \end{pmatrix}$$

$$C_{\mathrm{tetra\ II}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & & & C_{16} \\ \cdot & C_{11} & C_{13} & & & -C_{16} \\ \cdot & \cdot & C_{33} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ \cdot & \cdot & & & & C_{66} \end{pmatrix}$$

$$C_{\mathrm{rhombo\ II}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & \\ \cdot & C_{11} & C_{13} & -C_{14} & -C_{15} & \\ \cdot & \cdot & C_{33} & & & \\ \cdot & \cdot & & C_{44} & & -C_{15} \\ \cdot & \cdot & & & C_{44} & C_{14} \\ & & & \cdot & \cdot & C_{66} \end{pmatrix}$$

$$C_{\mathrm{rhombo\ I}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & & \\ \cdot & C_{11} & C_{13} & -C_{14} & & \\ \cdot & \cdot & C_{33} & & & \\ \cdot & \cdot & & C_{44} & & \\ & & & & C_{44} & C_{14} \\ & & & & \cdot & C_{66} \end{pmatrix}$$

$$C_{\mathrm{hexa/tetra\ I}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & & & \\ \cdot & C_{11} & C_{13} & & & \\ \cdot & \cdot & C_{33} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{66} \end{pmatrix}.$$

$$C_{\mathrm{cubic}} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & & & \\ \cdot & C_{11} & C_{12} & & & \\ \cdot & \cdot & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{pmatrix}$$

Workflow

CUBIC (I)

SG 207-230

Workflow

Cubic (I)

J. R. Cullen, A. E. Clark, and K. B. Hathaway, in Materials, Science and Technology (VCH Publishings, 1994), pp. 529 – 565.

Elastic energy

$$E_{el}|_{cubic} = \tfrac{1}{2} C_{11} (\varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{zz}^2) + $$
$$+ C_{12} (\varepsilon_{xx}\varepsilon_{yy} + \varepsilon_{xx}\varepsilon_{zz} + \varepsilon_{yy}\varepsilon_{zz}) + $$
$$+ \tfrac{1}{2} C_{44} (\varepsilon_{xy}^2 + \varepsilon_{xz}^2 + \varepsilon_{yz}^2) \qquad (16\text{-}15)$$

Magnetoelastic energy

$$E_{me}|_{cubic} = b_0 (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \qquad (16\text{-}14)$$
$$+ b_1 (\alpha_x^2 \varepsilon_{xx} + \alpha_y^2 \varepsilon_{yy} + \alpha_z^2 \varepsilon_{zz}) + $$
$$+ b_2 (\alpha_x \alpha_y \varepsilon_{xy} + \alpha_x \alpha_z \varepsilon_{xz} + \alpha_y \alpha_z \varepsilon_{yz})$$

$$\frac{\Delta l}{l} = \sum_{i,j} \varepsilon_{i,j} \beta_i \beta_j$$

$$\frac{\partial}{\partial \varepsilon_{ij}} (E_{el} + E_{me}) = 0$$

$$\frac{\Delta l}{l} = \frac{3}{2} \lambda_{100} \left(\alpha_x^2 \beta_x^2 + \alpha_y^2 \beta_y^2 + \alpha_z^2 \beta_z^2 - \frac{1}{3} \right) + $$
$$+ 3 \lambda_{111} (\alpha_x \alpha_y \beta_x \beta_y + \alpha_x \alpha_z \beta_x \beta_z + $$
$$+ \alpha_y \alpha_z \beta_y \beta_z) \qquad (16\text{-}6)$$

$$\lambda_{100} = -\frac{2 b_1}{3(C_{11} - C_{12})}$$

$$\lambda_{111} = -\frac{b_2}{3 C_{44}}$$

Workflow

$$\frac{\Delta l}{l} = \frac{3}{2}\lambda_{100}\left(\alpha_x^2\beta_x^2 + \alpha_y^2\beta_y^2 + \alpha_z^2\beta_z^2 - \frac{1}{3}\right) + \\ + 3\lambda_{111}(\alpha_x\alpha_y\beta_x\beta_y + \alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z)$$

POSCAR

Symmetry analysis

Space group: 207-230

Cubic (I)

λ_{001}

POSCAR_1_X (N POSCAR: Distortion along [0,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_1_1 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
INCAR_1_2 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])

OSZICAR_1_X_1

OSZICAR_1_X_2

λ_{111}

POSCAR_2_X (N POSCAR: Distortion along [1,1,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_2_1 (1 INCAR: non-collinear with SOC, SPIN=[1,1,1])
INCAR_2_2 (1 INCAR: non-collinear with SOC, SPIN=[1,0,-1])

OSZICAR_2_X_1

OSZICAR_2_X_2

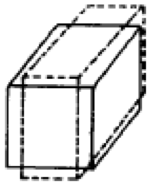
x=cell length along deformation

Fitting: $E(x)=a*x^2+b*x+c$
Minimum (E_{min}): $x_{min}=-b/(2*a)$

$$\lambda_{\substack{001\\111}} = \frac{2}{3}\cdot\frac{x_{min1}-x_{min2}}{x_{min1}}$$

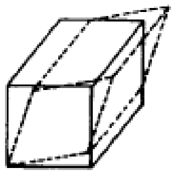
Polycrystal: $\lambda_S = \frac{2}{5}\lambda_{100} + \frac{3}{5}\lambda_{111}$

Volume-conserving transformations (determinant of transformation matrix = 1)



λ^{γ}

$$\begin{pmatrix} \frac{1}{\sqrt{1+\epsilon_z}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\epsilon_z}} & 0 \\ 0 & 0 & 1+\epsilon_z \end{pmatrix}$$



λ^{ϵ}

$$d\begin{pmatrix} 1 & \epsilon & \epsilon \\ \epsilon & 1 & \epsilon \\ \epsilon & \epsilon & 1 \end{pmatrix}$$

Workflow

CUBIC (II)

SG 195-206

Workflow

Cubic (II)

Elastic energy

$$E_{el}|_{cubic} = \tfrac{1}{2} C_{11}(\varepsilon_{xx}^2 + \varepsilon_{yy}^2 + \varepsilon_{zz}^2) + + C_{12}(\varepsilon_{xx}\varepsilon_{yy} + \varepsilon_{xx}\varepsilon_{zz} + \varepsilon_{yy}\varepsilon_{zz}) + + \tfrac{1}{2} C_{44}(\varepsilon_{xy}^2 + \varepsilon_{xz}^2 + \varepsilon_{yz}^2) \qquad (16\text{-}15)$$

$$\frac{\Delta l}{l} = \sum_{i,j} \varepsilon_{i,j}\beta_i\beta_j$$

$$\frac{\partial}{\partial \varepsilon_{ij}}(E_{el} + E_{me}) = 0$$

Magnetoelastic energy

$$E_{me}^{cub(II)} = b_0(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}) + [b_1(1-\alpha_x^2) + b_2(\alpha_z^2-\alpha_y^2)]\varepsilon_{xx} + [b_1(1-\alpha_y^2) + b_2(\alpha_x^2-\alpha_z^2)]\varepsilon_{yy} + [b_1(1-\alpha_z^2) + b_2(\alpha_y^2-\alpha_x^2)]\varepsilon_{zz} + b_3(\alpha_x\alpha_y\varepsilon_{xy} + \alpha_x\alpha_z\varepsilon_{xz} + \alpha_y\alpha_z\varepsilon_{yz})$$

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$$\delta l/l = \tfrac{1}{3}\lambda^{\alpha} + \tfrac{1}{2}\lambda_1{}^{\gamma}[3(\alpha_z{}^2-\tfrac{1}{3})(\beta_z{}^2-\tfrac{1}{3}) + (\alpha_x{}^2-\alpha_y{}^2)(\beta_x{}^2-\beta_y{}^2)] + (\sqrt{3}/2)\lambda_2{}^{\gamma}[(\alpha_x{}^2-\alpha_y{}^2)(\beta_z{}^2-\tfrac{1}{3}) - (\alpha_z{}^2-\tfrac{1}{3})(\beta_x{}^2-\beta_y{}^2)] + 2\lambda^{\epsilon}[\alpha_x\alpha_y\beta_x\beta_y + \alpha_y\alpha_z\beta_y\beta_z + \alpha_x\alpha_z\beta_x\beta_z]$$

$$b_0 = \frac{2}{3}(c_{12}-c_{11})\lambda_1^{\gamma} - \frac{1}{3}(2c_{12}+c_{11})\lambda^{\alpha}$$

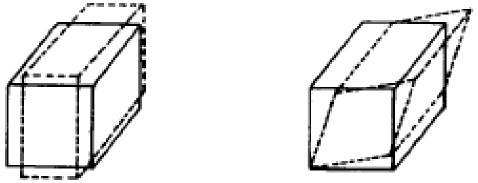
$$b_1 = (c_{11}-c_{12})\lambda_1^{\gamma}$$

$$b_2 = \frac{1}{\sqrt{3}}(c_{11}-c_{12})\lambda_2^{\gamma}$$

$$b_3 = -2c_{44}\lambda^{\epsilon}$$

Workflow

$$\delta l/l = \tfrac{1}{3}\lambda^{\alpha} + \tfrac{1}{2}\lambda_1^{\gamma}\left[3(\alpha_z^2 - \tfrac{1}{3})(\beta_z^2 - \tfrac{1}{3}) + (\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2)\right]$$
$$+ (\sqrt{3}/2)\lambda_2^{\gamma}\left[(\alpha_x^2 - \alpha_y^2)(\beta_z^2 - \tfrac{1}{3}) - (\alpha_z^2 - \tfrac{1}{3})(\beta_x^2 - \beta_y^2)\right]$$
$$+ 2\lambda^{\epsilon}\left[\alpha_x\alpha_y\beta_x\beta_y + \alpha_y\alpha_z\beta_y\beta_z + \alpha_x\alpha_z\beta_x\beta_z\right]$$



λ^{γ} λ^{ε}

$$\begin{pmatrix} \frac{1}{\sqrt{1+\epsilon_z}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\epsilon_z}} & 0 \\ 0 & 0 & 1+\epsilon_z \end{pmatrix} \qquad d\begin{pmatrix} 1 & \epsilon & \epsilon \\ \epsilon & 1 & \epsilon \\ \epsilon & \epsilon & 1 \end{pmatrix}$$

POSCAR → Symmetry analysis → SG: 195-206 → Cubic (II)

Volume-conserving transformations (determinant of transformation matrix = 1)

$$D = d \cdot \begin{pmatrix} 1 & \frac{\varepsilon_{xy}}{2} & 0 \\ \frac{\varepsilon_{xy}}{2} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

λ_1^{γ}

POSCAR_1_X (N POSCAR: Distortion along [0,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_1_1 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
INCAR_1_2 (1 INCAR: non-collinear with SOC, SPIN=[1,1,0])

→ OSZICAR_1_X_1, OSZICAR_1_X_2

λ_2^{γ}

POSCAR_2_X (N POSCAR: Distortion along [1,1,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_2_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
INCAR_2_2 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])

→ OSZICAR_2_X_1, OSZICAR_2_X_2

λ^{ε}

POSCAR_3_X (N POSCAR: Distortion along [1,1,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_3_1 (1 INCAR: non-collinear with SOC, SPIN=[1,1,1])
INCAR_3_2 (1 INCAR: non-collinear with SOC, SPIN=[1,0,-1])

→ OSZICAR_3_X_1, OSZICAR_3_X_2

x=cell length along deformation

Fitting: $E(x)=a*x^2+b*x+c$
Minimum (E_{min}): $x_{min}=-b/(2*a)$

$$\lambda_1^{\gamma} = \frac{x_{min1} - x_{min2}}{x_{min1}} \qquad \lambda_2^{\gamma} = \sqrt{3}\cdot\frac{x_{min1} - x_{min2}}{x_{min1}} \qquad \lambda^{\varepsilon} = \frac{x_{min1} - x_{min2}}{x_{min1}}$$

Workflow

HEXAGONAL (I)

SG 177-194

Workflow

Hexagonal (I)

Elastic energy

$$E_{\mathrm{el}}|_{\mathrm{hex}} = \tfrac{1}{2} C_{11} (\varepsilon_{xx}^2 \, \varepsilon_{yy}^2) + C_{12} \, \varepsilon_{xx} \, \varepsilon_{yy} + \\ + \tfrac{1}{2} C_{33} \, \varepsilon_{zz}^2 + C_{13} (\varepsilon_{xx} + \varepsilon_{yy}) \, \varepsilon_{zz} + \\ + \tfrac{1}{2} C_{44} (\varepsilon_{yz}^2 + \varepsilon_{xz}^2) + \\ + \tfrac{1}{4} (C_{11} - C_{12}) \, \varepsilon_{xy}^2 \qquad (16\text{-}28)$$

J. R. Cullen, A. E. Clark, and K. B. Hathaway, in Materials, Science and Technology (VCH Publishings, 1994), pp. 529 – 565.

Magnetoelastic energy

$$E_{\mathrm{me}}|_{\mathrm{hex}} = b_{11} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12} \, \varepsilon_{zz} + \\ + b_{21} (\alpha_z^2 - \tfrac{1}{3}) (\varepsilon_{xx} + \varepsilon_{yy}) + \\ + b_{22} (\alpha_z^2 - \tfrac{1}{3}) \, \varepsilon_{zz} \\ + \tfrac{1}{2} b_3 ((\alpha_x^2 - \alpha_y^2) (\varepsilon_{xx} - \varepsilon_{yy}) + 2 \, \alpha_x \, \alpha_y \, \varepsilon_{xy}) + \\ + b_4 (\alpha_x \, \alpha_z \, \varepsilon_{xz} + \alpha_y \, \alpha_z \, \varepsilon_{yz}) \qquad (16\text{-}29)$$

$$\frac{\Delta l}{l} = \sum_{i,j} \varepsilon_{i,j} \beta_i \beta_j$$

$$\frac{\partial}{\partial \varepsilon_{ij}} (E_{\mathrm{el}} + E_{\mathrm{me}}) = 0$$

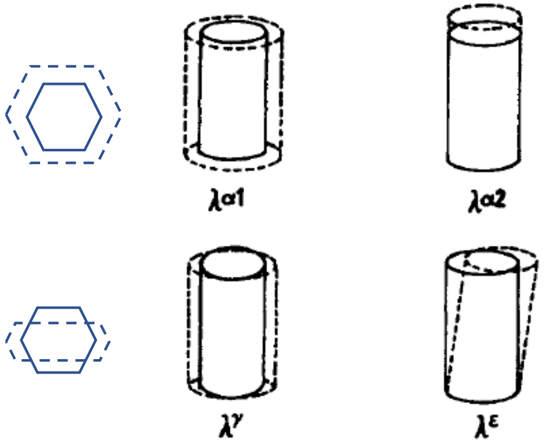
$$\left.\frac{\Delta l}{l}\right|_{\mathrm{Hex}} = \lambda^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0} + \\ + \lambda^{\alpha 1,2} (\alpha_z^2 - \tfrac{1}{3}) (\beta_x^2 + \beta_y^2) + \\ + \lambda^{\alpha 2,2} (\alpha_z^2 - \tfrac{1}{3}) \, \beta_z^2 + \\ + \lambda^{\gamma,2} (\tfrac{1}{2} (\alpha_x^2 - \alpha_y^2) (\beta_x^2 - \beta_y^2) + 2 \, \alpha_x \, \alpha_y \, \beta_x \, \beta_y) + \\ + 2\lambda^{\varepsilon,2} (\alpha_x \, \alpha_z \, \beta_x \, \beta_z + \alpha_y \, \alpha_z \, \beta_y \, \beta_z) \qquad (16\text{-}30)$$

$\lambda^{\alpha 1,0}$	$(b_{11} \, c_{33} + b_{12} \, c_{13})/D$
$\lambda^{\alpha 2,0}$	$[2 b_{11} \, c_{13} - b_{12} \, (c_{11} + c_{22})]/D$
$\lambda^{\alpha 1,2}$	$(- b_{21} \, c_{33} + b_{22} \, c_{13})/D$
$\lambda^{\alpha 2,2}$	$[2 b_{21} \, c_{13} - b_{22} \, (c_{11} + c_{12})]/D$
$\lambda^{\gamma,2}$	$- b_3/(c_{11} - c_{12})$
$\lambda^{\varepsilon,2}$	$- b_4/(2 c_{44})$

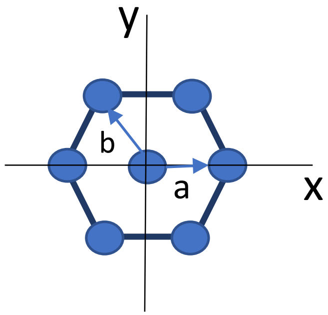
[a] $D \equiv c_{33} (c_{11} + c_{12}) - 2 c_{13}^2$.

Workflow

$$\left.\frac{\Delta l}{l}\right|_{\mathrm{Hex}} = \lambda^{\alpha 1,0}(\beta_x^2+\beta_y^2) + \lambda^{\alpha 2,0} + \lambda^{\alpha 1,2}(\alpha_z^2 - \tfrac{1}{3})(\beta_x^2+\beta_y^2) + \lambda^{\alpha 2,2}(\alpha_z^2-\tfrac{1}{3})\beta_z^2 + \lambda^{\gamma,2}\left(\tfrac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2)+2\alpha_x\alpha_y\beta_x\beta_y\right) + 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z+\alpha_y\alpha_z\beta_y\beta_z) \qquad (16\text{-}30)$$



POSCAR → Symmetry analysis → (Space group: 177-194) → Hexagonal (I)



$\lambda^{\alpha 1,2}$:
POS_1_X (N POSCAR: Distortion along [1,0,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_1_1 (1 INCAR: non-collinear with SOC, SPIN=[1,1,1])
INCAR_1_2 (1 INCAR: non-collinear with SOC, SPIN=[1,1,0])
→ OSZICAR_1_X_1, OSZICAR_1_X_2

$\lambda^{\alpha 2,2}$:
POS_2_X (N POSCAR: Distortion along [0,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_2_1 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
INCAR_2_2 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
→ OSZICAR_2_X_1, OSZICAR_2_X_2

$\lambda^{\gamma,2}$:
POS_3_X (N POSCAR: Distortion along [1,0,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_3_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
INCAR_3_2 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
→ OSZICAR_3_X_1, OSZICAR_3_X_2

$\lambda^{\varepsilon,2}$:
POS_4_X (N x POSCAR: Distortion along [1,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_4_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,1])
INCAR_4_2 (1 INCAR: non-collinear with SOC, SPIN=[-1,0,1])
→ OSZICAR_4_X_1, OSZICAR_4_X_2

Fitting: $E(x)=a*x^2+b*x+c$
Minimum (E_{min}): $x_{min}=-b/(2*a)$

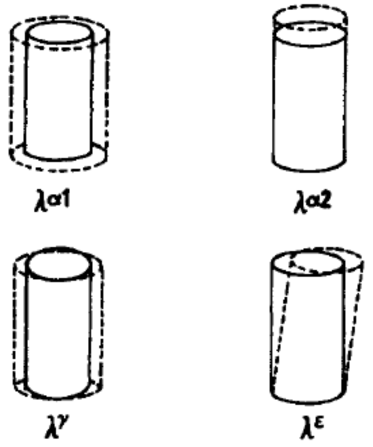
x=cell length along deformation

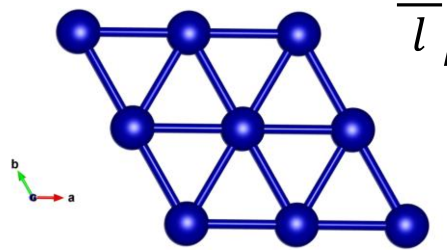
$$\lambda^{\alpha 1,2} = 3\cdot\frac{x_{min1}-x_{min2}}{x_{min1}} \qquad \lambda^{\alpha 2,2} = \frac{x_{min1}-x_{min2}}{x_{min1}} \qquad \lambda^{\gamma,2} = \frac{x_{min1}-x_{min2}}{x_{min1}} \qquad \lambda^{\varepsilon,2} = \frac{x_{min1}-x_{min2}}{x_{min1}}$$

Hexagonal

Distorted states

$$\left.\frac{\Delta l}{l}\right|_{\mathrm{Hex}} = \lambda^{\alpha 1,0}(\beta_x^2+\beta_y^2) + \lambda^{a 2,0} + \\ + \lambda^{\alpha 1,2}(\alpha_z^2 - 1/3)(\beta_x^2+\beta_y^2) + \\ + \lambda^{\alpha 2,2}(\alpha_z^2 - 1/3)\beta_z^2 + \\ + \lambda^{\gamma,2}\left(\tfrac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2) + 2\alpha_x\alpha_y\beta_x\beta_y\right) + \\ + 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z) \qquad (16\text{-}30)$$





$$\frac{\Delta l}{l}^{\alpha}_{\beta}$$

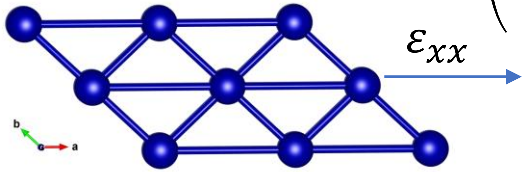
$$|\boldsymbol{\alpha}| = 1, |\boldsymbol{\beta}| = 1$$

strain along x-axis: $\beta = (1,0,0)$

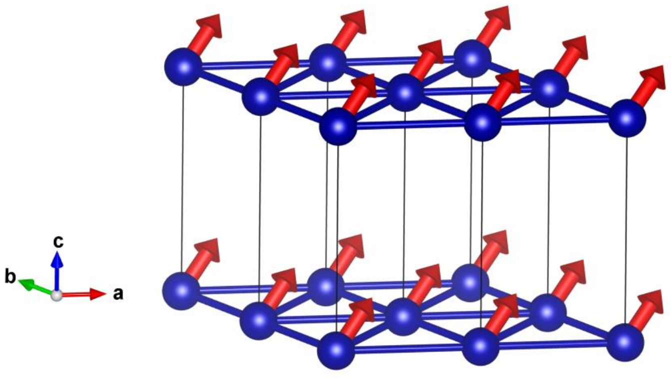
$$\frac{\Delta l}{l} = \varepsilon_{xx} = \lambda^{\alpha 1}\left(\alpha_z^2 - \frac{1}{3}\right) + \lambda^{\gamma}(\alpha_x^2 - \alpha_y^2)\,\frac{1}{2}$$

$$D=\begin{pmatrix} 1+\varepsilon_{xx} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\varepsilon_{xx}}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+\varepsilon_{xx}}} \end{pmatrix}$$

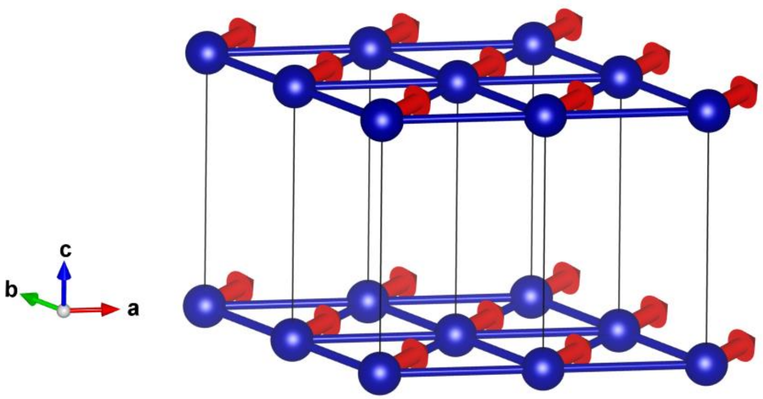
$$\boldsymbol{\lambda^{\alpha 1,2}} \Rightarrow \frac{\Delta l}{l}^{(1,1,1)}_{(1,0,0)} - \frac{\Delta l}{l}^{(1,1,0)}_{(1,0,0)} = \frac{1}{3}\cdot\lambda^{\alpha 1,2}$$



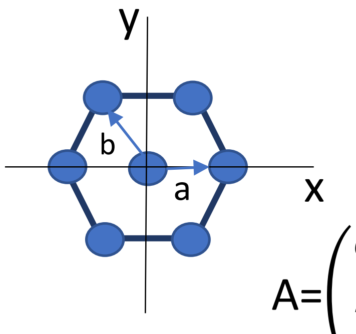
volume-conserving



S=(1,1,1)



S=(1,1,0)



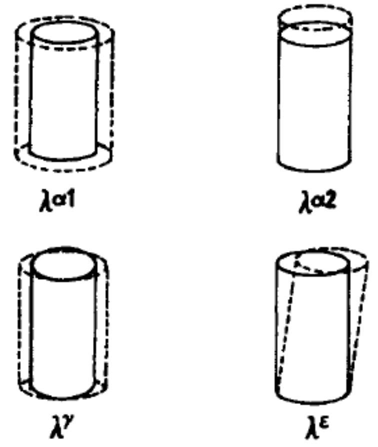
$$A=\begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

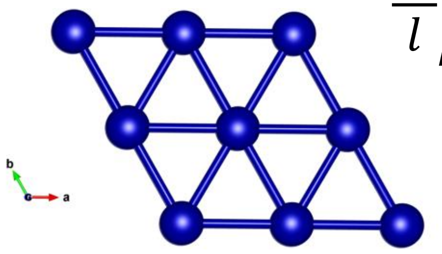
$$\lambda^{\alpha 1,2} = 3\cdot\frac{x_{min1} - x_{min2}}{x_{min1}}$$

Hexagonal

Distorted states

$$\left.\frac{\Delta l}{l}\right|_{\mathrm{Hex}} = \lambda^{\alpha1,0}(\beta_x^2+\beta_y^2) + \lambda^{\alpha2,0} +$$
$$+ \lambda^{\alpha1,2}(\alpha_z^2 - 1/3)(\beta_x^2+\beta_y^2) +$$
$$+ \lambda^{\alpha2,2}(\alpha_z^2 - 1/3)\beta_z^2 +$$
$$+ \lambda^{\gamma,2}\left(\tfrac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2) + 2\alpha_x\alpha_y\beta_x\beta_y\right) +$$
$$+ 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z) \qquad (16\text{-}30)$$



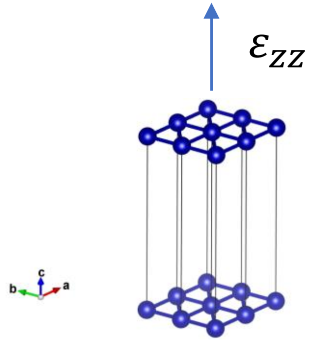


$$\frac{\Delta l^{\alpha}}{l_{\beta}}$$

$|\boldsymbol{\alpha}| = 1, |\boldsymbol{\beta}| = 1$

strain along z-axis: $\beta = (0,0,1)$

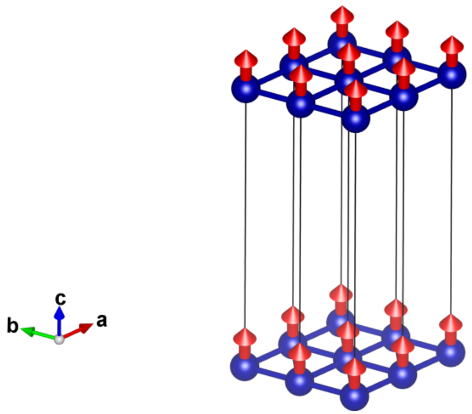
$$\frac{\Delta l}{l} = \varepsilon_{zz} = \lambda^{\alpha2}\left(\alpha_z^2 - \frac{1}{3}\right)$$



$$D=\begin{pmatrix} \frac{1}{\sqrt{1+\varepsilon_{xx}}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\varepsilon_{xx}}} & 0 \\ 0 & 0 & 1+\varepsilon_{xx} \end{pmatrix}$$

volume-conserving

$$\boldsymbol{\lambda^{\alpha2,2}} \Rightarrow \frac{\Delta l^{(0,0,1)}}{l_{(0,0,1)}} - \frac{\Delta l^{(1,0,0)}}{l_{(0,0,1)}} = \lambda^{\alpha2,2}$$



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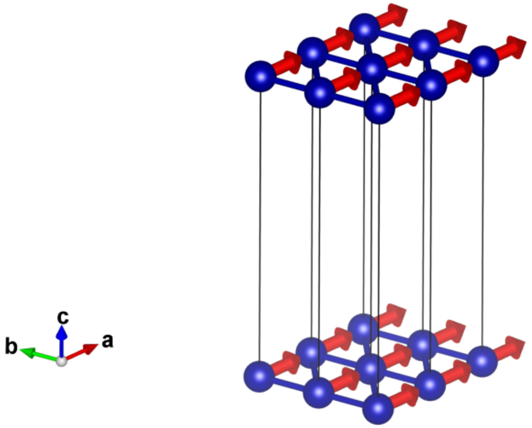
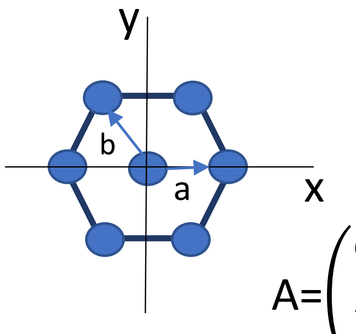


S=(1,0,0)



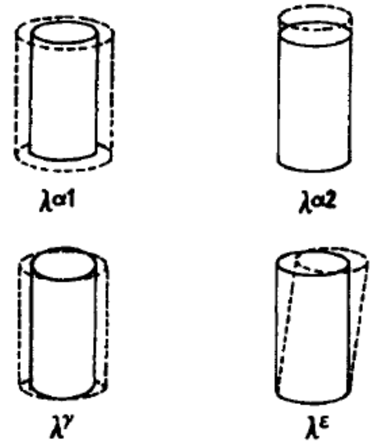
$$A=\begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

$$\lambda^{\alpha2,2} = \frac{x_{min1} - x_{min2}}{x_{min1}}$$

Hexagonal

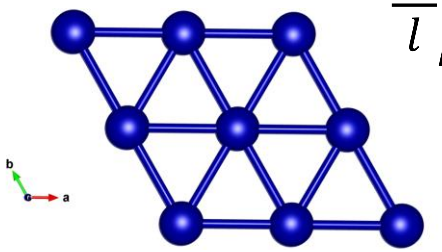
Distorted states

$$\left.\frac{\Delta l}{l}\right|_{\mathrm{Hex}} = \lambda^{\alpha 1,0}(\beta_x^2+\beta_y^2) + \lambda^{\alpha 2,0} + \lambda^{\alpha 1,2}(\alpha_z^2 - 1/3)(\beta_x^2+\beta_y^2) + \lambda^{\alpha 2,2}(\alpha_z^2 - 1/3)\beta_z^2 + \lambda^{\gamma,2}\left(\tfrac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2) + 2\alpha_x\alpha_y\beta_x\beta_y\right) + 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z) \qquad (16\text{-}30)$$



$$\frac{\Delta l^{\alpha}}{l}_{\beta}$$

$$|\boldsymbol{\alpha}| = 1, |\boldsymbol{\beta}| = 1$$

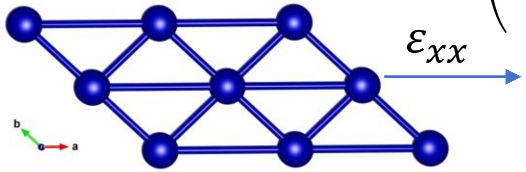


strain along x-axis: $\beta = (1,0,0)$

$$\frac{\Delta l}{l} = \varepsilon_{xx} = \lambda^{\alpha 1}\left(\alpha_z^2 - \frac{1}{3}\right) + \lambda^{\gamma}(\alpha_x^2 - \alpha_y^2)\,\frac{1}{2}$$

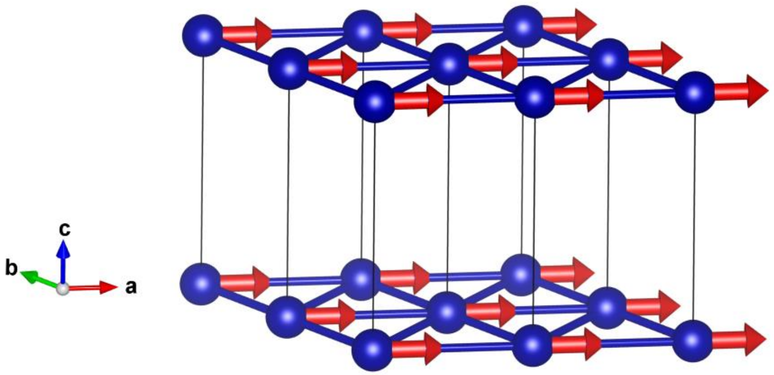
$$D=\begin{pmatrix} 1+\varepsilon_{xx} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\varepsilon_{xx}}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+\varepsilon_{xx}}} \end{pmatrix}$$

$$\lambda^{\gamma,2} \Rightarrow \frac{\Delta l^{(1,0,0)}}{l}_{(1,0,0)} - \frac{\Delta l^{(0,1,0)}}{l}_{(1,0,0)} = \lambda^{\gamma,2}$$

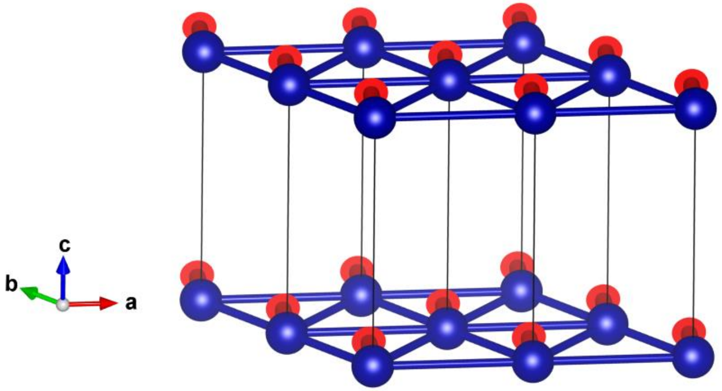


ε_{xx}

volume-conserving



S=(1,0,0)



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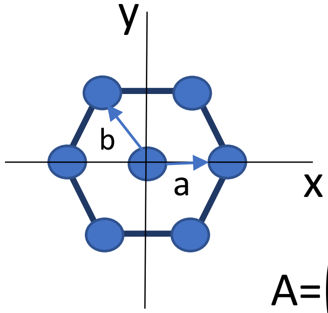
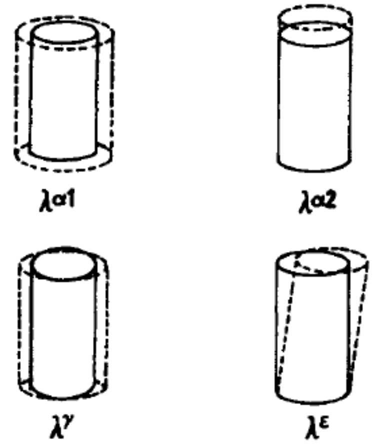


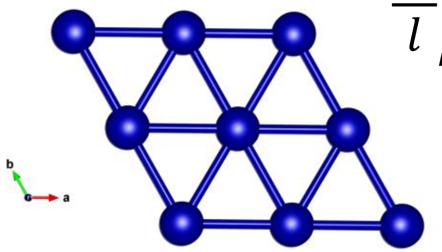
$$A=\begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

$$\lambda^{\gamma,2} = \frac{x_{min1} - x_{min2}}{x_{min1}}$$

Hexagonal

Distorted states





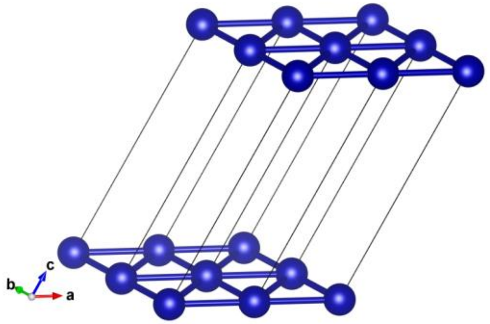
$$\frac{\Delta l^{\alpha}}{l}_{\beta} \qquad |\boldsymbol{\alpha}| = 1, |\boldsymbol{\beta}| = 1$$

shear along xz: $\beta = (1,0,1)$

$$\left.\frac{\Delta l}{l}\right|_{\mathrm{Hex}} = \lambda^{\alpha 1,0}(\beta_x^2+\beta_y^2) + \lambda^{a 2,0} + \\ + \lambda^{\alpha 1,2}(\alpha_z^2 - 1/3)(\beta_x^2+\beta_y^2) + \\ + \lambda^{\alpha 2,2}(\alpha_z^2 - 1/3)\beta_z^2 + \\ + \lambda^{\gamma,2}\left(\tfrac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2) + 2\alpha_x\alpha_y\beta_x\beta_y\right) + \\ + 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z) \qquad (16\text{-}30)$$

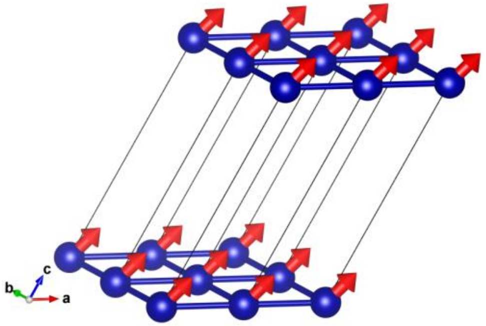
$$\boldsymbol{\lambda^{\varepsilon,2}} \Rightarrow \frac{\Delta l^{(1,0,1)}}{l}_{(1,0,1)} - \frac{\Delta l^{(-1,0,1)}}{l}_{(1,0,1)} = \lambda^{\varepsilon,2}$$

ε_{xz}

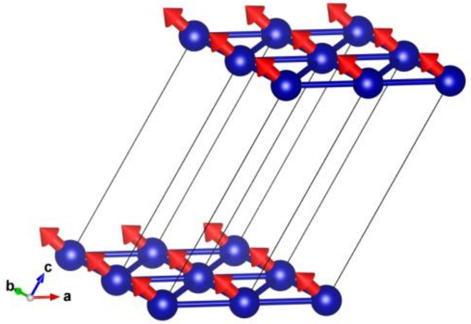


$$\mathrm{D} = \mathrm{d}\cdot\begin{pmatrix} 1 & 0 & \frac{\varepsilon_{xz}}{2} \\ 0 & 1 & 0 \\ \frac{\varepsilon_{xz}}{2} & 0 & 1 \end{pmatrix}$$

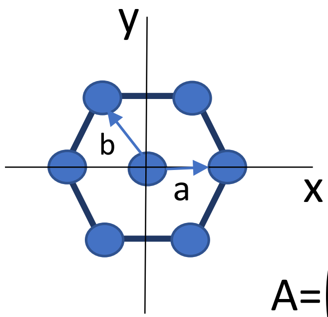
volume-conserving



S=(1,0,1)



S=(-1,0,1)



$$\mathrm{A}=\begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

$$\lambda^{\varepsilon,2} = \frac{x_{min1} - x_{min2}}{x_{min1}}$$

Relation between different notations

Clark

PHYSICAL REVIEW
VOLUME 138, NUMBER 1A
5 APRIL 1965

Hexagonal system

Gauge direction			Magnetization direction Initial			Final				Magnetostriction coefficients		
β_x	β_y	β_z	α_x	α_y	α_z	α_x	α_y	α_z	$\lambda(x,y)_0-\lambda(x,y)_f$	Eq. (3)	Mason[a]	Birss[b]
1	0	0	1	0	0	0	1	0	$\lambda(a,a)-\lambda(b,a)$	$\lambda^{\gamma,2}$	$\lambda_A-\lambda_B$	Q_8
0	0	1	0	0	1	1	0	0	$\lambda(c,c)-\lambda(a,c)$	$\lambda_2^{\alpha,2}$	$-\lambda_C$	$-Q_2-Q_4$
1	0	0	1	0	0	0	0	1	$\lambda(a,a)-\lambda(c,a)$	$-\lambda_1^{\alpha,2}+\frac{1}{2}\lambda^{\gamma,2}$	λ_A	$-Q_2$
$\frac{\sqrt{2}}{2}$	0	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	0	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	0	$\frac{\sqrt{2}}{2}$	$\lambda(d,d)-\lambda(e,d)$	$\lambda^{\epsilon,2}$	$-\frac{1}{2}\lambda_A-\frac{1}{2}\lambda_C+2\lambda_D$	$\frac{1}{2}Q_6$

[a] W. P. Mason, Phys. Rev. **96**, 302 (1954).
[b] R. R. Birss, *Advances in Physics* (Francis & Taylor, Ltd., London, 1959), Vol. 8, p. 252.

MAELAS notation

PHYSICAL REVIEW
VOLUME 139, NUMBER 2A
19 JULY 1965

Callen

$$\lambda_{11}^{\alpha}=2\lambda_1^{\alpha,0}+\lambda_2^{\alpha,0}+2\lambda_1^{\alpha,2}+\lambda_2^{\alpha,2}$$

$$(\sqrt{3}/2)\lambda_{12}^{\alpha}=2\lambda_1^{\alpha,2}+\lambda_2^{\alpha,2},$$

$$2\lambda_{21}^{\alpha}=-\lambda_1^{\alpha,0}+\lambda_2^{\alpha,0},$$

$$\sqrt{3}\lambda_{22}^{\alpha}=-\lambda_1^{\alpha,2}+\lambda_2^{\alpha,2}.$$

$$\lambda^{\epsilon}=\lambda^{\epsilon,2}$$

$$\lambda^{\gamma}=\lambda^{\gamma,2}$$

The calculated magnetostriction coefficients are written in Clark, Mason, Birss and Callen notation in MAELAS code

HEXAGONAL (II) – point group 6/m

SG 175-176

Workflow

Hexagonal (II) - point group 6/m

J. R. Cullen, A. E. Clark, and K. B. Hathaway, in Materials, Science and Technology (VCH Publishings, 1994), pp. 529 – 565.

Elastic energy

$$\begin{aligned} E_{\mathrm{el}}|_{\mathrm{hex}} = {} & \tfrac{1}{2} C_{11} (\varepsilon_{xx}^2\, \varepsilon_{yy}^2) + C_{12}\, \varepsilon_{xx}\, \varepsilon_{yy} + \\ & + \tfrac{1}{2} C_{33}\, \varepsilon_{zz}^2 + C_{13} (\varepsilon_{xx} + \varepsilon_{yy})\, \varepsilon_{zz} + \\ & + \tfrac{1}{2} C_{44} (\varepsilon_{yz}^2 + \varepsilon_{xz}^2) + \\ & + \tfrac{1}{4} (C_{11} - C_{12})\, \varepsilon_{xy}^2 \end{aligned} \qquad (16\text{-}28)$$

Magnetoelastic energy

$$\begin{aligned} E_{\mathrm{me}}|_{\mathrm{hex}} = {} & b_{11} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12}\, \varepsilon_{zz} + \\ & + b_{21} (\alpha_z^2 - 1/3) (\varepsilon_{xx} + \varepsilon_{yy}) + \\ & + b_{22} (\alpha_z^2 - 1/3)\, \varepsilon_{zz} \\ & + \tfrac{1}{2} b_3 ((\alpha_x^2 - \alpha_y^2) (\varepsilon_{xx} - \varepsilon_{yy}) + 2\, \alpha_x\, \alpha_y\, \varepsilon_{xy}) + \\ & + b_4 (\alpha_x\, \alpha_z\, \varepsilon_{xz} + \alpha_y\, \alpha_z\, \varepsilon_{yz}) \qquad (16\text{-}29) \\ & + b_5 (\alpha_x \alpha_z \varepsilon_{yz} - \alpha_y \alpha_z \varepsilon_{xz}) \end{aligned}$$

$$\frac{\Delta l}{l} = \sum_{i,j} \varepsilon_{i,j}\, \beta_i\, \beta_j$$

$$\frac{\partial}{\partial \varepsilon_{ij}} (E_{\mathrm{el}} + E_{\mathrm{me}}) = 0$$

$$\begin{aligned} \left.\frac{\Delta l}{l}\right|_{\mathrm{Hex}} = {} & \lambda^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0} + \\ & + \lambda^{\alpha 1,2} (\alpha_z^2 - 1/3) (\beta_x^2 + \beta_y^2) + \\ & + \lambda^{\alpha 2,2} (\alpha_z^2 - 1/3)\, \beta_z^2 + \\ & + \lambda^{\gamma,2} (\tfrac{1}{2} (\alpha_x^2 - \alpha_y^2) (\beta_x^2 - \beta_y^2) + 2\, \alpha_x\, \alpha_y\, \beta_x\, \beta_y) + \\ & + 2\lambda^{\varepsilon,2} (\alpha_x\, \alpha_z\, \beta_x\, \beta_z + \alpha_y\, \alpha_z\, \beta_y\, \beta_z) \end{aligned} \qquad (16\text{-}30)$$

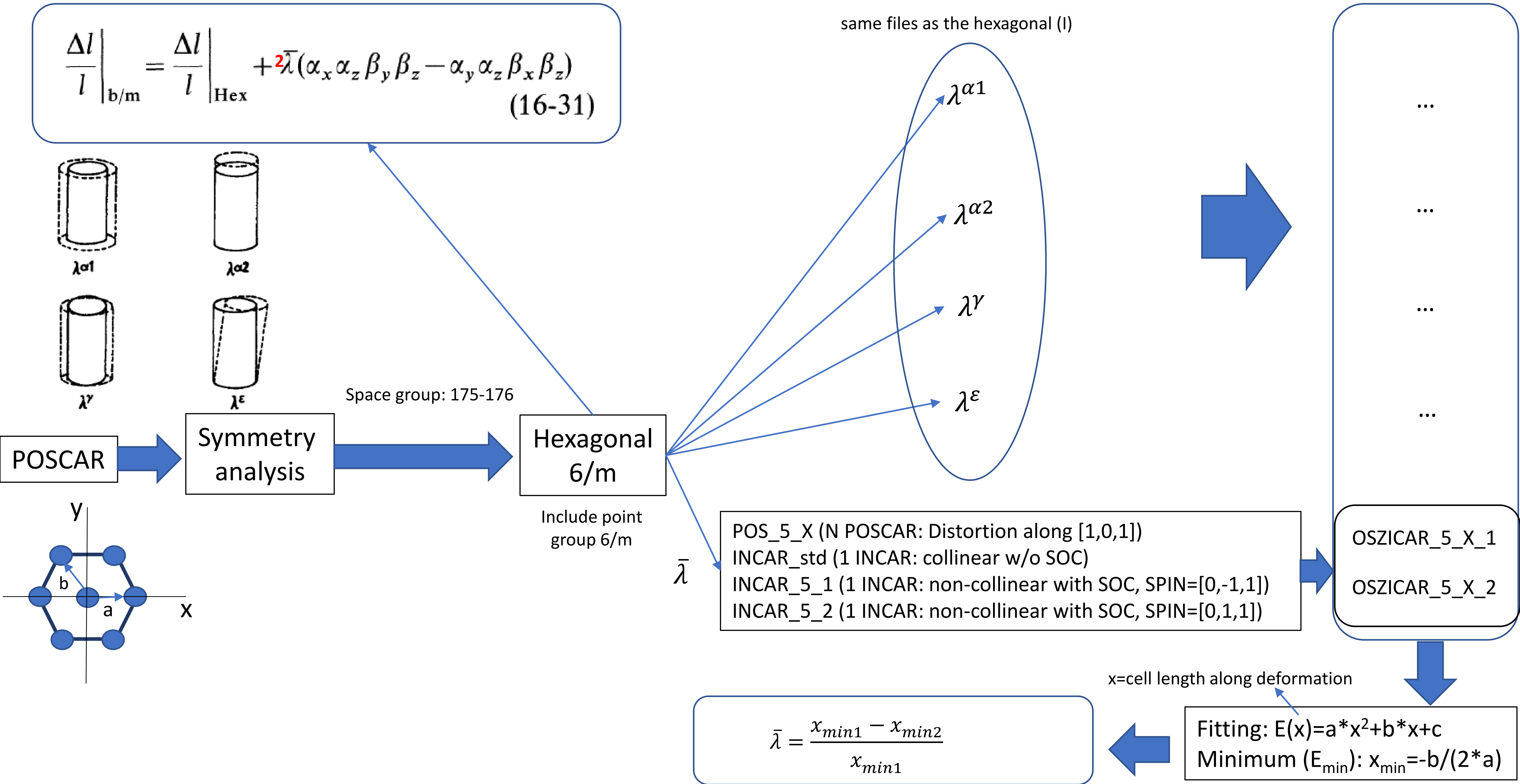
$$\left.\frac{\Delta l}{l}\right|_{\mathrm{b/m}} = \left.\frac{\Delta l}{l}\right|_{\mathrm{Hex}} + 2\bar{\lambda} (\alpha_x \alpha_z \beta_y \beta_z - \alpha_y \alpha_z \beta_x \beta_z) \qquad (16\text{-}31)$$

$\lambda^{\alpha 1,0}$	$(b_{11}\, c_{33} + b_{12}\, c_{13})/D$
$\lambda^{\alpha 2,0}$	$[2\, b_{11}\, c_{13} - b_{12} (c_{11} + c_{22})]/D$
$\lambda^{\alpha 1,2}$	$(-\, b_{21}\, c_{33} + b_{22}\, c_{13})/D$
$\lambda^{\alpha 2,2}$	$[2\, b_{21}\, c_{13} - b_{22} (c_{11} + c_{12})]/D$
$\lambda^{\gamma,2}$	$-\, b_3/(c_{11} - c_{12})$
$\lambda^{\varepsilon,2}$	$-\, b_4/(2\, c_{44})$

[a] $D \equiv c_{33} (c_{11} + c_{12}) - 2\, c_{13}^2$.

$$\bar{\lambda} = \frac{-b_5}{2c_{44}}$$

Workflow



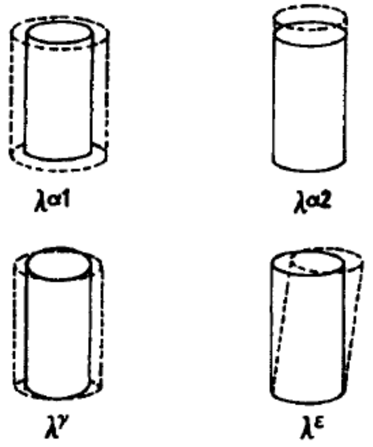
$\frac{\Delta l}{l}\Big|_{b/m} = \frac{\Delta l}{l}\Big|_{Hex} + 2\bar{\lambda}(\alpha_x\alpha_z\beta_y\beta_z - \alpha_y\alpha_z\beta_x\beta_z)$ (16-31)
$\lambda^{\alpha 1}$
$\lambda^{\alpha 2}$
λ^{γ}
λ^{ε}
POSCAR
Symmetry analysis
Space group: 175-176
Hexagonal 6/m
Include point group 6/m
y
b
a
x
same files as the hexagonal (I)
$\lambda^{\alpha 1}$
$\lambda^{\alpha 2}$
λ^{γ}
λ^{ε}
...
...
...
...
$\bar{\lambda}$
POS_5_X (N POSCAR: Distortion along [1,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_5_1 (1 INCAR: non-collinear with SOC, SPIN=[0,-1,1])
INCAR_5_2 (1 INCAR: non-collinear with SOC, SPIN=[0,1,1])
OSZICAR_5_X_1
OSZICAR_5_X_2
x=cell length along deformation
Fitting: $E(x)=a*x^2+b*x+c$
Minimum (E_{min}): $x_{min}=-b/(2*a)$
$\bar{\lambda} = \frac{x_{min1} - x_{min2}}{x_{min1}}$

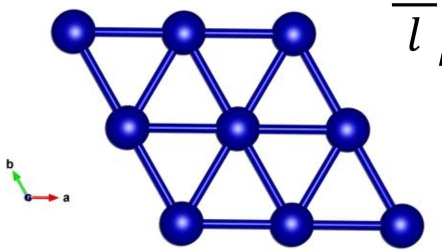
Hexagonal (II)
point group 6/m

Distorted states

Include point group 6/m

Space group: 175,191,192





$$\frac{\Delta l^{\alpha}}{l}_{\beta}$$

$$|\boldsymbol{\alpha}| = 1, |\boldsymbol{\beta}| = 1$$

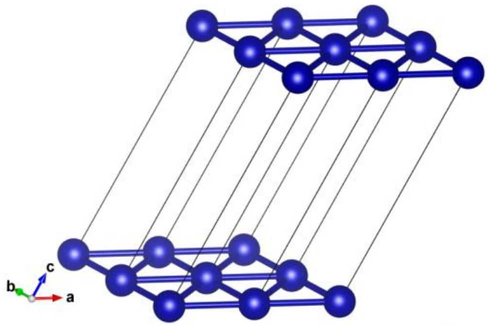
$$\left.\frac{\Delta l}{l}\right|_{\mathrm{b/m}} = \left.\frac{\Delta l}{l}\right|_{\mathrm{Hex}} + \bar{\lambda}(\alpha_x\alpha_z\beta_y\beta_z - \alpha_y\alpha_z\beta_x\beta_z) \qquad (16\text{-}31)$$

shear along xz: $\beta = (1,0,1)$

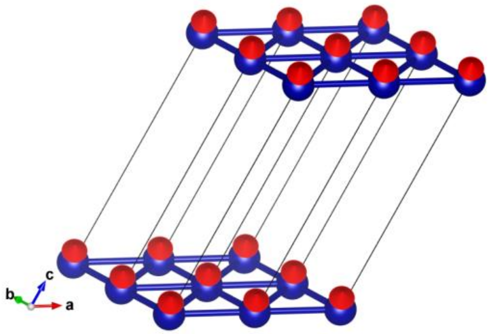
ε_{xz}

$$D = \mathrm{d}\cdot\begin{pmatrix} 1 & 0 & \frac{\varepsilon_{xz}}{2} \\ 0 & 1 & 0 \\ \frac{\varepsilon_{xz}}{2} & 0 & 1 \end{pmatrix}$$

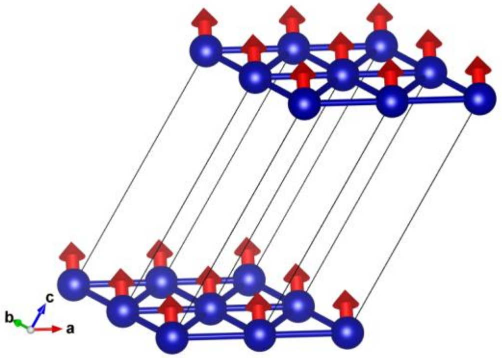
volume-conserving



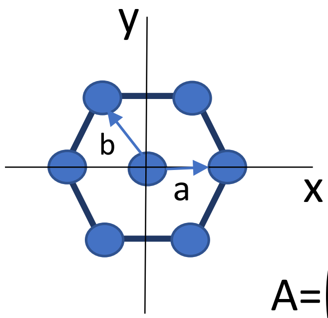
$$\bar{\lambda} \Rightarrow \frac{\Delta l^{(0,-1,1)}}{l}_{(1,0,1)} - \frac{\Delta l^{(0,1,1)}}{l}_{(1,0,1)} = \frac{1}{2}\cdot\bar{\lambda}$$



S=(0,-1,1)



S=(0,1,1)



$$A=\begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

$$\bar{\lambda} = 2\cdot\frac{x_{min1} - x_{min2}}{x_{min1}}$$

Workflow

HEXAGONAL (II) – point groups $\bar{6}, 6$

SG 168-174

WARNING: Current version doesn’t calculate the magnetostriction coefficients for these point groups

TRIGONAL (I)

SG 149-167

Trigonal (I)

Workflow

Elastic energy

$$E_{el}^{trig(I)} = \frac{\mathrm{c11}\epsilon_{\mathrm{xx}}^2}{2} + \frac{1}{4}(\mathrm{c11}-\mathrm{c12})\epsilon_{\mathrm{xy}}^2 + \mathrm{c12}\epsilon_{\mathrm{xx}}\epsilon_{\mathrm{yy}}$$
$$+\frac{\mathrm{c11}\epsilon_{\mathrm{yy}}^2}{2} + \mathrm{c14}\left(\epsilon_{\mathrm{xy}}\epsilon_{\mathrm{xz}} + \epsilon_{\mathrm{xx}}\epsilon_{\mathrm{yz}} - \epsilon_{\mathrm{yy}}\epsilon_{\mathrm{yz}}\right)$$
$$+\mathrm{c44}\left(\frac{\epsilon_{\mathrm{xz}}^2}{2} + \frac{\epsilon_{\mathrm{yz}}^2}{2}\right) + \frac{\mathrm{c33}\epsilon_{\mathrm{zz}}^2}{2} + \mathrm{c13}\left(\epsilon_{\mathrm{xx}}\epsilon_{\mathrm{zz}} + \epsilon_{\mathrm{yy}}\epsilon_{\mathrm{zz}}\right)$$

J. R. Cullen, A. E. Clark, and K. B. Hathaway, in Materials, Science and Technology (VCH Publishings, 1994), pp. 529 – 565.

$$\frac{\Delta l}{l} = \sum_{i,j} \varepsilon_{i,j}\beta_i\beta_j$$

$$\frac{\partial}{\partial \varepsilon_{ij}}(E_{\mathrm{el}} + E_{\mathrm{me}}) = 0$$

$$\left.\frac{\Delta l}{l}\right|_{\mathrm{trigonal}} =$$
$$= (\beta_x^2 + \beta_y^2)\cdot[\lambda^{\alpha 1,0} + \lambda^{\alpha 1,2}(\alpha_z^2 - 1/3)] +$$
$$+ \beta_z^2[\lambda^{\alpha 2,0} + \lambda^{\alpha 2,2}(\alpha_z^2 - 1/3)] +$$
$$+ \lambda^{\gamma 1}[\tfrac{1}{2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + \cancel{2}\alpha_x\alpha_y\beta_x\beta_y] +$$
$$+ \lambda^{\gamma 2}[\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z] +$$
$$+ \lambda_{12}[\tfrac{1}{2}\alpha_y\alpha_z(\beta_x^2 - \beta_y^2) + \alpha_x\alpha_z\beta_x\beta_y] +$$
$$+ \lambda_{21}[\tfrac{1}{2}(\alpha_x^2 - \alpha_y^2)\beta_y\beta_z + \alpha_x\alpha_y\beta_x\beta_z] \quad (16\text{-}40)$$

Magnetoelastic energy

$$E_{\mathrm{me}}|_{\mathrm{trigonal}} = b_{11}(\varepsilon_{xx} + \varepsilon_{yy}) + b_{12}\varepsilon_{zz} +$$
$$+ b_{21}(\alpha_z^2 - 1/3)(\varepsilon_{xx} + \varepsilon_{yy}) +$$
$$+ b_{22}(\alpha_z^2 - 1/3)\varepsilon_{zz} + \quad (16\text{-}39)$$
$$+ \tfrac{1}{2}b_3[(\alpha_x^2 - \alpha_y^2)(\varepsilon_{xx} - \varepsilon_{yy}) + 2\alpha_x\alpha_y\varepsilon_{xy}] +$$
$$+ b_4(\alpha_x\alpha_z\varepsilon_{xz} + \alpha_y\alpha_z\varepsilon_{yz}) +$$
b14 $+ \cancel{b_{34}}[\tfrac{1}{2}(\alpha_x^2 - \alpha_y^2)\varepsilon_{yz} + \alpha_x\alpha_y\varepsilon_{xz} +$

b34 [1/2 $+\alpha_y\alpha_z(\varepsilon_{xx} - \varepsilon_{yy}) + \alpha_x\alpha_z\varepsilon_{xy}]$

$$\lambda^{\alpha 1,0} = (b_{11}c_{33} + b_{12}c_{13})/D$$
$$\lambda^{\alpha 2,0} = [2b_{11}c_{13} - b_{12}(c_{11} + c_{22})]/D$$
$$\lambda^{\alpha 1,2} = (-b_{21}c_{33} + b_{22}c_{13})/D$$
$$\lambda^{\alpha 2,2} = [2b_{21}c_{13} - b_{22}(c_{11} + c_{12})]/D$$

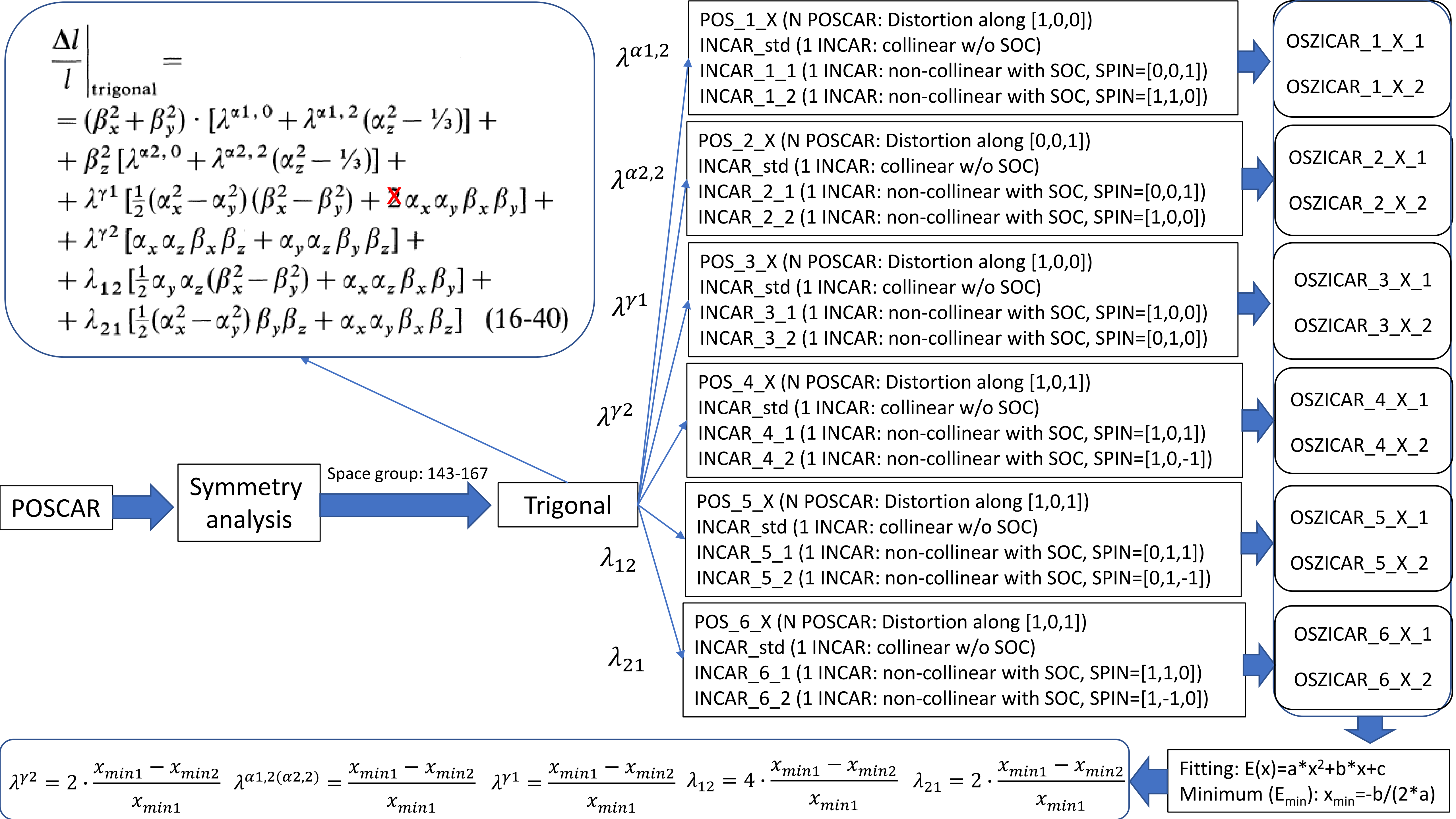
$$D \equiv c_{33}(c_{11} + c_{12}) - 2c_{13}^2$$

b14 b3

$$\lambda^{\gamma 1} = (C_{14}\cancel{b_{34}} - C_{44}\cancel{b_2})/D^{\gamma} \quad (16\text{-}41\,\mathrm{a})$$
$$\lambda^{\gamma 2} = \left(\frac{b_4}{2}(C_{11} - C_{12}) - b_{34}C_{14}\right)\Big/ D^{\gamma} \quad (16\text{-}41\,\mathrm{b})$$
$$\lambda_{12} = (C_{14}b_4 - C_{44}b_{34})/D^{\gamma} \quad (16\text{-}41\,\mathrm{c})$$
$$\lambda_{21} = \left(\frac{b_{14}}{2}(C_{11} - C_{12}) - C_{14}b_3\right)\Big/ D^{\gamma} \quad (16\text{-}41\,\mathrm{d})$$

where

$$D^{\gamma} = \frac{C_{44}}{2}(C_{11} - C_{12}) - C_{14}^2 \quad (16\text{-}42)$$



$\left.\frac{\Delta l}{l}\right|_{\text{trigonal}} =$
$= (\beta_x^2+\beta_y^2)\cdot[\lambda^{\alpha1,0}+\lambda^{\alpha1,2}(\alpha_z^2-1/3)] +$
$+ \beta_z^2[\lambda^{\alpha2,0}+\lambda^{\alpha2,2}(\alpha_z^2-1/3)] +$
$+ \lambda^{\gamma1}[\frac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2)+\cancel{2}\alpha_x\alpha_y\beta_x\beta_y] +$
$+ \lambda^{\gamma2}[\alpha_x\alpha_z\beta_x\beta_z+\alpha_y\alpha_z\beta_y\beta_z] +$
$+ \lambda_{12}[\frac{1}{2}\alpha_y\alpha_z(\beta_x^2-\beta_y^2)+\alpha_x\alpha_z\beta_x\beta_y] +$
$+ \lambda_{21}[\frac{1}{2}(\alpha_x^2-\alpha_y^2)\beta_y\beta_z+\alpha_x\alpha_y\beta_x\beta_z]$ (16-40)
POSCAR
Symmetry analysis
Space group: 143-167
Trigonal
$\lambda^{\alpha1,2}$
$\lambda^{\alpha2,2}$
$\lambda^{\gamma1}$
$\lambda^{\gamma2}$
λ_{12}
λ_{21}
POS_1_X (N POSCAR: Distortion along [1,0,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_1_1 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
INCAR_1_2 (1 INCAR: non-collinear with SOC, SPIN=[1,1,0])
POS_2_X (N POSCAR: Distortion along [0,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_2_1 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
INCAR_2_2 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
POS_3_X (N POSCAR: Distortion along [1,0,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_3_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
INCAR_3_2 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
POS_4_X (N POSCAR: Distortion along [1,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_4_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,1])
INCAR_4_2 (1 INCAR: non-collinear with SOC, SPIN=[1,0,-1])
POS_5_X (N POSCAR: Distortion along [1,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_5_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,1])
INCAR_5_2 (1 INCAR: non-collinear with SOC, SPIN=[0,1,-1])
POS_6_X (N POSCAR: Distortion along [1,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_6_1 (1 INCAR: non-collinear with SOC, SPIN=[1,1,0])
INCAR_6_2 (1 INCAR: non-collinear with SOC, SPIN=[1,-1,0])
OSZICAR_1_X_1
OSZICAR_1_X_2
OSZICAR_2_X_1
OSZICAR_2_X_2
OSZICAR_3_X_1
OSZICAR_3_X_2
OSZICAR_4_X_1
OSZICAR_4_X_2
OSZICAR_5_X_1
OSZICAR_5_X_2
OSZICAR_6_X_1
OSZICAR_6_X_2
Fitting: $E(x)=a*x^2+b*x+c$
Minimum (E_{min}): $x_{min}=-b/(2*a)$
$\lambda^{\gamma2} = 2\cdot\frac{x_{min1}-x_{min2}}{x_{min1}}$ $\lambda^{\alpha1,2(\alpha2,2)} = \frac{x_{min1}-x_{min2}}{x_{min1}}$ $\lambda^{\gamma1} = \frac{x_{min1}-x_{min2}}{x_{min1}}$ $\lambda_{12} = 4\cdot\frac{x_{min1}-x_{min2}}{x_{min1}}$ $\lambda_{21} = 2\cdot\frac{x_{min1}-x_{min2}}{x_{min1}}$

Workflow

TRIGONAL (II)

SG 143-148

WARNING: Current version doesn’t calculate the magnetostriction coefficients for these space groups

TETRAGONAL (I)

SG 89-142

Workflow

Tetragonal (I)

J. R. Cullen, A. E. Clark, and K. B. Hathaway, in Materials, Science and Technology (VCH Publishings, 1994), pp. 529 – 565.

Elastic energy

$$E_{el}^{tet} = \mathrm{c12}\epsilon_{\mathrm{xx}}\epsilon_{\mathrm{yy}} + \mathrm{c11}\left(\frac{\epsilon_{\mathrm{xx}}^2}{2} + \frac{\epsilon_{\mathrm{yy}}^2}{2}\right) + \mathrm{c44}\left(\frac{\epsilon_{\mathrm{xz}}^2}{2} + \frac{\epsilon_{\mathrm{yz}}^2}{2}\right) + \frac{\mathrm{c33}\epsilon_{\mathrm{zz}}^2}{2} + \mathrm{c13}(\epsilon_{\mathrm{xx}}\epsilon_{\mathrm{zz}} + \epsilon_{\mathrm{yy}}\epsilon_{\mathrm{zz}}) + \frac{\mathrm{c66}\epsilon_{\mathrm{xy}}^2}{2}$$

Magnetoelastic energy

$$f_{\mathrm{me}}^{\mathrm{tet}} = b_{11}(\varepsilon_{xx} + \varepsilon_{yy}) + b_{12}\varepsilon_{zz} + b_{21}(\alpha_z^2 - {}^1/_3)(\varepsilon_{xx} + \varepsilon_{yy}) + b_{22}(\alpha_z^2 - {}^1/_3)\varepsilon_{zz} + \frac{1}{2}b_3(\alpha_x^2 - \alpha_y^2)(\varepsilon_{xx} - \varepsilon_{yy}) + b_3'\alpha_x\alpha_y\varepsilon_{xy} + b_4(\alpha_x\alpha_z\varepsilon_{xz} + \alpha_y\alpha_z\varepsilon_{yz}) \;,$$

$$\frac{\Delta l}{l} = \sum_{i,j} \varepsilon_{i,j}\beta_i\beta_j$$

$$\frac{\partial}{\partial\varepsilon_{ij}}(E_{\mathrm{el}} + E_{\mathrm{me}}) = 0$$

$$\left.\frac{\Delta l}{l}\right|_{\mathrm{tetragonal}} = \lambda^{\alpha1,0}(\beta_x^2 + \beta_y^2) + \lambda^{\alpha2,0}\beta_z^2 + \lambda^{\alpha1,2}(\alpha_z^2 - {}^1/_3)(\beta_x^2 + \beta_y^2) + \lambda^{\alpha2,2}(\alpha_z^2 - {}^1/_3)\beta_z^2 + \tfrac{1}{2}\lambda^{\gamma,2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + 2\lambda^{\delta,2}\alpha_x\alpha_y\beta_x\beta_y + 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z) \qquad (16\text{-}34)$$

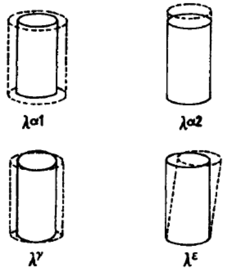
$\lambda^{\alpha1,0}$	$(b_{11}c_{33} + b_{12}c_{13})/D$
$\lambda^{\alpha2,0}$	$[2b_{11}c_{13} - b_{12}(c_{11} + c_{22})]/D$
$\lambda^{\alpha1,2}$	$(-b_{21}c_{33} + b_{22}c_{13})/D$
$\lambda^{\alpha2,2}$	$[2b_{21}c_{13} - b_{22}(c_{11} + c_{12})]/D$
$\lambda^{\gamma,2}$	$-b_3/(c_{11} - c_{12})$
$\lambda^{\varepsilon,2}$	$-b_4/(2c_{44})$

[a] $D \equiv c_{33}(c_{11} + c_{12}) - 2c_{13}^2$.

$$\lambda^{\delta,2} = \frac{-b_3'}{2C_{66}}$$

Workflow

$$\left.\frac{\Delta l}{l}\right|_{\text{tetragonal}} = \lambda^{\alpha 1,0}(\beta_x^2+\beta_y^2) + \lambda^{\alpha 2,0}\beta_z^2 + $$
$$+ \lambda^{\alpha 1,2}(\alpha_z^2 - 1/3)(\beta_x^2+\beta_y^2) +$$
$$+ \lambda^{\alpha 2,2}(\alpha_z^2 - 1/3)\beta_z^2 +$$
$$+ \tfrac{1}{2}\lambda^{\gamma,2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2) +$$
$$+ 2\lambda^{\delta,2}\alpha_x\alpha_y\beta_x\beta_y +$$
$$+ 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z) \quad (16\text{-}34)$$



POSCAR → Symmetry analysis → Tetragonal

Space group: 75-142

same files as the hexagonal case

$\lambda^{\alpha 1}$

$\lambda^{\alpha 2}$

λ^{γ}

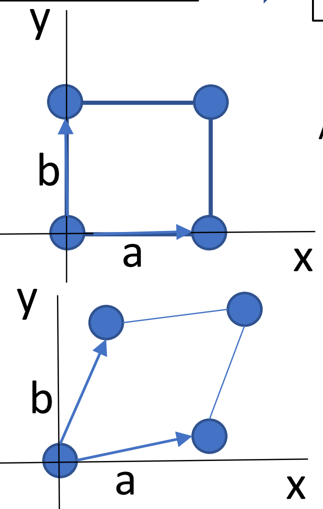
λ^{ε}

...

...

...

...



$$A = \begin{pmatrix} a1 & 0 & 0 \\ 0 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

$$a1 = b2$$

$\lambda^{\delta,2}$

POS_5_X (N POSCAR: Distortion along [1,1,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_5_1 (1 INCAR: non-collinear with SOC, SPIN=[1,1,0])
INCAR_5_2 (1 INCAR: non-collinear with SOC, SPIN=[-1,1,0])

OSZICAR_5_X_1

OSZICAR_5_X_2

shear along xy: $\beta = (1,1,0)$

$$D = d\cdot\begin{pmatrix} 1 & \frac{\varepsilon_{xy}}{2} & 0 \\ \frac{\varepsilon_{xy}}{2} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

volume-conserving

x=cell length along deformation

Fitting: $E(x)=a*x^2+b*x+c$

Minimum (E_{min}): $x_{min}=-b/(2*a)$

$$\lambda^{\delta,2} = \frac{x_{min1} - x_{min2}}{x_{min1}}$$

Relation between different notations

Tetragonal (I)

Cullen

$$\left.\frac{\Delta l}{l}\right|_{\text{tetragonal}} = \lambda^{\alpha 1,0}(\beta_x^2+\beta_y^2)+\lambda^{\alpha 2,0}\,\beta_z^2 + \\ +\lambda^{\alpha 1,2}(\alpha_z^2-1/3)(\beta_x^2+\beta_y^2)+ \\ +\lambda^{\alpha 2,2}(\alpha_z^2-1/3)\,\beta_z^2+ \\ +\tfrac{1}{2}\lambda^{\gamma,2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2)+ \\ +2\lambda^{\delta,2}\,\alpha_x\alpha_y\beta_x\beta_y+ \\ +2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z+\alpha_y\alpha_z\beta_y\beta_z) \qquad (16\text{-}34)$$

Mason

$$\lambda=\tfrac{1}{2}\lambda_1[(\alpha_1\beta_1-\alpha_2\beta_2)^2-(\alpha_1\beta_2+\alpha_2\beta_1)^2+(1-\beta_3^2)(1-\alpha_3^2) \\ -2\alpha_3\beta_3(\alpha_1\beta_1+\alpha_2\beta_2)]+4\lambda_2\alpha_3\beta_3(\alpha_1\beta_1+\alpha_2\beta_2) \\ +4\lambda_3\alpha_1\alpha_2\beta_1\beta_2+\lambda_4[\beta_3^2(1-\alpha_3^2)-\alpha_3\beta_3(\alpha_1\beta_1+\alpha_2\beta_2)] \\ +\tfrac{1}{2}\lambda_5[(\alpha_1\beta_2-\alpha_2\beta_1)^2-(\alpha_1\beta_1+\alpha_2\beta_2)^2 \\ +(1-\beta_3^2)(1-\alpha_3^2)], \qquad (74)$$

$$\lambda_1=\lambda(\alpha_1=1,\beta_1=1);\quad \lambda_2=\lambda(\alpha_1=\beta_1=\alpha_3=\beta_3=1/\sqrt{2});$$
$$\lambda_3=\lambda(\alpha_1=\alpha_2=\beta_1=\beta_2=1/\sqrt{2});$$
$$\lambda_4=\lambda(\alpha_1=1,\beta_3=1);\quad \lambda_5=\lambda(\alpha_1=1,\beta_2=1)$$

$$\frac{\Delta l^{111}}{l}_{100}-\frac{\Delta l^{110}}{l}_{100}=\frac{1}{3}\lambda^{\alpha1,2}=-\frac{1}{6}\lambda_1-\frac{1}{6}\lambda_5$$

$$\frac{\Delta l^{100}}{l}_{100}-\frac{\Delta l^{010}}{l}_{100}=\lambda^{\gamma,2}=\lambda_1-\lambda_5$$

$$\lambda_1=-\lambda^{\alpha1,2}+\frac{1}{2}\lambda^{\gamma,2}$$

$$\lambda_5=-\lambda^{\alpha1,2}-\frac{1}{2}\lambda^{\gamma,2}$$

$$\frac{\Delta l^{001}}{l}_{001}-\frac{\Delta l^{100}}{l}_{001}=\lambda^{\alpha2,2}=-\lambda_4 \longrightarrow \lambda_4=-\lambda^{\alpha2,2}$$

$$\frac{\Delta l^{101}}{l}_{101}-\frac{\Delta l^{-101}}{l}_{101}=\lambda^{\varepsilon,2}=2\lambda_2-\frac{1}{2}\lambda_4 \longrightarrow \lambda_2=\frac{1}{2}\left[\lambda^{\varepsilon,2}-\frac{1}{2}\lambda^{\alpha2,2}\right]$$

$$\frac{\Delta l^{110}}{l}_{110}-\frac{\Delta l^{-110}}{l}_{110}=\lambda^{\delta,2}=-\lambda_1+2\lambda_3-\lambda_5 \longrightarrow \lambda_3=\frac{1}{2}\lambda^{\delta,2}-\lambda^{\alpha1,2}$$

TETRAGONAL (II)

SG 75-88

WARNING: Current version doesn't calculate the magnetostriction coefficients for these space groups

Workflow

ORTHORHOMBIC

SG 16-74

Workflow

Orthorhombic

Elastic energy

$$E_{el}^{ortho} = \frac{\mathrm{c11}\epsilon_{\mathrm{xx}}^2}{2} + \frac{\mathrm{c66}\epsilon_{\mathrm{xy}}^2}{2} + \frac{\mathrm{c55}\epsilon_{\mathrm{xz}}^2}{2} + \mathrm{c12}\epsilon_{\mathrm{xx}}\epsilon_{\mathrm{yy}} + \frac{\mathrm{c22}\epsilon_{\mathrm{yy}}^2}{2} + \frac{\mathrm{c44}\epsilon_{\mathrm{yz}}^2}{2} + \mathrm{c13}\epsilon_{\mathrm{xx}}\epsilon_{\mathrm{zz}} + \mathrm{c23}\epsilon_{\mathrm{yy}}\epsilon_{\mathrm{zz}} + \frac{\mathrm{c33}\epsilon_{\mathrm{zz}}^2}{2}$$

$$\frac{\Delta l}{l} = \sum_{i,j} \varepsilon_{i,j}\beta_i\beta_j$$

$$\frac{\partial}{\partial \varepsilon_{ij}}(E_{\mathrm{el}} + E_{\mathrm{me}}) = 0$$

Magnetoelastic energy

$$E_{me}^{ortho} = (\alpha_x^2 b_1 + \alpha_y^2 b_2)\epsilon_{\mathrm{xx}} + (\alpha_x^2 b_3 + \alpha_y^2 b_4)\epsilon_{\mathrm{yy}} + (\alpha_x^2 b_5 + \alpha_y^2 b_6)\epsilon_{\mathrm{zz}} + \alpha_y\alpha_z b_7\epsilon_{\mathrm{yz}} + \alpha_x\alpha_z b_8\epsilon_{\mathrm{xz}} + \alpha_x\alpha_y b_9\epsilon_{\mathrm{xy}}$$

PHYSICAL REVIEW

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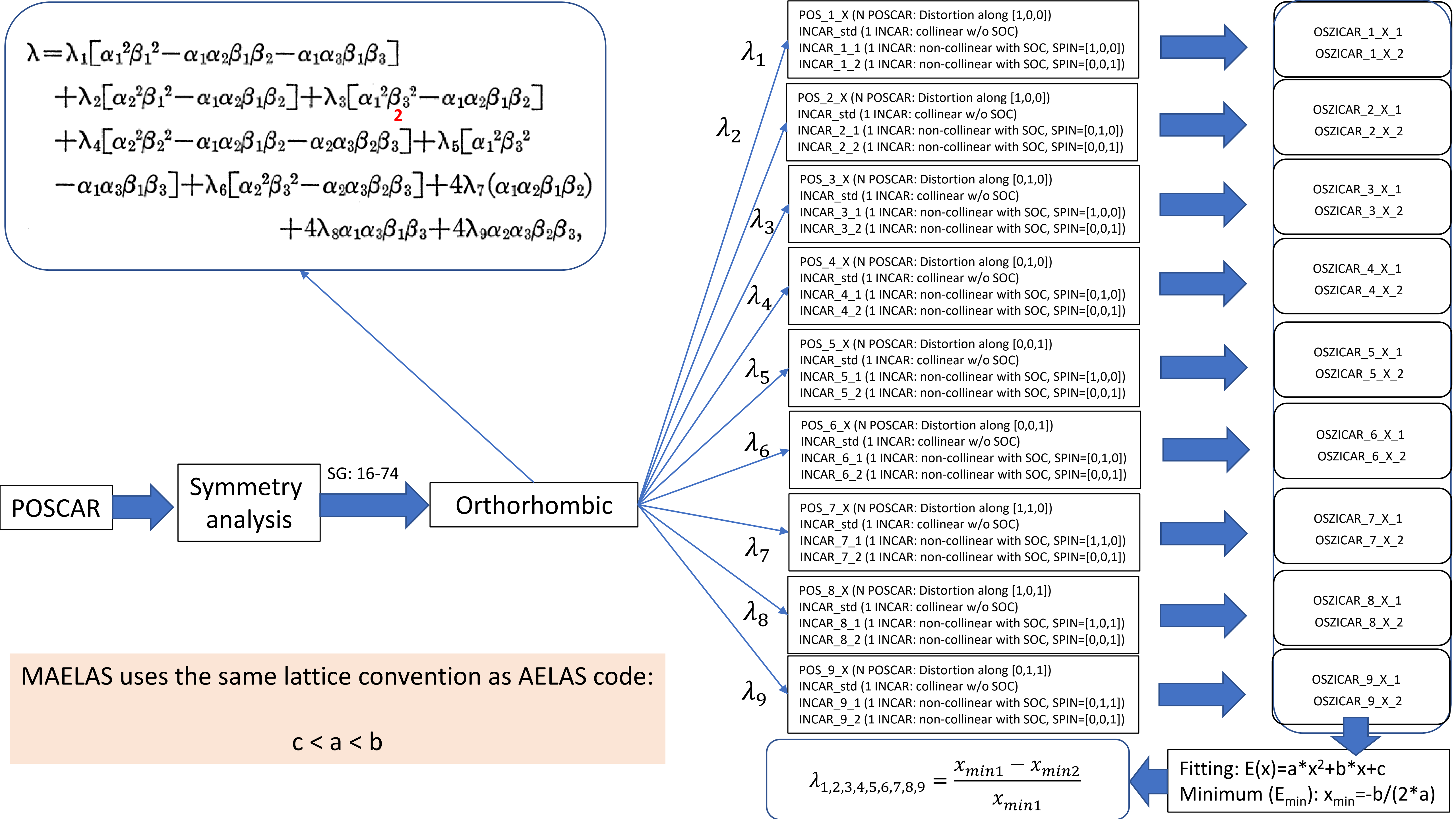
OCTOBER 15, 1954

$$\lambda = \lambda_1[\alpha_1^2\beta_1^2 - \alpha_1\alpha_2\beta_1\beta_2 - \alpha_1\alpha_3\beta_1\beta_3] + \lambda_2[\alpha_2^2\beta_1^2 - \alpha_1\alpha_2\beta_1\beta_2] + \lambda_3[\alpha_1^2\beta_3^2 - \alpha_1\alpha_2\beta_1\beta_2] + \lambda_4[\alpha_2^2\beta_2^2 - \alpha_1\alpha_2\beta_1\beta_2 - \alpha_2\alpha_3\beta_2\beta_3] + \lambda_5[\alpha_1^2\beta_3^2 - \alpha_1\alpha_3\beta_1\beta_3] + \lambda_6[\alpha_2^2\beta_3^2 - \alpha_2\alpha_3\beta_2\beta_3] + 4\lambda_7(\alpha_1\alpha_2\beta_1\beta_2) + 4\lambda_8\alpha_1\alpha_3\beta_1\beta_3 + 4\lambda_9\alpha_2\alpha_3\beta_2\beta_3,$$

$b_1 = -\mathrm{c11}\ \lambda_1 - \mathrm{c12}\ \lambda_3 - \mathrm{c13}\ \lambda_5$
$b_2 = -\ \mathrm{c11}\ \lambda_2 - \mathrm{c12}\ \lambda_4 - \mathrm{c13}\ \lambda_6$
$b_3 = -\ \mathrm{c12}\ \lambda_1 - \mathrm{c22}\ \lambda_3 - \mathrm{c23}\ \lambda_5$
$b_4 = -\ \mathrm{c12}\ \lambda_2 - \mathrm{c22}\ \lambda_4 - \mathrm{c23}\ \lambda_6$
$b_5 = -\ \mathrm{c13}\ \lambda_1 - \mathrm{c23}\ \lambda_3 - \mathrm{c33}\ \lambda_5$
$b_6 = -\ \mathrm{c13}\ \lambda_2 - \mathrm{c23}\ \lambda_4 - \mathrm{c33}\ \lambda_6$
$b_7 = \mathrm{c44}\ (\lambda_4 + \lambda_6 - 4\ \lambda_9)$
$b_8 = \mathrm{c55}\ (\lambda_1 + \lambda_5 - 4\ \lambda_8)$
$b_9 = \mathrm{c66}\ (\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 - 4\ \lambda_7)$



λ=λ1[α1²β1²−α1α2β1β2−α1α3β1β3] +λ2[α2²β1²−α1α2β1β2]+λ3[α1²β3²−α1α2β1β2] +λ4[α2²β2²−α1α2β1β2−α2α3β2β3]+λ5[α1²β3² −α1α3β1β3]+λ6[α2²β3²−α2α3β2β3]+4λ7(α1α2β1β2) +4λ8α1α3β1β3+4λ9α2α3β2β3,
2
POSCAR
Symmetry analysis
SG: 16-74
Orthorhombic
λ1
λ2
λ3
λ4
λ5
λ6
λ7
λ8
λ9
POS_1_X (N POSCAR: Distortion along [1,0,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_1_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
INCAR_1_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
POS_2_X (N POSCAR: Distortion along [1,0,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_2_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
INCAR_2_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
POS_3_X (N POSCAR: Distortion along [0,1,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_3_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
INCAR_3_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
POS_4_X (N POSCAR: Distortion along [0,1,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_4_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
INCAR_4_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
POS_5_X (N POSCAR: Distortion along [0,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_5_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
INCAR_5_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
POS_6_X (N POSCAR: Distortion along [0,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_6_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
INCAR_6_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
POS_7_X (N POSCAR: Distortion along [1,1,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_7_1 (1 INCAR: non-collinear with SOC, SPIN=[1,1,0])
INCAR_7_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
POS_8_X (N POSCAR: Distortion along [1,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_8_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,1])
INCAR_8_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
POS_9_X (N POSCAR: Distortion along [0,1,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_9_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,1])
INCAR_9_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
OSZICAR_1_X_1
OSZICAR_1_X_2
OSZICAR_2_X_1
OSZICAR_2_X_2
OSZICAR_3_X_1
OSZICAR_3_X_2
OSZICAR_4_X_1
OSZICAR_4_X_2
OSZICAR_5_X_1
OSZICAR_5_X_2
OSZICAR_6_X_1
OSZICAR_6_X_2
OSZICAR_7_X_1
OSZICAR_7_X_2
OSZICAR_8_X_1
OSZICAR_8_X_2
OSZICAR_9_X_1
OSZICAR_9_X_2
Fitting: E(x)=a*x²+b*x+c
Minimum (Emin): xmin=-b/(2*a)
λ1,2,3,4,5,6,7,8,9 = (xmin1 − xmin2)/xmin1
MAELAS uses the same lattice convention as AELAS code:
c < a < b

Workflow

MONOCLINIC

SG 3-15

WARNING: Current version doesn’t calculate the magnetostriction coefficients for these point groups

Workflow

TRICLINIC

SG 1-2

WARNING: Current version doesn't calculate the magnetostriction coefficients for these point groups

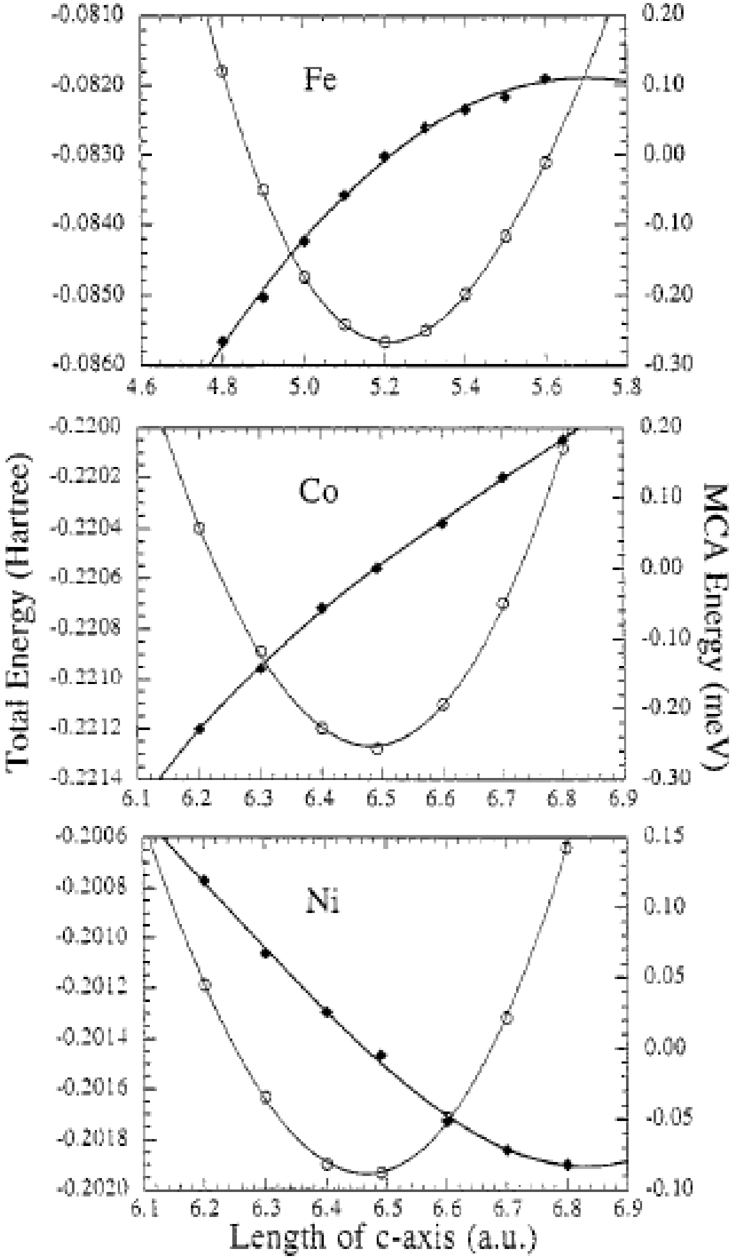
BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

Cubic systems: Itenerant magnets

R.Q. Wu et al. / Journal of Magnetism and Magnetic Materials 177–181 (1998) 1216–1219

	a (a.u.)	σ	$M_s(\mu_B)$	$M_L(\mu_B)$	$\lambda_{001}(10^{-6})$
bcc Fe					
LDA	5.20	-0.409	2.05	0.048	52
GGA	5.37	-0.486	2.17	0.045	29
EXP	5.41	-0.368	2.22	0.08	21
fcc Co					
LDA	6.48	-0.374	1.59	0.076	92
GGA	6.67	-0.396	1.66	0.073	56
EXP	6.70	---	1.72	0.12	79
fcc Ni					
LDA	6.46	-0.332	0.62	0.049	-63
GGA	6.64	-0.3376	0.66	0.050	-56
EXP	6.66	-0.376	0.57	0.05	-49

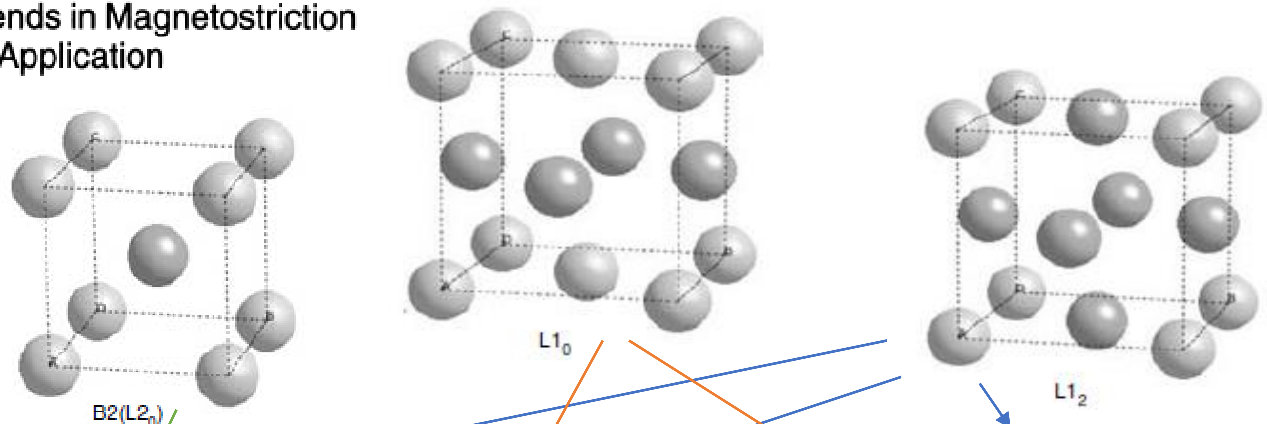
	$T = 4.2$ K		Room Temperature		
	$\lambda_{100}(\lambda^{\gamma,2})$	$\lambda_{111}(\lambda^{\varepsilon,2})$	$\lambda_{100}(\lambda^{\gamma,2})$	$\lambda_{111}(\lambda^{\varepsilon,2})$	Polycrystal λ_s
3d Metals					
BCC-Fe	26	−30	21	−21	−7
HCP-Co[a]	(−150)	(45)	(−140)	(50)	(−62)
FCC-Ni	−60	−35	−46	−24	−34
BCC-FeCo	—	—	140	30	—
a-$Fe_{80}B_{20}$	48 (isotropic)	—	—	—	+32
a-$Fe_{40}Ni_{40}B_{20}$	+20	—	—	—	+14
a-$Cos_{80}B_{20}$	−4	—	—	—	−4



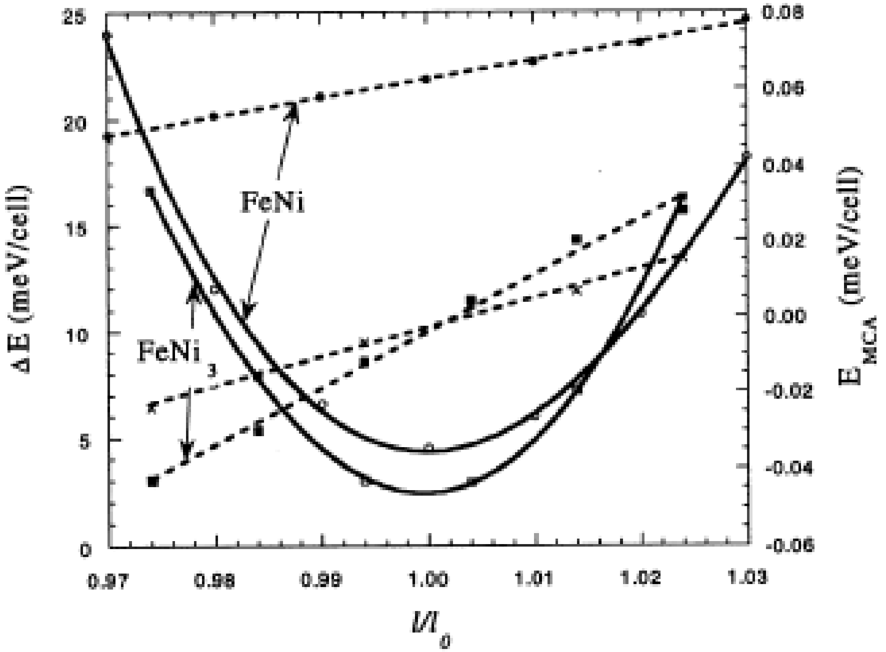
BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

Cubic systems: Itenerant magnets

Modern Trends in Magnetostriction
Study and Application



	bcc	fcc	fcc	fcc	fcc	fcc
	FeCo	$FeCo_3$	FeNi	$FeNi_3$	CoNi	$CoNi_3$
a (a.u.)	5.38 (5.39)	6.70	6.76 (6.76)	6.70 (6.71)	6.62 (6.67)	6.66 (6.65)
c (a.u.)	5.38 (5.39)	6.70	6.76 (6.76)	6.70 (6.71)	6.78 (6.67)	6.66 (6.65)
E_{MCA}(μeV)	0	0	63	0	143	0
σ	-0.35	-0.36	-0.33	-0.35	-0.34	-0.36
λ_{001} (10^{-6})	83 (125)	-68	10 (12)	27 (13)	42 (42-100)	33



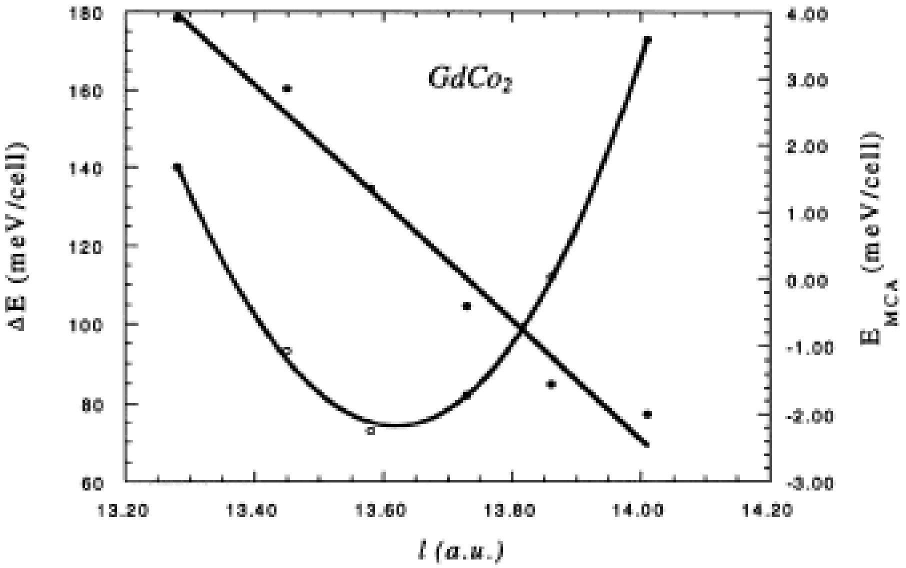
BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

Cubic systems: Rare-Earth magnets

Modern Trends in Magnetostriction
Study and Application

C15 cubic Laves phase

	Theory	Experiment
λ_{001} ($GdCo_2$)	-407	-1200
λ_{111} ($GdCo_2$)	19	< 10
λ_{001} ($SmCo_2$)	-290	---
λ_{001} ($ErCo_2$)	-516	-1000
λ_{001} ($GdFe_2$)	44	39



$DyFe_2$

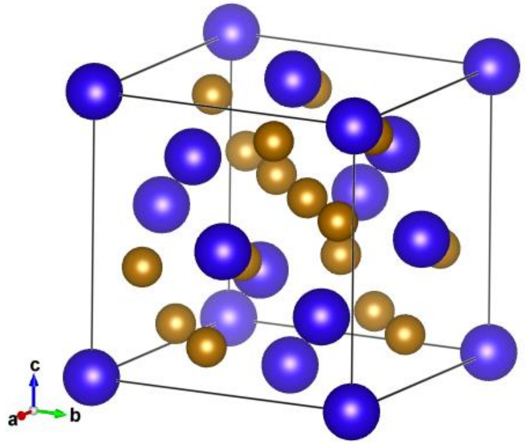


Table 16-10. Low-temperature magnetostriction constants for RCo_2 crystals [from Levitin and Markosyan (1990) unless otherwise noted].

R in RCo_2	$10^6\ \lambda_{111}$	$10^6\ \lambda_{100}$	T_c (K)[a]
Gd	$<10^{-5}$	−1200	409
Tb	4500	−1200[b]	256
Dy	5000[b, c]	−2000[d]	159
		−1300[e]	
Ho	300, 600[c]	−2000	85
Er	−2500	−1000	36
Tm	−4100[b]	750[c]	18

Table 1.6. Magnetostriction of Cubic Laves Phase Compounds with Rare Earths at $T = 0$

Compound	$\lambda_{111}\,(10^{-6})$	$\lambda_{100}\,(10^{-6})$	T_c (K)
$NdAl_2$	—	−700	61
$TbAl_2$	−3000	—	114
$DyAl_2$	—	−1700	68
$TbMn_2$	−3000	—	40
$TbFe_2$	4000, 4500	—	711
$DyFe_2$	—	−70	635
$HoFe_2$	—	−750	612
$TmFe_2$	−3500, −2600	—	610
$TbCo_2$	4400	—	256
$DyCo_2$	—	−2000	159
$HoCo_2$	—	−2200	85
$ErCo_2$	−2500	—	36
$TbNi_2$	1500	—	45
$DyNi_2$	—	−1300	30
$HoNi_2$	—	−1000	22

Table 1.7. Magnitudes of Single-Crystal Magnetostriction in Rare Earth–Fe_2 Compounds

Compound	$\frac{3}{2}\lambda_{111}$ (10^{-6}) (calculated at 0 K)	$\frac{3}{2}\lambda_{111}$ (10^{-6}) (measured at room temperature)	T_c
$SmFe_2$	−4800	−3150	676
$TbFe_2$	6600	3690	697, 711
$DyFe_2$	6300	1890	635
$HoFe_2$	2400	288	606
$ErFe_2$	−2250	−450	590, 597
$TmFe_2$	−5550	−315	560

BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

Hexagonal Rare-Earth

TABLE 6

Magnetostriction coefficients at zero Kelvin in units of 10^{-3}

Element	$\lambda_1^{\alpha,2}$	$\lambda_2^{\alpha,2}$	$\lambda^{\gamma,2}$	$\lambda^{\epsilon,2}$	$\lambda_1^{\alpha,0}-\frac{1}{3}\lambda_1^{\alpha,2}$	$\lambda_2^{\alpha,0}-\frac{1}{3}\lambda_2^{\alpha,2}$	$\lambda^{\gamma,4}$
Gadolinium[a)]	0.14	−0.13	0.11	0.02	–	–	–
Terbium[b)]	−2.6[c)]	9.0[c)]	8.7	15.0[c)]	−0.8	4.3	−2.1
Dysprosium[b)]	–	–	9.4	5.5	−2.0	7.3	1.5
Holmium[b)]	–	–	2.5[c)]	–	−3.9	7.1	–
Erbium[b)]	–	–	−5.1[c)]	–	+0.3	6.2	–

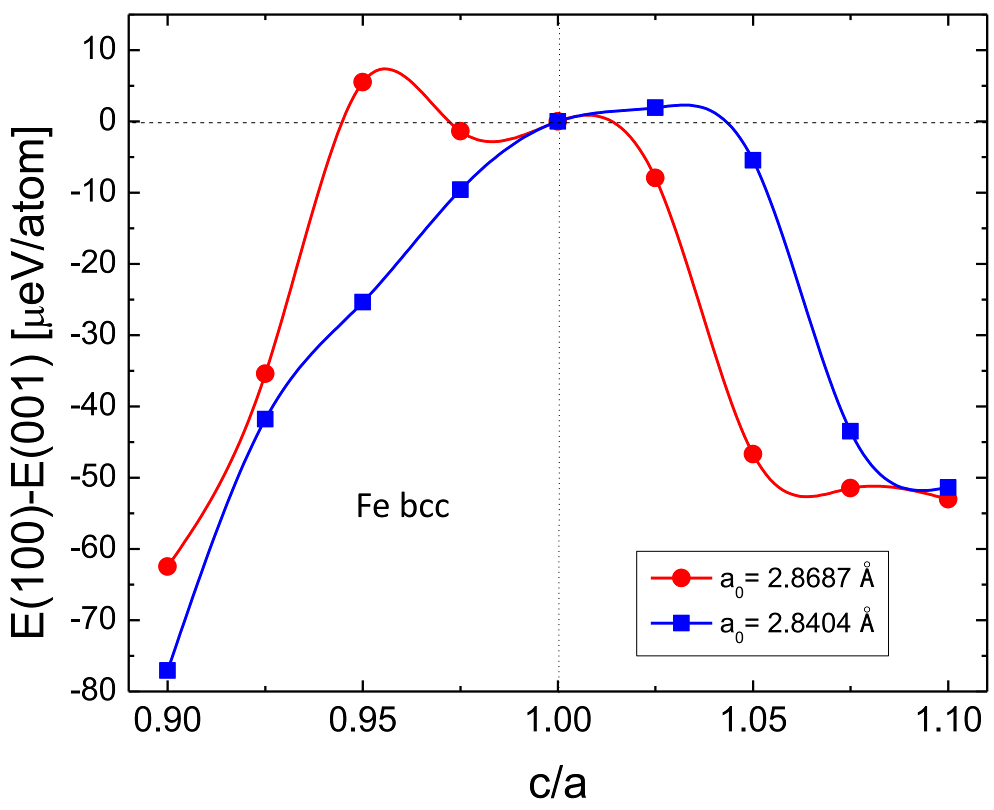
[a)] After Mishima et al. (1976).
[b)] After Rhyne (1972).
[c)] Extrapolated from paramagnetic range using single-ion theory.

Oxide magnets

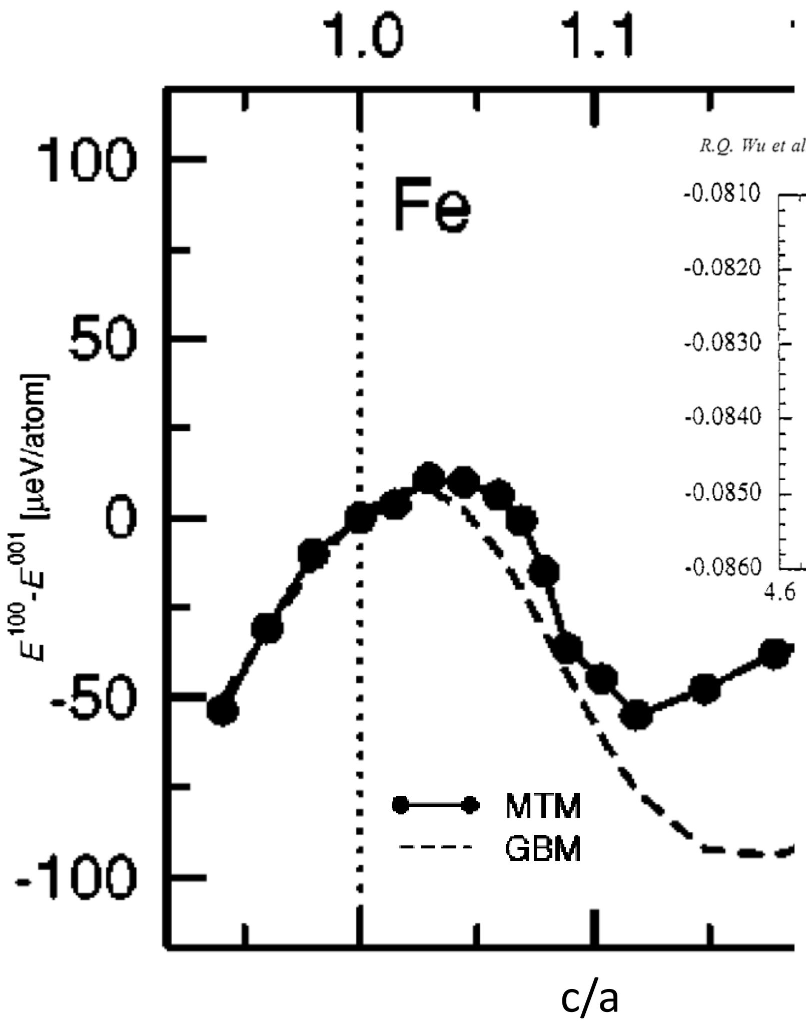
	$T = 4.2\,K$		Room Temperature		
	$\lambda_{100}(\lambda^{\gamma,2})$	$\lambda_{111}(\lambda^{\varepsilon,2})$	$\lambda_{100}(\lambda^{\gamma,2})$	$\lambda_{111}(\lambda^{\varepsilon,2})$	Polycrystal λ_s
		Spinel Ferrites			
Fe_3O_4	0	50	−15	56	+40
$MnFe_2O_4^{\prime\prime}$	—	—	(−54)	(10)	—
$CoFe_2O_4$	—	—	−670	120	−110
		Garnets			
YIG	−0.6	−2.5	−1.4	−1.6	−2

MAELAS TESTS: Fe bcc

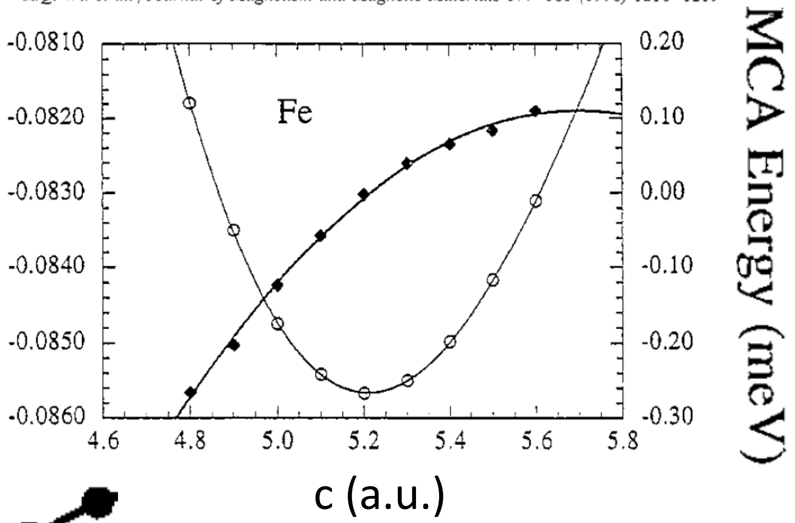
MAELAS code



PHYSICAL REVIEW B **69**, 104426 (2004)



R.Q. Wu et al. / Journal of Magnetism and Magnetic Materials 177–181 (1998) 1216–1219

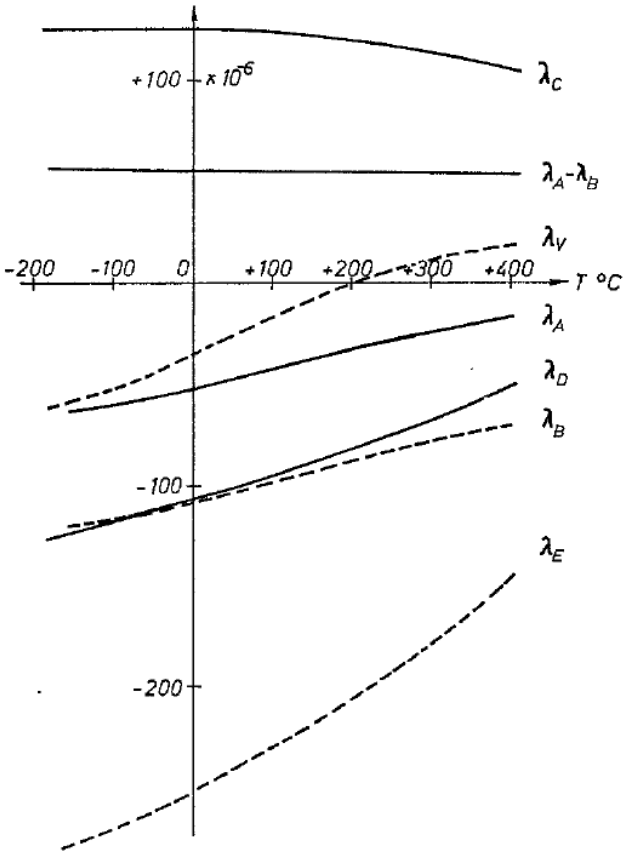


MAELAS (kp=185) $\lambda_{001} = 13 \cdot 10^{-6}$

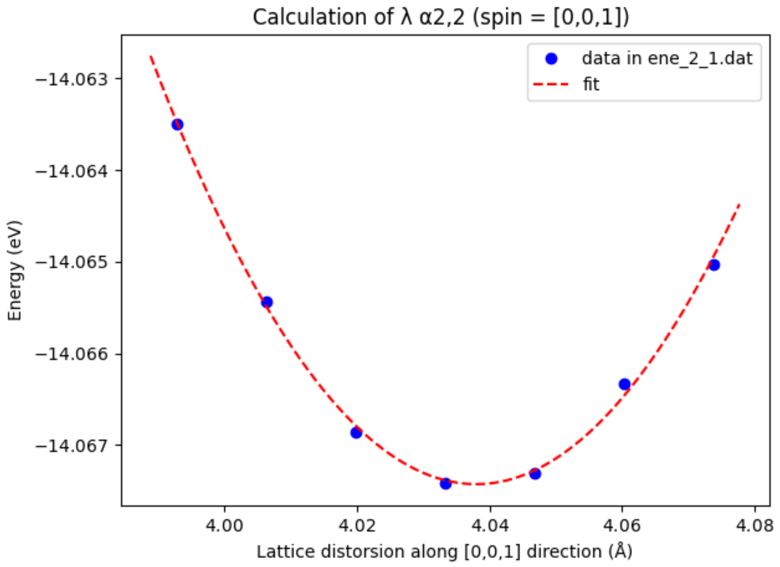
Exp. $\lambda_{001} = 26 \cdot 10^{-6}$

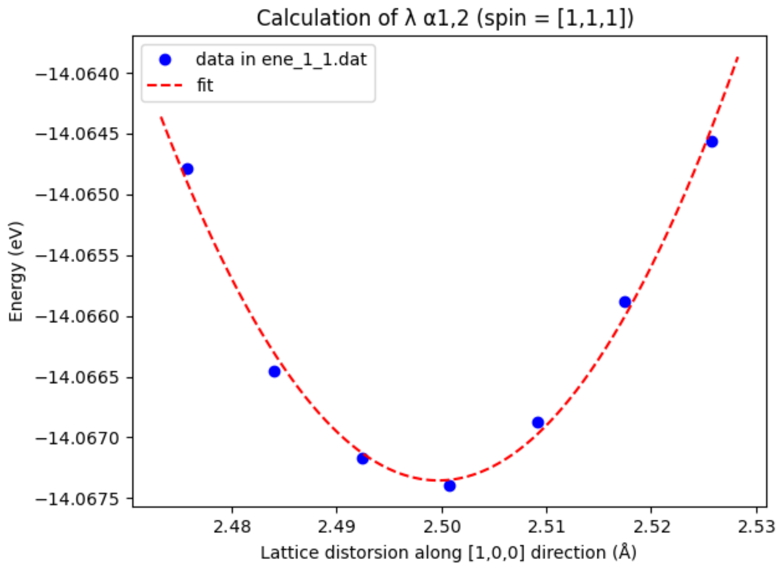
MAELAS TESTS: Co hcp

Z. Physik 224, 148—155 (1969)



	Experiment (x 10^{-6})	MAELAS kp=70 (x 10^{-6})
λA	-66	-10
λB	-123	-26
λC	126	25
λD	-128	-11



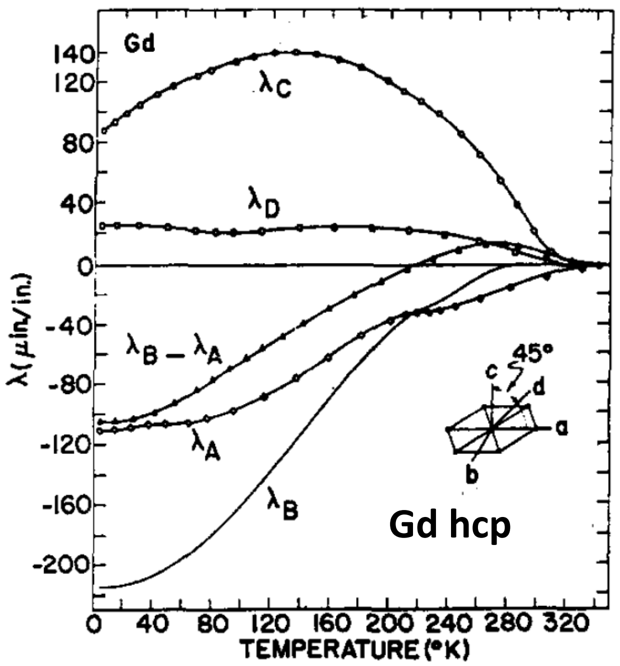


Magnetocrystalline anisotropy energy ratio for the relaxed structure: K1 exp. / K1 theory = 0.7 / 0.13 = 5.38

MAELAS TESTS: Gd hcp

Experiments

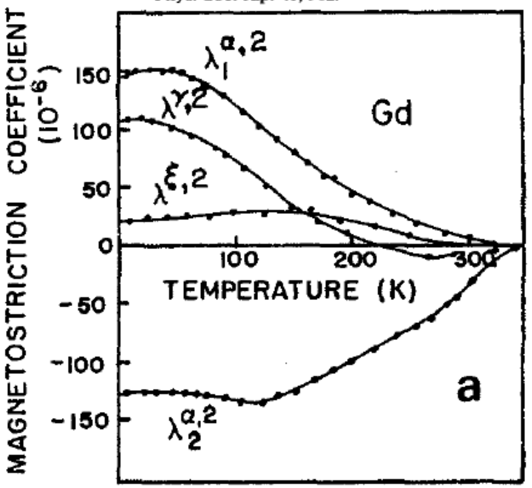
Journal of Applied Physics **35**, 1752 (1964)

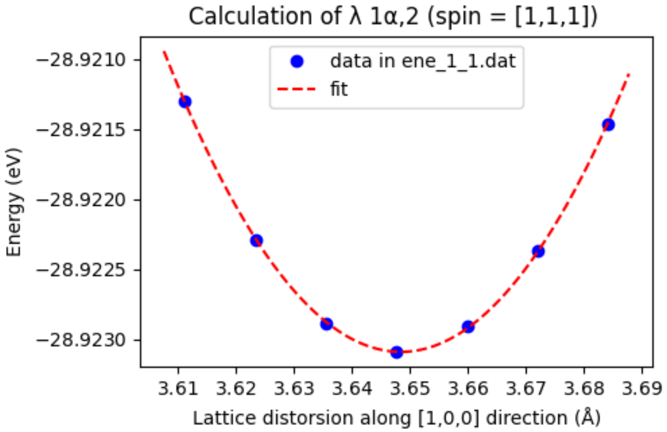


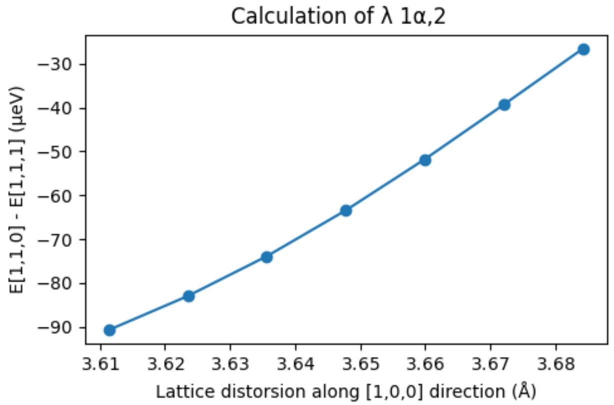
	Experiment (x 10^{-6})	MAELAS (x 10^{-6})
λA	-110	-262
λB	-215	-305
λC	85	521
λD	22	22

LDAUU=6.7
LDAUJ=0.7
kpoints 22x22x11

Mishima, A., H. Fujii and T. Okamoto, 1976, J. Phys. Soc. Jap. 40, 962.



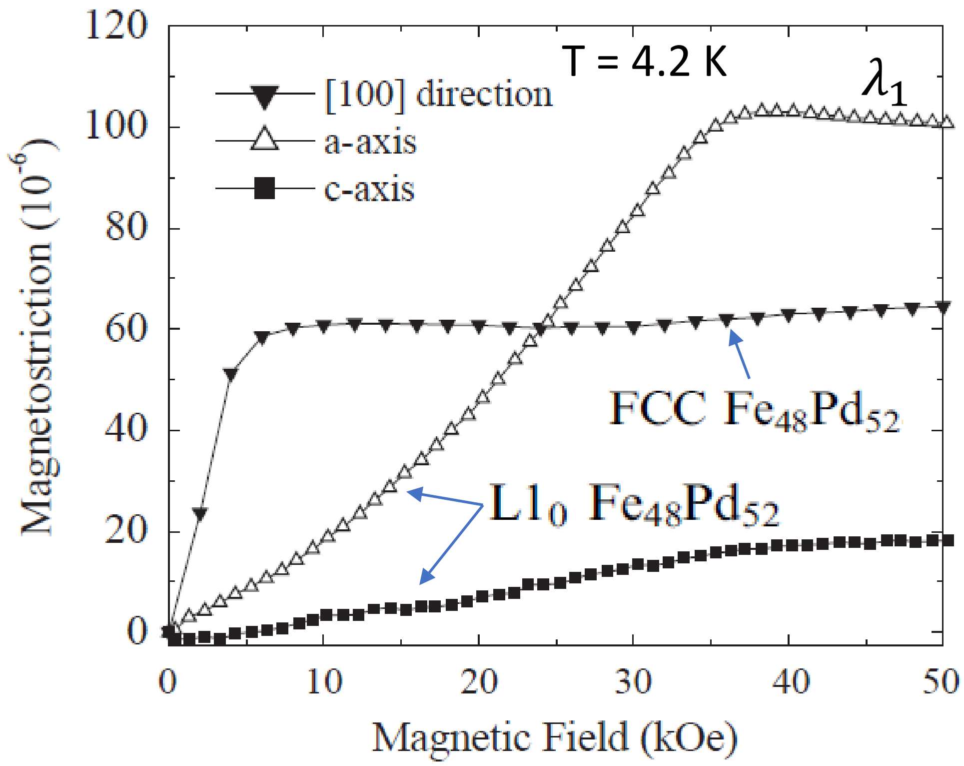




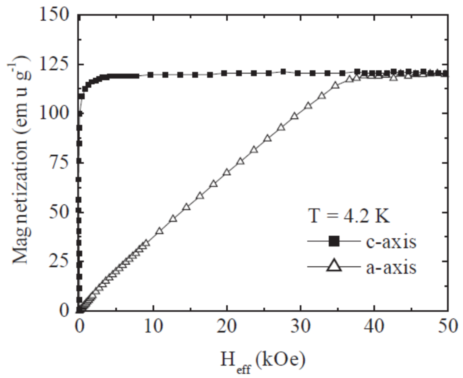
MAELAS TESTS: $L1_0$ FePd

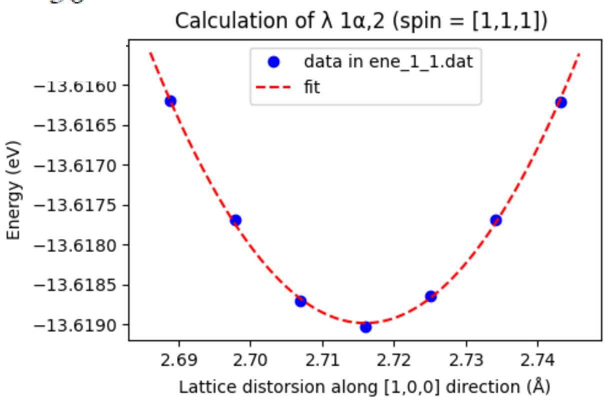
Experiment

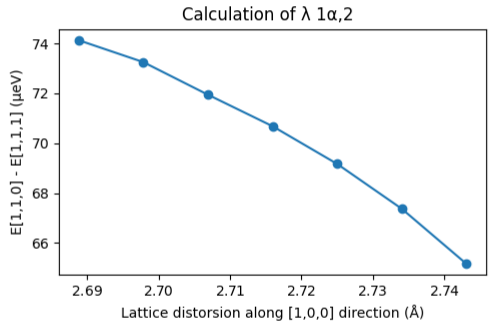
H. Shima et al. / Journal of Magnetism and Magnetic Materials 272–276 (2004) 2173–2174



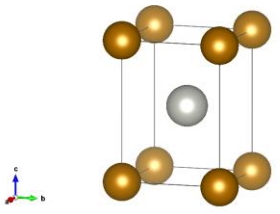
	Experiment (x 10^{-6})	MAELAS kp=70 (x 10^{-6})
λ1	100	28
λ2	-	-10
λ3	-	83
λ4	-	-75
λ5	-	20







$L1_0$ FePd



Crystal system=tetragonal
Space group=123

Magnetocrystalline anisotropy energy ratio for the relaxed structure: K1 exp. / K1 theory = 2.5 / 1.2 = 2.1

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