

MAELAS code

User manual v1.0

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- INSTALLATION
- HOW TO USE MAELAS CODE
- WORKFLOW
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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
```

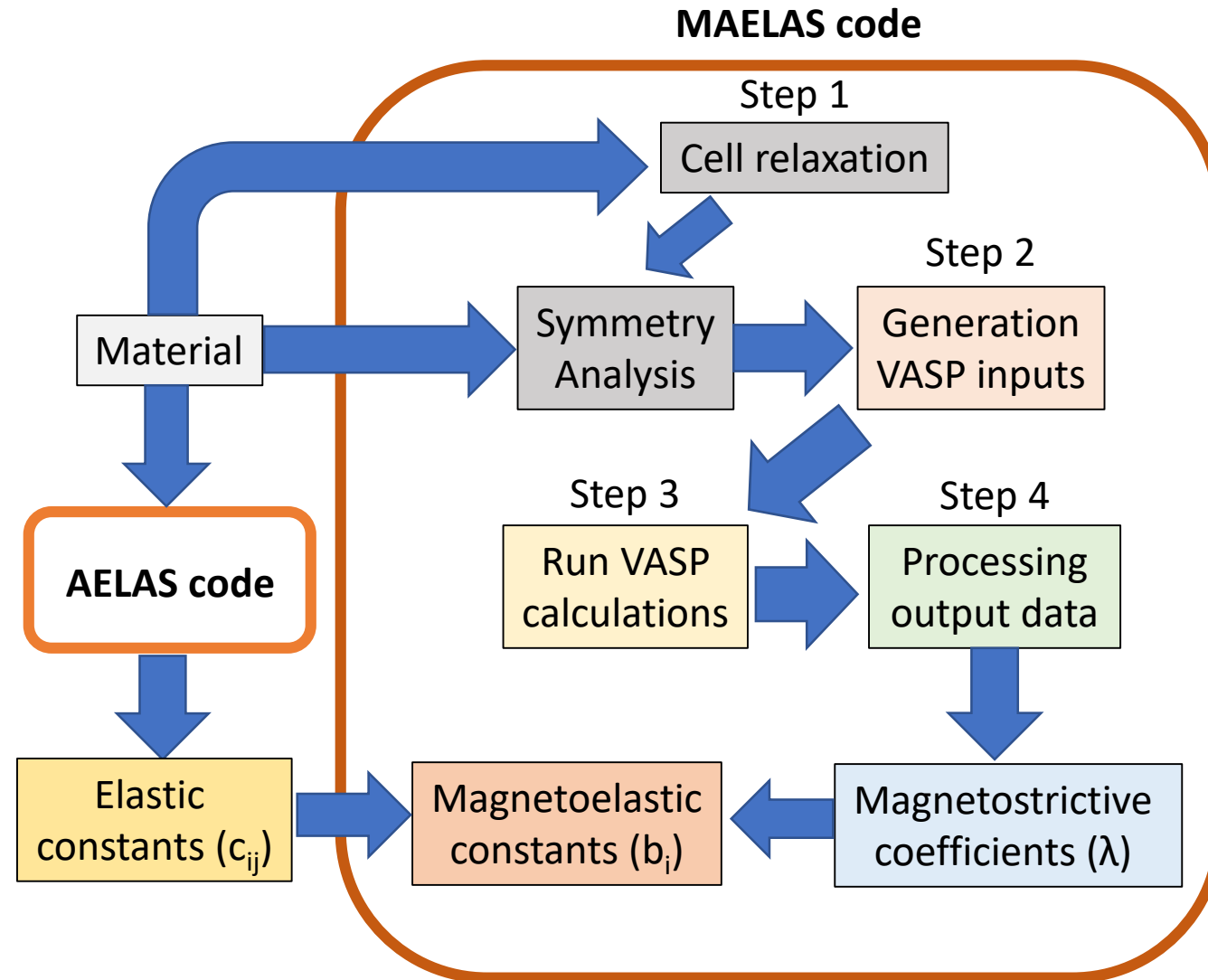
Additionally, MAELAS makes use of the following python libraries: pymatgen, scikit-learn, pyfiglet, argparse, numpy, matplotlib, scipy, math, os and stat. In case you need to install them, you can do it using pip3 as:

```
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 magnetostriction 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 queue the 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 immediately 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 magnetostriction 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 magnetostriction 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 queue the 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 and 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 magnetostriction 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
```

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

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

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).
- 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

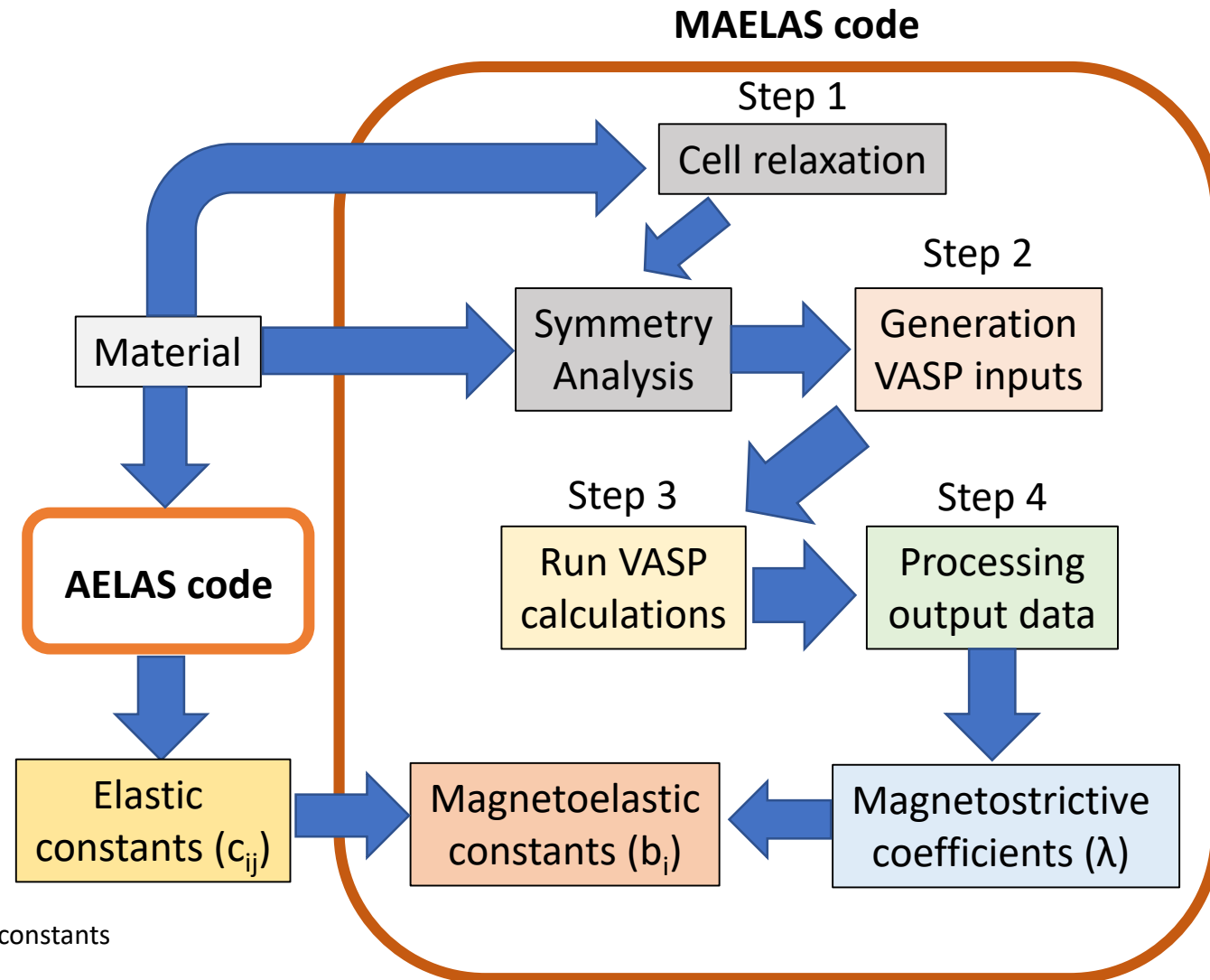
```
python3 maelas.py -d -i POSCAR_rlx -n 7
```

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
```



HOW TO USE MAELAS CODE

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-09	868760	0.143E-04	
1 F=	-0.21909285E+02	E0= -0.21909330E+02	d E =	0.135168E-03	mag=	0.0000	0.0000 2.5077

HOW TO USE MAELAS CODE

Crystal systems supported by MAELAS v1.0

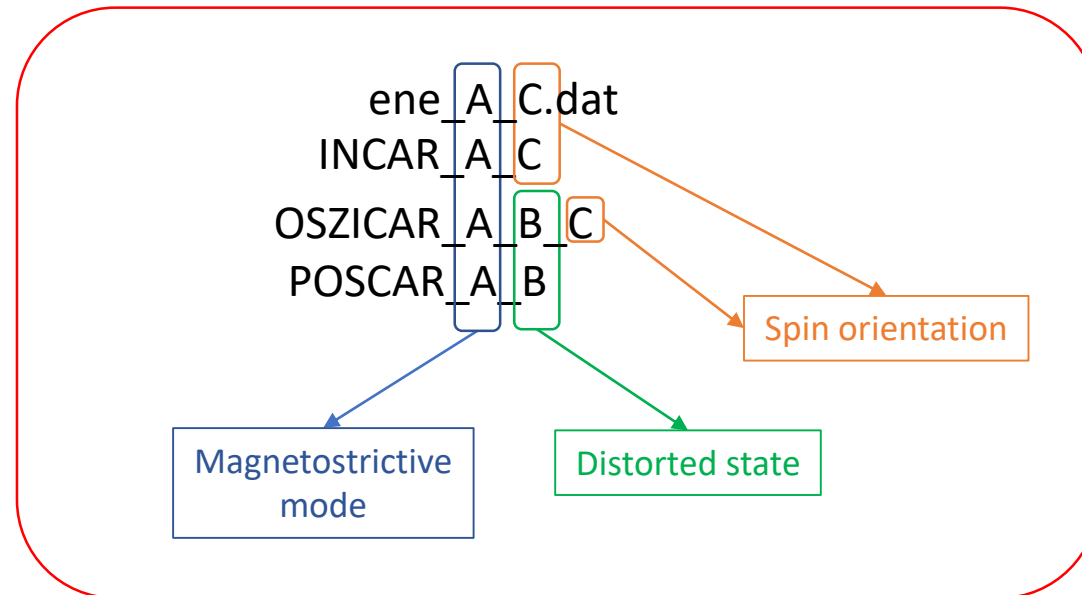
Current version supports the following crystal systems:

- 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

MAELAS file notation



Magnetostriction coefficients

Not supported by MAELAS v1.0

PHYSICAL REVIEW
VOLUME 139, NUMBER 2A
19 JULY 1965

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 magnetostriction 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
Monoclinic SG 3-15	2, m , $2/m$	x^2, y^2, z^2, xy xz, yz	1 1	10 3	13	12 4
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
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 7 1	3 4 9	4 4 10
Tetragonal SG 89-142	422, $4/mmm$, $4mm$, $42m$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $\frac{1}{2}(x^2-y^2)$ xy $[yz, xz]$	1 1 1 2	3 6 1 1	3 6 1 1	4 7 1 1
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
Trigonal SG 149-167	32, $3m$, $3m$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $[(x^2-y^2)/2, xy]$, $[yz, xz]$	1 2	3 6	3 7	4 8
SG 168-174	6, $\bar{6}$, $6/m$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $\{xy, xz\}$	1 1 complex 1 complex	3 1 5	3 2 7	4 2 8
Hexagonal SG 175-176	622, $6mm$, $6m2$, $6/mmm$	$x^2+y^2+z^2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $[yz, xz]$ $[(x^2-y^2)/2, xy]$	1 2 2	3 5 1	3 5 1	4 6 1
SG 195-206	23, $m\bar{3}$	$x^2+y^2+z^2$ $\{(x^2-y^2)/2, (\sqrt{3}/2)(z^2-\frac{1}{3}r^2)\}$	1 1 complex 1 complex	1 3 3	0 3 3	1 2 4
Cubic SG 207-230	432, $\bar{4}3m$, $m\bar{3}m$	$x^2+y^2+z^2$ $[xy, yz, xz]$ $(x^2-y^2)/2$, $(\sqrt{3}/2)(z^2-\frac{1}{3}r^2)$ $[xy, yz, xz]$	1 3 2 3	1 1 3 1	0 2 2 1	1 1 3 1

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

$$\frac{\Delta l}{l} \Big|_{\text{tetragonal}} = \lambda^{1,0}(\beta_x^2 + \beta_y^2) + \lambda^{2,0}\beta_z^2 + \lambda^{1,2}(\alpha_z^2 - \frac{1}{3})(\beta_x^2 + \beta_y^2) + \lambda^{2,2}(\alpha_z^2 - \frac{1}{3})\beta_z^2 + \frac{1}{2}\lambda^{\gamma,2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + 2\lambda^{\delta,2}\alpha_x\alpha_y\beta_x\beta_y + 2\lambda^{\epsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z) \quad (16-34)$$

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

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

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

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

$$\frac{\Delta l}{l} \Big|_{\text{cubic}} = \lambda\alpha + \frac{3}{2}\lambda_{100}(\alpha_x^2\beta_x^2 + \alpha_y^2\beta_y^2 + \alpha_z^2\beta_z^2 - \frac{1}{3}) + 3\lambda_{111}(\alpha_x\alpha_y\beta_x\beta_y + \alpha_y\alpha_z\beta_y\beta_z + \alpha_x\alpha_z\beta_x\beta_z)$$

Elastic constants

Not supported by MAELAS v1.0

PHYSICAL REVIEW B 90, 224104 (2014)

	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

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

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

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

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

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

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

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

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

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

Workflow

CUBIC (I)

SG 207-230

Cubic (I)

Workflow

Elastic energy

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

Magnetoelastic energy

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

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

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

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

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

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

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

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}

λ_{111}

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])

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_1_X_1
OSZICAR_1_X_2

OSZICAR_2_X_1
OSZICAR_2_X_2

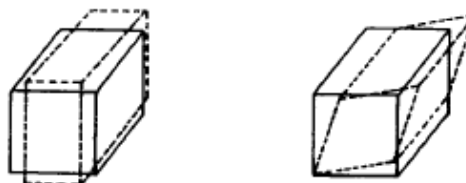
x=cell length along deformation

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

$$\lambda_{001} = \frac{2}{3} \cdot \frac{x_{\min 1} - x_{\min 2}}{x_{\min 1}}$$

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

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



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

Workflow

CUBIC (II)

SG 195-206

Cubic (II)

Workflow

Elastic energy

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

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

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

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

Magnetoelastic energy

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

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

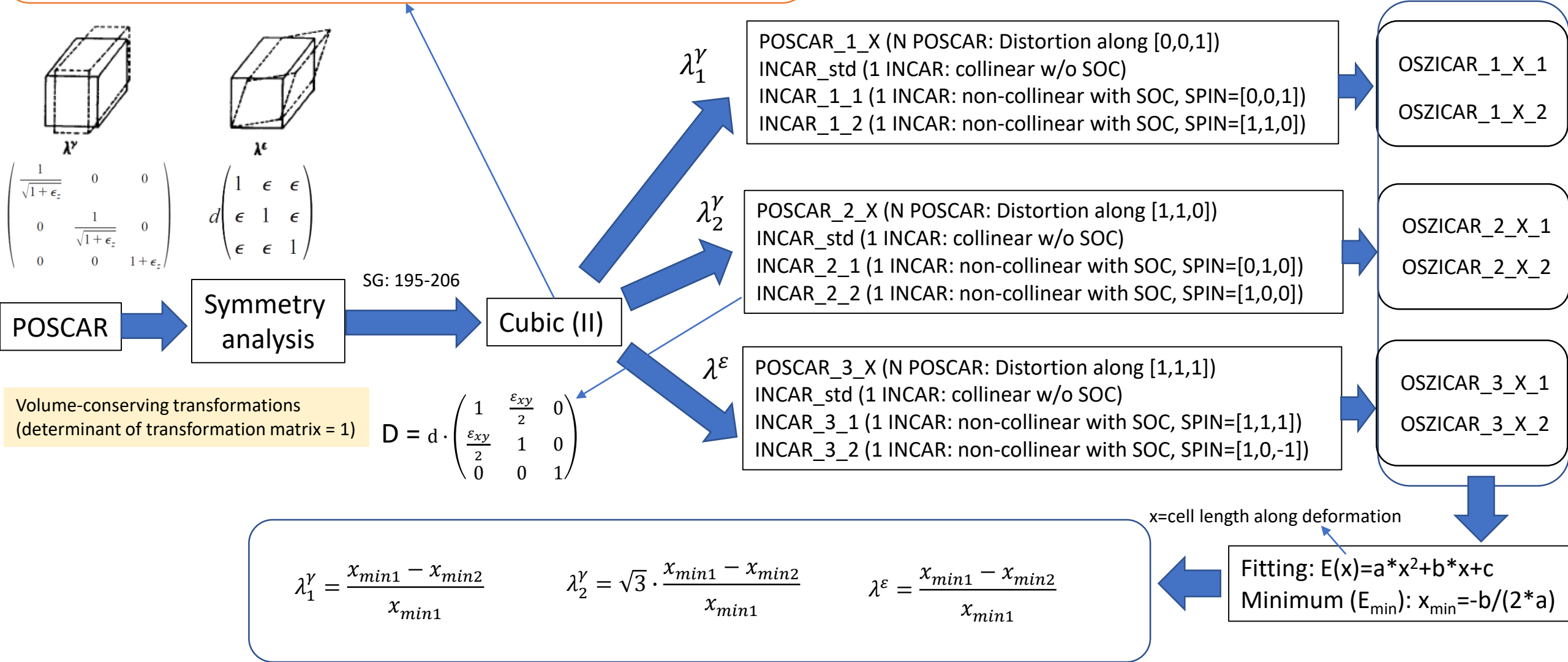
$$b_1 = (c_{11} - c_{12}) \lambda_1^\gamma$$

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

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

Workflow

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



Workflow

HEXAGONAL (I)

SG 177-194

Hexagonal (I)

Workflow

Elastic energy

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

Magnetoelastic energy

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

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

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

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

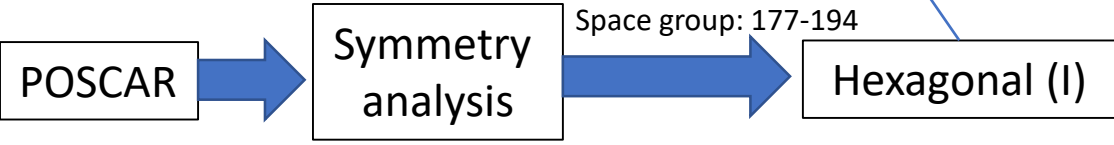
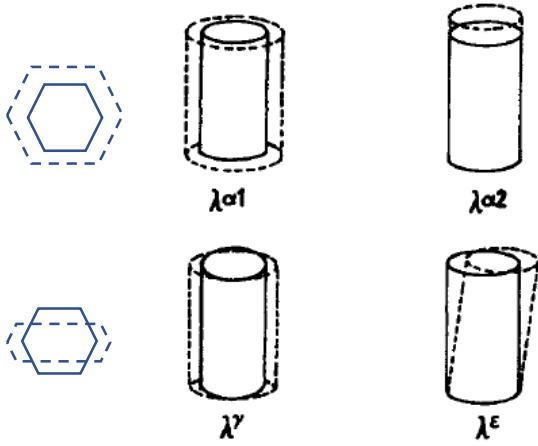
$$\left. \frac{\Delta l}{l} \right|_{\text{Hex}} = \lambda^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0} + \lambda^{\alpha 1,2} (\alpha_z^2 - 1/3) (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,2} (\alpha_z^2 - 1/3) \beta_z^2 + \lambda^{\gamma,2} (\frac{1}{2} (\alpha_x^2 - \alpha_y^2) (\beta_x^2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

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

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

Workflow

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



$\lambda^{\alpha 1,2}$

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

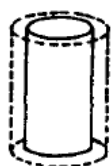
x=cell length along deformation

$$\lambda^{\alpha 1,2} = 3 \cdot \frac{x_{\min 1} - x_{\min 2}}{x_{\min 1}} \quad \lambda^{\alpha 2,2} = \frac{x_{\min 1} - x_{\min 2}}{x_{\min 1}} \quad \lambda^{\gamma,2} = \frac{x_{\min 1} - x_{\min 2}}{x_{\min 1}} \quad \lambda^{\varepsilon,2} = \frac{x_{\min 1} - x_{\min 2}}{x_{\min 1}}$$

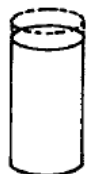
Fitting: $E(x)=a \cdot x^2+b \cdot x+c$
 Minimum (E_{\min}): $x_{\min}=-b/(2 \cdot a)$

Hexagonal

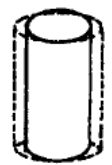
Distorted states



$\lambda^{\alpha 1}$



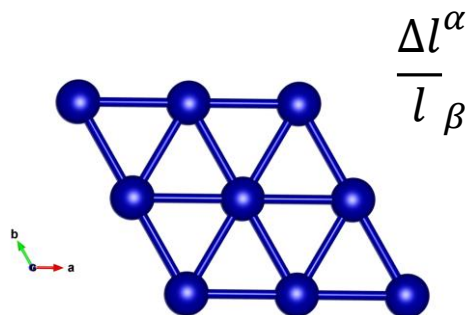
$\lambda^{\alpha 2}$



λ^γ



λ^ϵ



$$|\alpha| = 1, |\beta| = 1$$

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

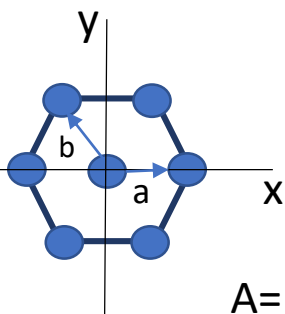
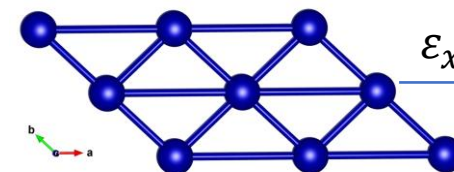
$$\frac{\Delta l}{l} = \epsilon_{xx} = \lambda^{\alpha 1} \left(\alpha_z^2 - \frac{1}{3} \right) + \lambda^\gamma (\alpha_x^2 - \alpha_y^2) \frac{1}{2}$$

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

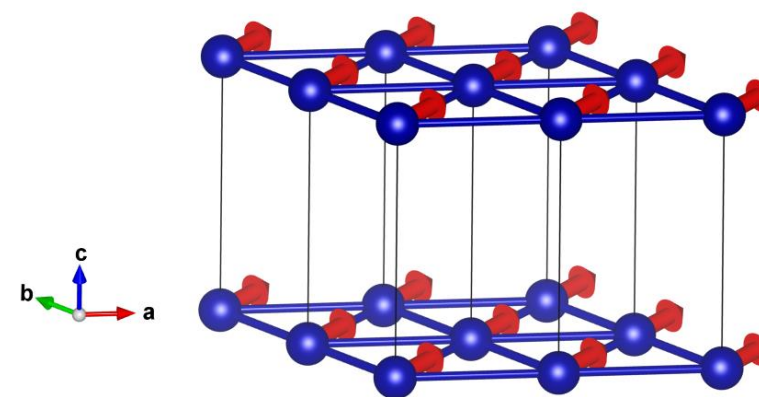
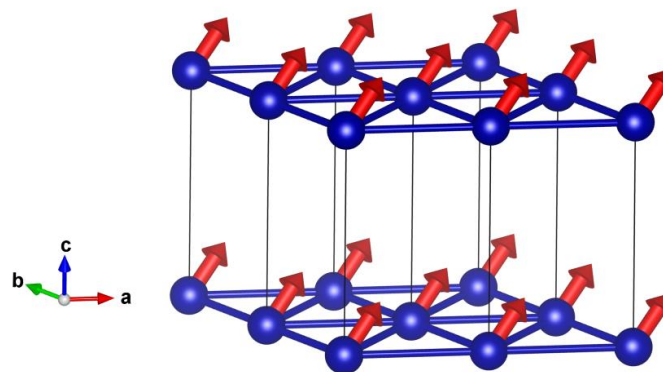
$$\begin{aligned} \left. \frac{\Delta l}{l} \right|_{\text{Hex}} &= \lambda^{\alpha 1, 0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2, 0} + \\ &+ \lambda^{\alpha 1, 2} (\alpha_z^2 - \frac{1}{3}) (\beta_x^2 + \beta_y^2) + \\ &+ \lambda^{\alpha 2, 2} (\alpha_z^2 - \frac{1}{3}) \beta_z^2 + \\ &+ \lambda^{\gamma,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

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

volume-conserving



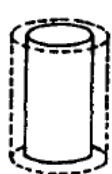
$$A = \begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$



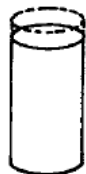
$$\lambda^{\alpha 1, 2} = 3 \cdot \frac{x_{min1} - x_{min2}}{x_{min1}}$$

Hexagonal

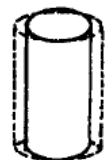
Distorted states



$\lambda^{\alpha 1}$



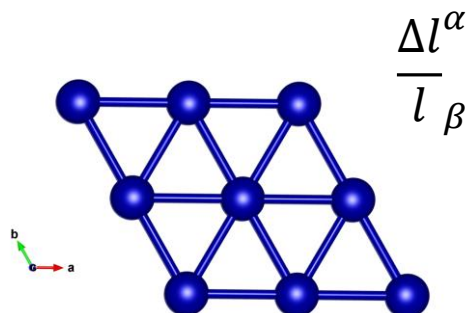
$\lambda^{\alpha 2}$



λ^{γ}



λ^{ϵ}



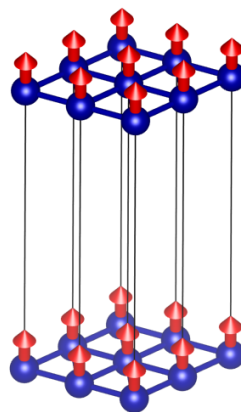
$$\frac{\Delta l^{\alpha}}{l} \beta$$

$$|\alpha| = 1, |\beta| = 1$$

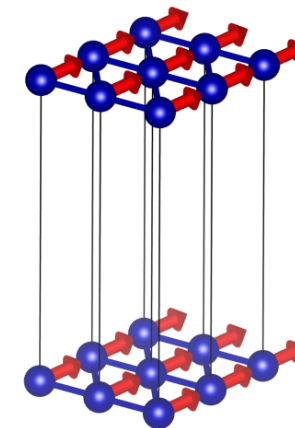
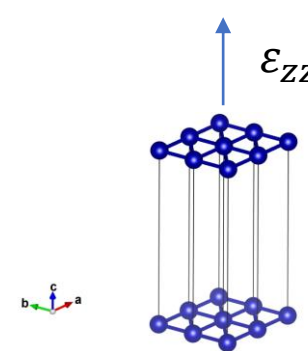
strain along z-axis: $\beta = (0,0,1)$

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

$$\lambda^{\alpha 2,2} \rightarrow \frac{\Delta l^{(0,0,1)}}{l_{(0,0,1)}} - \frac{\Delta l^{(1,0,0)}}{l_{(0,0,1)}} = \lambda^{\alpha 2,2}$$



$$S=(0,0,1)$$



$$S=(1,0,0)$$



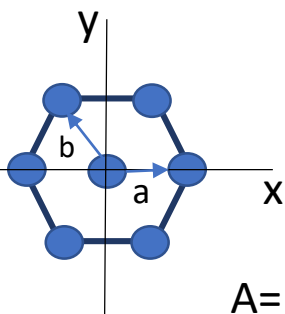
$$\begin{aligned} \left. \frac{\Delta l}{l} \right|_{\text{Hex}} &= \lambda^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0} + \\ &+ \lambda^{\alpha 1,2} (\alpha_z^2 - \frac{1}{3}) (\beta_x^2 + \beta_y^2) + \\ &+ \lambda^{\alpha 2,2} (\alpha_z^2 - \frac{1}{3}) \beta_z^2 + \\ &+ \lambda^{\gamma,2}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

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

volume-conserving

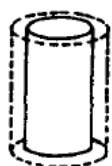
$$A = \begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

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

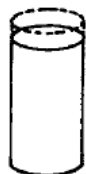


Hexagonal

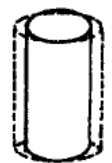
Distorted states



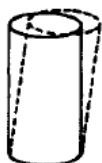
$\lambda^{\alpha 1}$



$\lambda^{\alpha 2}$

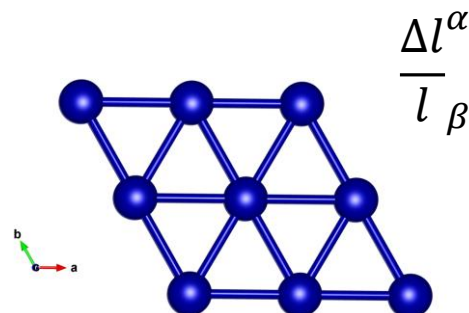


λ^{γ}



λ^{ϵ}

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



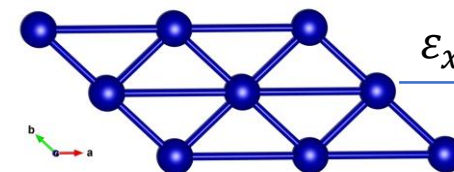
$$|\alpha| = 1, |\beta| = 1$$

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

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

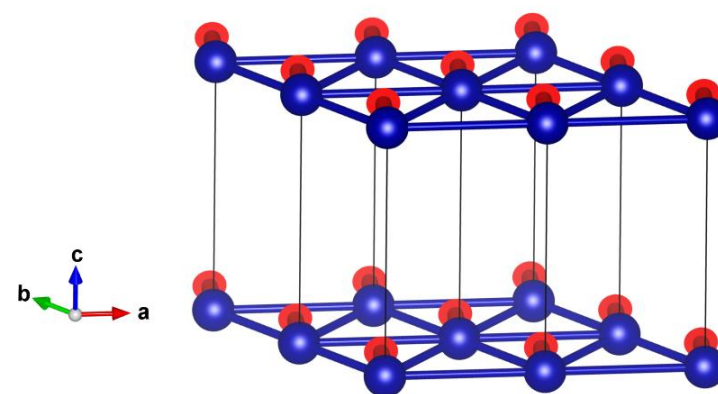
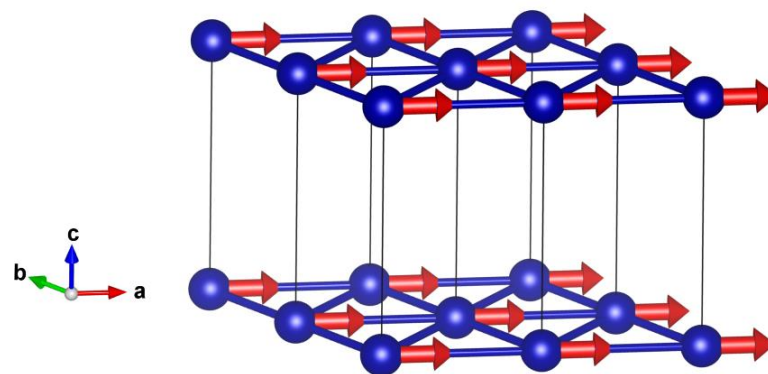
$$\lambda^{\gamma, 2} \Rightarrow \frac{\Delta l^{(1,0,0)}}{l_{(1,0,0)}} - \frac{\Delta l^{(0,1,0)}}{l_{(1,0,0)}} = \lambda^{\gamma, 2}$$

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



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

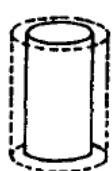
volume-conserving



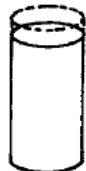
$$\lambda^{\gamma, 2} = \frac{x_{min1} - x_{min2}}{x_{min1}}$$

Hexagonal

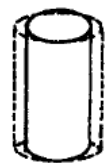
Distorted states



$\lambda^{\alpha 1}$



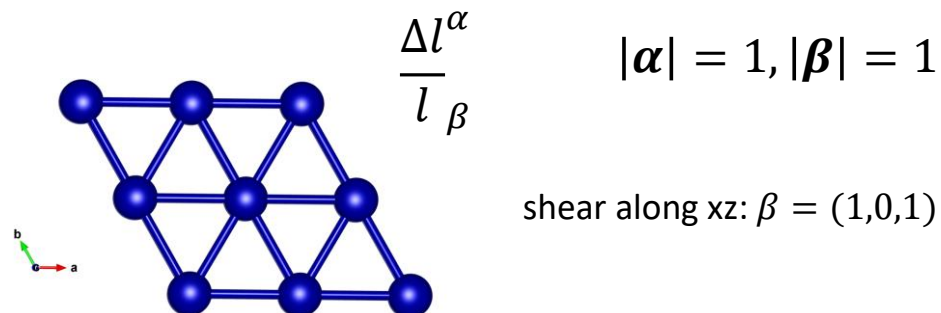
$\lambda^{\alpha 2}$



λ^{γ}

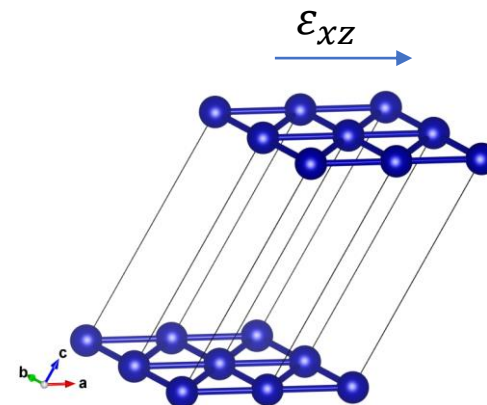


λ^{ϵ}



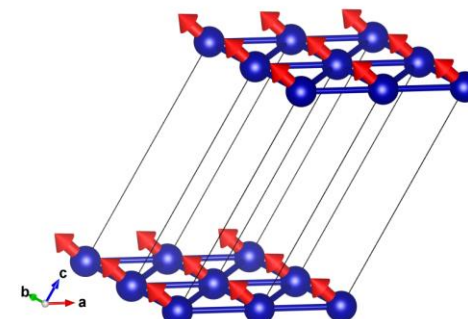
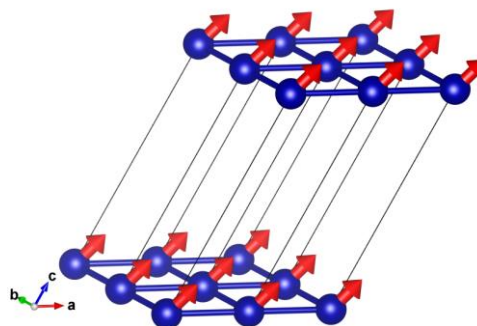
$$\lambda^{\epsilon, 2} \rightarrow \frac{\Delta l^{(1,0,1)}}{l_{(1,0,1)}} - \frac{\Delta l^{(-1,0,1)}}{l_{(1,0,1)}} = \lambda^{\epsilon, 2}$$

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



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

volume-conserving



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

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

Relation between different notations

Clark

Hexagonal system

PHYSICAL REVIEW
VOLUME 138, NUMBER 1A
5 APRIL 1965

PHYSICAL REVIEW
VOLUME 139, NUMBER 2A
19 JULY 1965

Callen

$$\begin{aligned}\lambda_{11}^\alpha &= 2\lambda_1^{\alpha,0} + \lambda_2^{\alpha,0} + 2\lambda_1^{\alpha,2} + \lambda_2^{\alpha,2}, \\ (\sqrt{3}/2)\lambda_{12}^\alpha &= 2\lambda_1^{\alpha,2} + \lambda_2^{\alpha,2}, \\ 2\lambda_{21}^\alpha &= -\lambda_1^{\alpha,0} + \lambda_2^{\alpha,0}, \\ \sqrt{3}\lambda_{22}^\alpha &= -\lambda_1^{\alpha,2} + \lambda_2^{\alpha,2}.\end{aligned}$$

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

^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

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

Workflow

HEXAGONAL (II) – point group 6/m

SG 175-176

Elastic energy

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

Magnetoelastic energy

$$E_{me}|_{hex} = b_{11} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12} \varepsilon_{zz} + b_{21} (\alpha_z^2 - \frac{1}{3}) (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12} (\alpha_z^2 - \frac{1}{3}) \varepsilon_{zz} + \frac{1}{2} b_3 ((\alpha_x^2 - \alpha_y^2) (\varepsilon_{xx} - \varepsilon_{yy}) + 2 \alpha_x \alpha_y \varepsilon_{xy}) + b_4 (\alpha_x \alpha_z \varepsilon_{xz} + \alpha_y \alpha_z \varepsilon_{yz}) + b_5 (\alpha_x \alpha_z \varepsilon_{yz} - \alpha_y \alpha_z \varepsilon_{xz}) \quad (16-29)$$

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

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

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

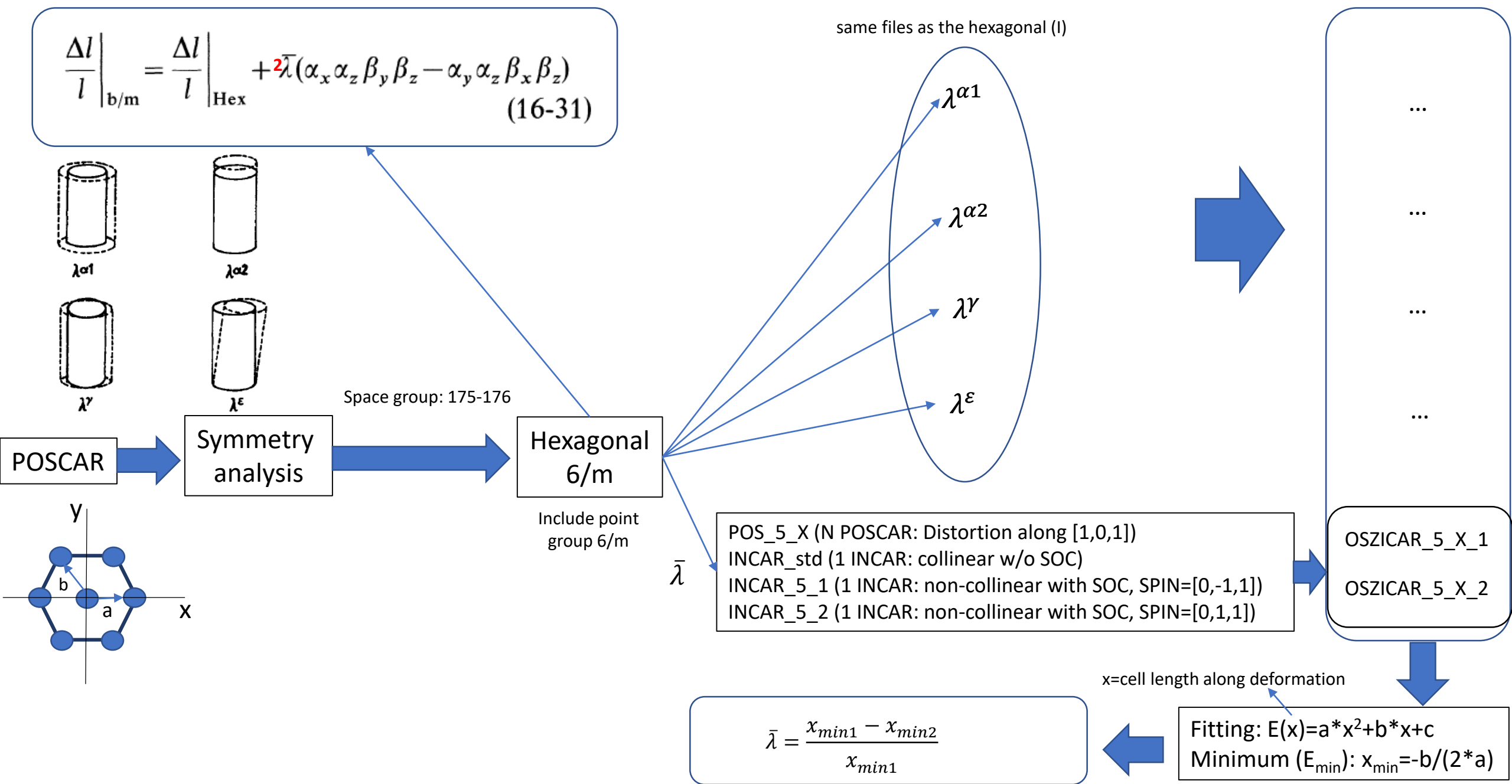
$$\left. \frac{\Delta l}{l} \right|_{b/m} = \left. \frac{\Delta l}{l} \right|_{Hex} + \bar{\lambda} (\alpha_x \alpha_z \beta_y \beta_z - \alpha_y \alpha_z \beta_x \beta_z) \quad (16-31)$$

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

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

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

Workflow

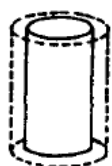


Hexagonal (II)
point group 6/m

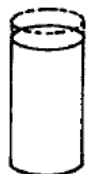
Distorted states

Include point
group 6/m

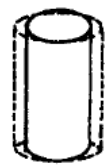
Space group: 175,191,192



$\lambda^{\alpha 1}$



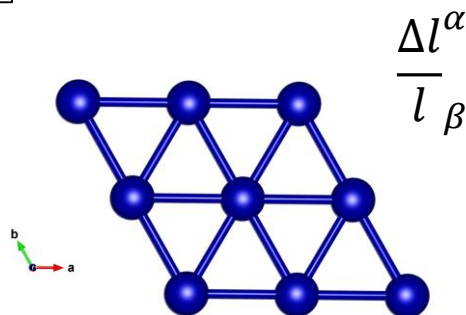
$\lambda^{\alpha 2}$



λ^{γ}



λ^{ϵ}

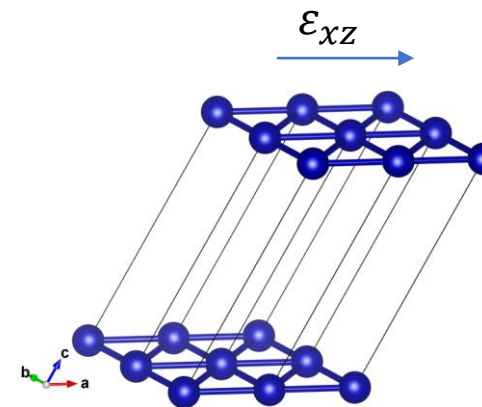


$$|\alpha| = 1, |\beta| = 1$$

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

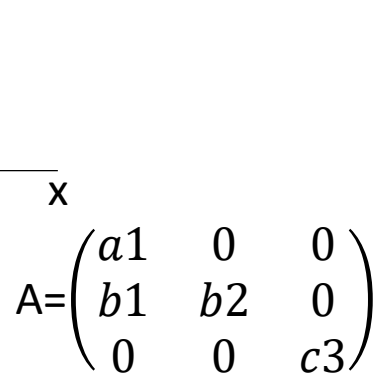
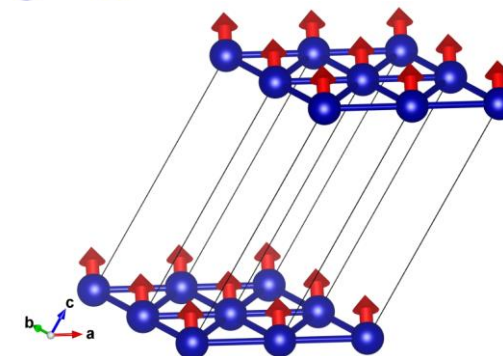
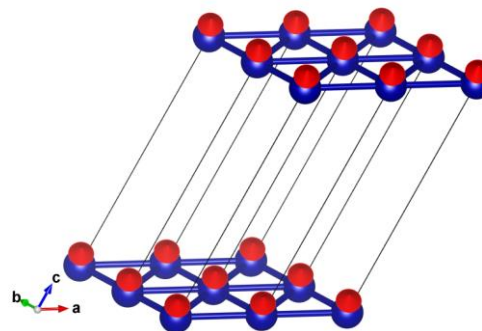
$$\bar{\lambda} \rightarrow \frac{\Delta l^{(0,-1,1)}}{l_{(1,0,1)}} - \frac{\Delta l^{(0,1,1)}}{l_{(1,0,1)}} = \frac{1}{2} \cdot \bar{\lambda}$$

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



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

volume-conserving



$$\bar{\lambda} = 2 \cdot \frac{x_{\min 1} - x_{\min 2}}{x_{\min 1}}$$

Workflow

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

SG 168-174

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

Workflow

TRIGONAL (I)

SG 149-167

Trigonal (I)

Elastic energy

$$E_{el}^{trig(I)} = \frac{c_{11}\epsilon_{xx}^2}{2} + \frac{1}{4}(c_{11} - c_{12})\epsilon_{xy}^2 + c_{12}\epsilon_{xx}\epsilon_{yy} + \frac{c_{11}\epsilon_{yy}^2}{2} + c_{14}(\epsilon_{xy}\epsilon_{xz} + \epsilon_{xx}\epsilon_{yz} - \epsilon_{yy}\epsilon_{yz}) + c_{44}\left(\frac{\epsilon_{xz}^2}{2} + \frac{\epsilon_{yz}^2}{2}\right) + \frac{c_{33}\epsilon_{zz}^2}{2} + c_{13}(\epsilon_{xx}\epsilon_{zz} + \epsilon_{yy}\epsilon_{zz})$$

Magnetoelastic energy

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

Workflow

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

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

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

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

$$\lambda^{\gamma 1} = (C_{14}b_{34} - C_{44}b_3)/D^{\gamma} \quad (16-41 a)$$

$$\lambda^{\gamma 2} = \left(\frac{b_4}{2}(C_{11} - C_{12}) - b_{34}C_{14} \right) / D^{\gamma} \quad (16-41 b)$$

$$\lambda_{12} = (C_{14}b_4 - C_{44}b_{34})/D^{\gamma} \quad (16-41 c)$$

$$\lambda_{21} = \left(\frac{b_{14}}{2}(C_{11} - C_{12}) - C_{14}b_3 \right) / D^{\gamma} \quad (16-41 d)$$

where

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

$$\lambda^{\alpha 1,0} = (b_{11}c_{33} + b_{12}c_{13})/D$$

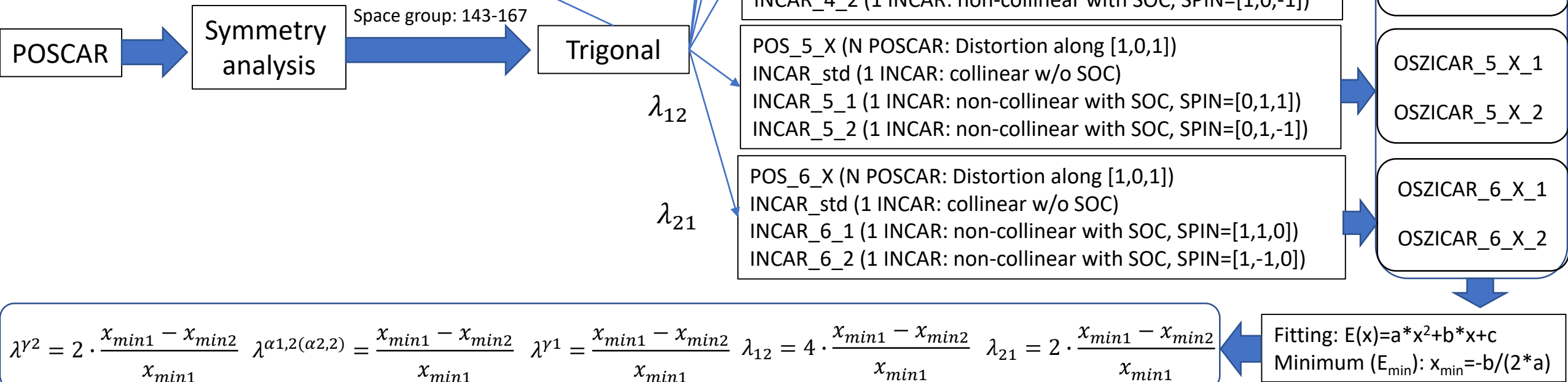
$$\lambda^{\alpha 2,0} = [2b_{11}c_{13} - b_{12}(c_{11} + c_{22})]/D$$

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

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

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

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



Workflow

TRIGONAL (II)

SG 143-148

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

Workflow

TETRAGONAL (I)

SG 89-142

Workflow

Tetragonal (I)

Elastic energy

$$E_{el}^{tet} = c_{12}\epsilon_{xx}\epsilon_{yy} + c_{11}\left(\frac{\epsilon_{xx}^2}{2} + \frac{\epsilon_{yy}^2}{2}\right) + c_{44}\left(\frac{\epsilon_{xz}^2}{2} + \frac{\epsilon_{yz}^2}{2}\right) + \frac{c_{33}\epsilon_{zz}^2}{2} + c_{13}(\epsilon_{xx}\epsilon_{zz} + \epsilon_{yy}\epsilon_{zz}) + \frac{c_{66}\epsilon_{xy}^2}{2}$$

Magnetoelastic energy

$$f_{me}^{tet} = b_{11}(\epsilon_{xx} + \epsilon_{yy}) + b_{12}\epsilon_{zz} + b_{21}(\alpha_z^2 - 1/3)(\epsilon_{xx} + \epsilon_{yy}) + b_{22}(\alpha_z^2 - 1/3)\epsilon_{zz} + \frac{1}{2}b_3(\alpha_x^2 - \alpha_y^2)(\epsilon_{xx} - \epsilon_{yy}) + b'_3\alpha_x\alpha_y\epsilon_{xy} + b_4(\alpha_x\alpha_z\epsilon_{xz} + \alpha_y\alpha_z\epsilon_{yz}),$$

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

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

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

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

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

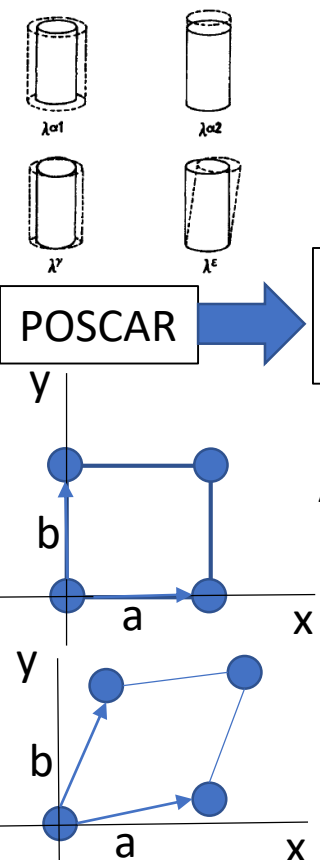
$$\lambda^{\delta,2} = \frac{-b'_3}{2c_{66}}$$

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

Workflow

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

same files as the hexagonal case



POSCAR

Space group: 75-142

Tetragonal

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

$a1 = b2$

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

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

volume-conserving

$\lambda^{\delta, 2}$

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])

$$\lambda^{\delta, 2} = \frac{x_{\min 1} - x_{\min 2}}{x_{\min 1}}$$

x=cell length along deformation

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

OSZICAR_5_X_1
 OSZICAR_5_X_2

Relation between different notations

Tetragonal (I)

Cullen

Mason

$$\left. \frac{\Delta l}{l} \right|_{\text{tetragonal}} = \lambda^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0} \beta_z^2 +$$

$$+ \lambda^{\alpha 1,2} (\alpha_z^2 - \frac{1}{3}) (\beta_x^2 + \beta_y^2) +$$

$$+ \lambda^{\alpha 2,2} (\alpha_z^2 - \frac{1}{3}) \beta_z^2 +$$

$$+ \frac{1}{2} \lambda^{\gamma,2} (\alpha_x^2 - \alpha_y^2) (\beta_x^2 - \beta_y^2) +$$

$$+ 2 \lambda^{\delta,2} \alpha_x \alpha_y \beta_x \beta_y +$$

$$+ 2 \lambda^{\epsilon,2} (\alpha_x \alpha_z \beta_x \beta_z + \alpha_y \alpha_z \beta_y \beta_z) \quad (16-34)$$

$$\lambda = \frac{1}{2} \lambda_1 [(\alpha_1 \beta_1 - \alpha_2 \beta_2)^2 - (\alpha_1 \beta_2 + \alpha_2 \beta_1)^2 + (1 - \beta_3^2)(1 - \alpha_3^2)$$

$$- 2 \alpha_3 \beta_3 (\alpha_1 \beta_1 + \alpha_2 \beta_2)] + 4 \lambda_2 \alpha_3 \beta_3 (\alpha_1 \beta_1 + \alpha_2 \beta_2)$$

$$+ 4 \lambda_3 \alpha_1 \alpha_2 \beta_1 \beta_2 + \lambda_4 [\beta_3^2 (1 - \alpha_3^2) - \alpha_3 \beta_3 (\alpha_1 \beta_1 + \alpha_2 \beta_2)]$$

$$+ \frac{1}{2} \lambda_5 [(\alpha_1 \beta_2 - \alpha_2 \beta_1)^2 - (\alpha_1 \beta_1 + \alpha_2 \beta_2)^2$$

$$+ (1 - \beta_3^2)(1 - \alpha_3^2)], \quad (74)$$

$$\left. \begin{aligned} \frac{\Delta l^{111}}{l_{100}} - \frac{\Delta l^{110}}{l_{100}} &= \frac{1}{3} \lambda^{\alpha 1,2} = -\frac{1}{6} \lambda_1 - \frac{1}{6} \lambda_5 \\ \frac{\Delta l^{100}}{l_{100}} - \frac{\Delta l^{010}}{l_{100}} &= \lambda^{\gamma,2} = \lambda_1 - \lambda_5 \\ \frac{\Delta l^{001}}{l_{001}} - \frac{\Delta l^{100}}{l_{001}} &= \lambda^{\alpha 2,2} = -\lambda_4 \end{aligned} \right\} \begin{aligned} \lambda_1 &= -\lambda^{\alpha 1,2} + \frac{1}{2} \lambda^{\gamma,2} \\ \lambda_5 &= -\lambda^{\alpha 1,2} - \frac{1}{2} \lambda^{\gamma,2} \end{aligned}$$

$$\longrightarrow \lambda_4 = -\lambda^{\alpha 2,2}$$

$$\frac{\Delta l^{101}}{l_{101}} - \frac{\Delta l^{-101}}{l_{101}} = \lambda^{\epsilon,2} = 2\lambda_2 - \frac{1}{2} \lambda_4 \longrightarrow \lambda_2 = \frac{1}{2} \left[\lambda^{\epsilon,2} - \frac{1}{2} \lambda^{\alpha 2,2} \right]$$

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

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

$$\lambda_3 = \lambda(\alpha_1=\alpha_2=\beta_1=\beta_2=1/\sqrt{2});$$

$$\lambda_4 = \lambda(\alpha_1=1, \beta_3=1); \quad \lambda_5 = \lambda(\alpha_1=1, \beta_2=1)$$

Workflow

TETRAGONAL (II)

SG 75-88

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

Workflow

ORTHORHOMBIC

SG 16-74

Orthorhombic

Workflow

Elastic energy

$$E_{el}^{ortho} = \frac{c_{11}\epsilon_{xx}^2}{2} + \frac{c_{66}\epsilon_{xy}^2}{2} + \frac{c_{55}\epsilon_{xz}^2}{2} + c_{12}\epsilon_{xx}\epsilon_{yy} + \frac{c_{22}\epsilon_{yy}^2}{2} + \frac{c_{44}\epsilon_{yz}^2}{2} + c_{13}\epsilon_{xx}\epsilon_{zz} + c_{23}\epsilon_{yy}\epsilon_{zz} + \frac{c_{33}\epsilon_{zz}^2}{2}$$

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

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

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

Magnetoelastic energy

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

$$\begin{aligned} b_1 &= -c_{11} \lambda_1 - c_{12} \lambda_3 - c_{13} \lambda_5 \\ b_2 &= -c_{11} \lambda_2 - c_{12} \lambda_4 - c_{13} \lambda_6 \\ b_3 &= -c_{12} \lambda_1 - c_{22} \lambda_3 - c_{23} \lambda_5 \\ b_4 &= -c_{12} \lambda_2 - c_{22} \lambda_4 - c_{23} \lambda_6 \\ b_5 &= -c_{13} \lambda_1 - c_{23} \lambda_3 - c_{33} \lambda_5 \\ b_6 &= -c_{13} \lambda_2 - c_{23} \lambda_4 - c_{33} \lambda_6 \\ b_7 &= c_{44} (\lambda_4 + \lambda_6 - 4 \lambda_9) \\ b_8 &= c_{55} (\lambda_1 + \lambda_5 - 4 \lambda_8) \\ b_9 &= c_{66} (\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 - 4 \lambda_7) \end{aligned}$$

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

POSCAR

Symmetry
analysis

SG: 16-74

Orthorhombic

MAELAS uses the same lattice convention as AELAS code:

$$c < a < b$$

λ_1
 λ_2
 λ_3
 λ_4
 λ_5
 λ_6
 λ_7
 λ_8
 λ_9

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])

$$\lambda_{1,2,3,4,5,6,7,8,9} = \frac{x_{min1} - x_{min2}}{x_{min1}}$$

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

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

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

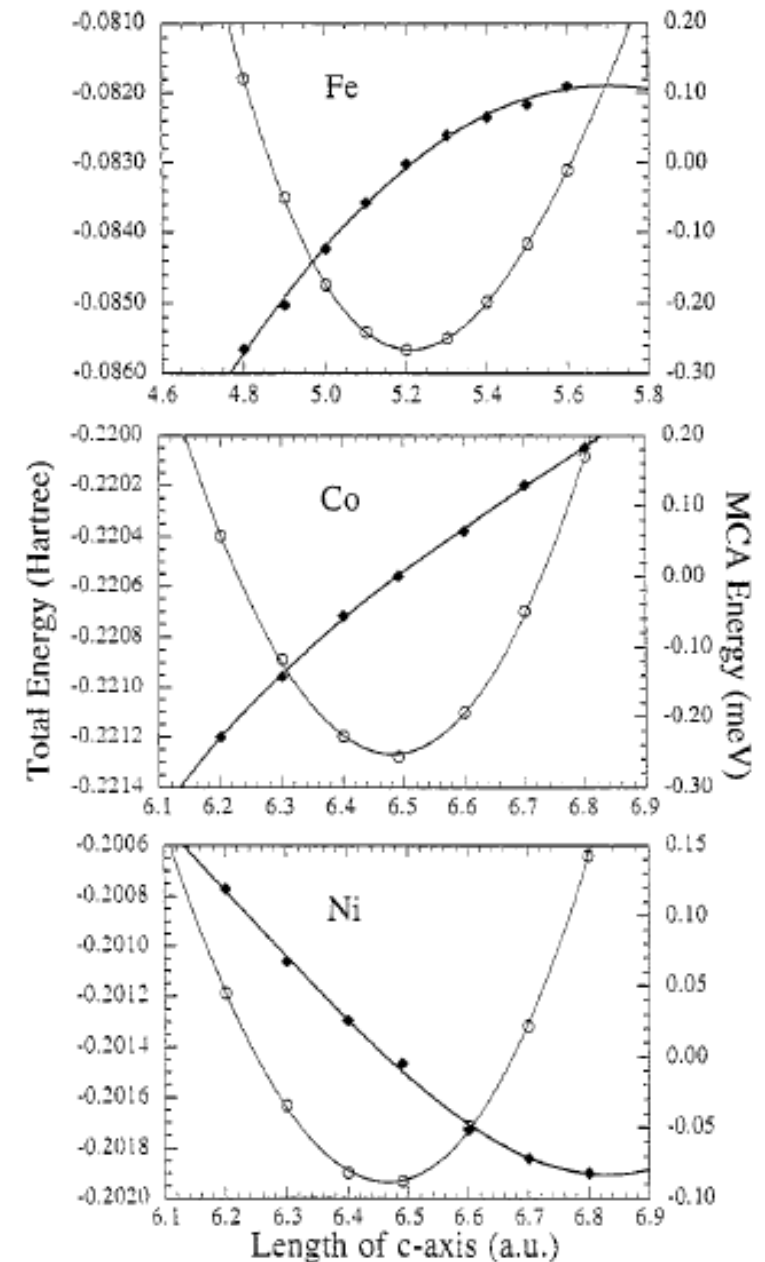
R.Q. Wu et al. / Journal of Magnetism and Magnetic Materials 177–181 (1998) 1216–1219

	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

	$T = 4.2\text{ K}$		Room Temperature		
	$\lambda_{100}(\lambda^{r,2})$	$\lambda_{111}(\lambda^{r,2})$	$\lambda_{100}(\lambda^{r,2})$	$\lambda_{111}(\lambda^{r,2})$	Polycrystal λ_s

3d Metals

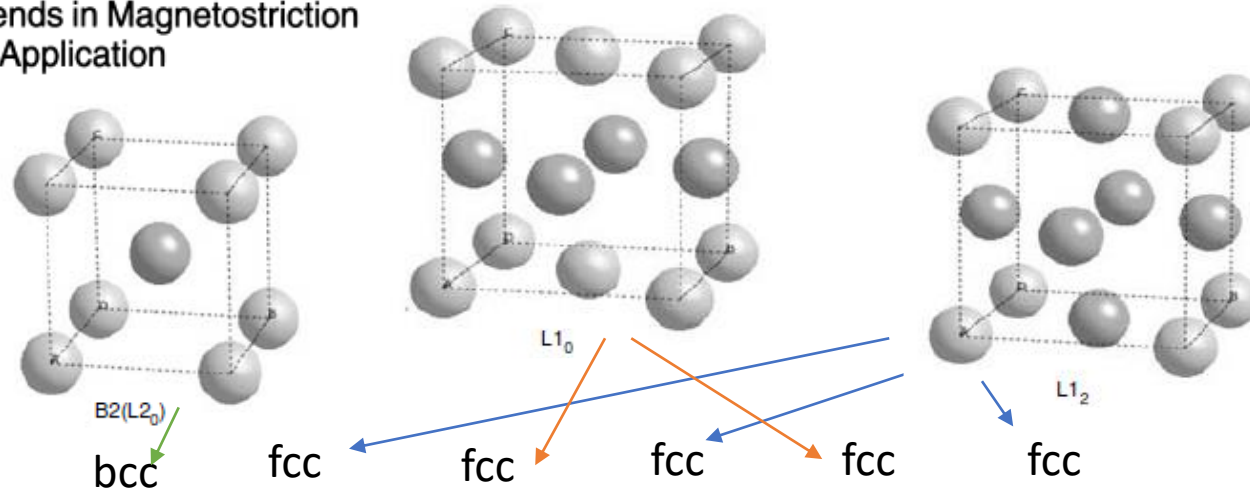
BCC-Fe	26	-30	21	-21	-7
HCP-Co ^u	(-150)	(45)	(-140)	(50)	(-62)
FCC-Ni	-60	-35	-46	-24	-34
BCC-FeCo	—	—	140	30	—
a-Fe ₈₀ B ₂₀	48 (isotropic)	—	—	—	+32
a-Fe ₄₀ Ni ₄₀ B ₂₀	+20	—	—	—	+14
a-Cos ₈₀ B ₂₀	-4	—	—	—	-4



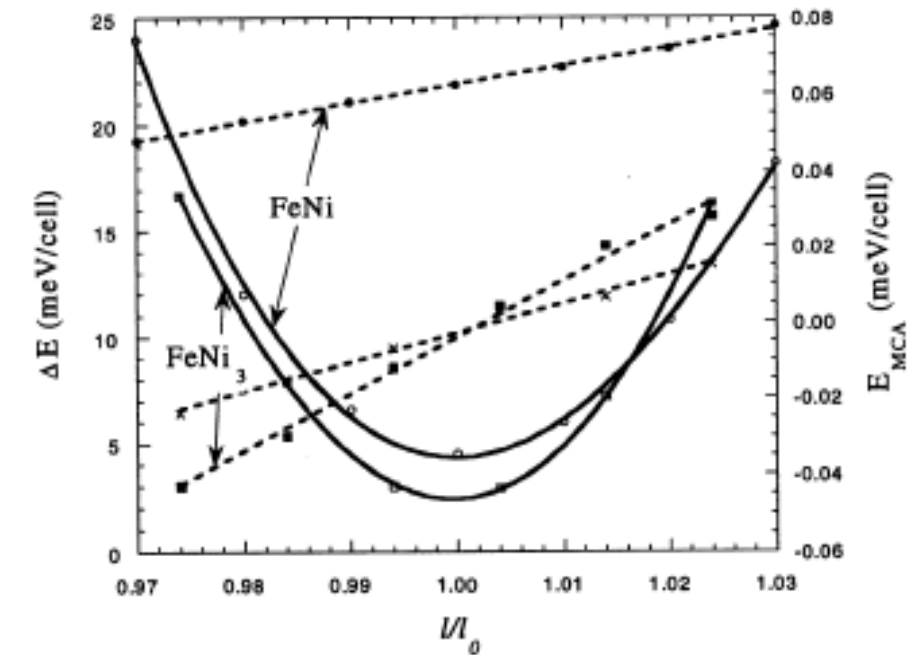
BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

Cubic systems: Itenerant magnets

Modern Trends in Magnetostriction
Study and Application



	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

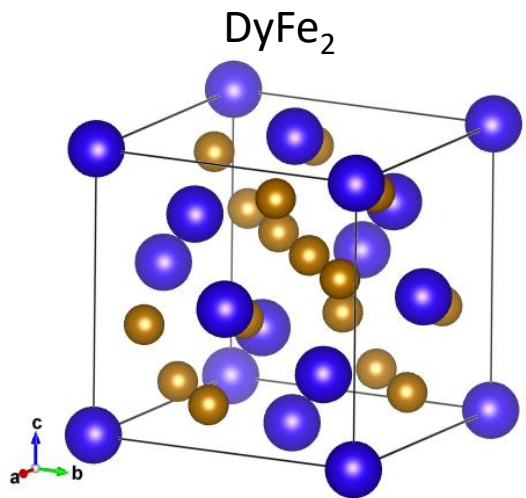
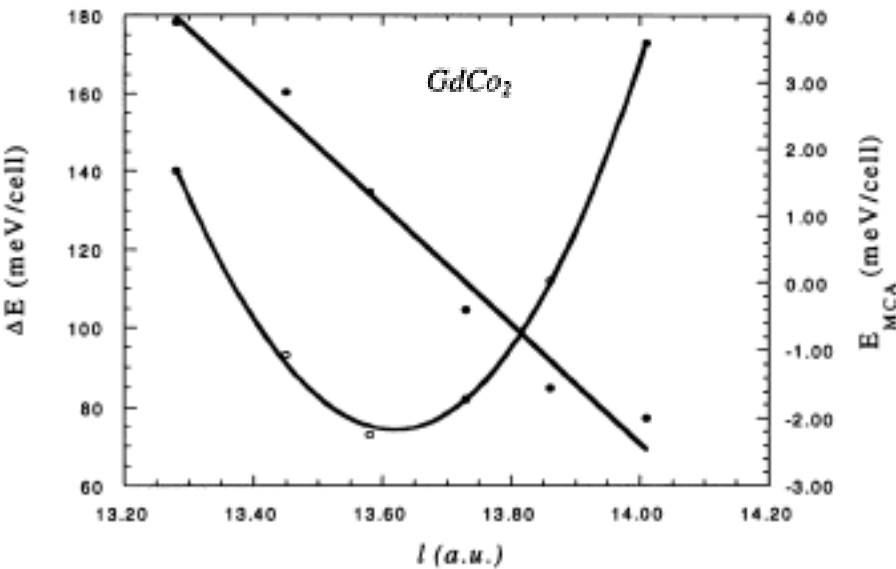


Table 16-10. Low-temperature magnetostriction constants for RCo₂ crystals [from Levitin and Markosyan (1990) unless otherwise noted].

R in RCo ₂	10 ⁶ λ_{111}	10 ⁶ λ_{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-Fe₂ Compounds

Compound	$\frac{2}{3}\lambda_{111}(10^{-6})$ (calculated at 0 K)	$\frac{2}{3}\lambda_{111}(10^{-6})$ (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

TABLE 6
Magnetostriiction coefficients at zero Kelvin in units of 10^{-3}

Hexagonal
Rare-Earth

Element	$\lambda_1^{a,2}$	$\lambda_2^{a,2}$	$\lambda^{\gamma,2}$	$\lambda^{\epsilon,2}$	$\lambda_1^{a,0} - \frac{1}{3}\lambda_1^{a,2}$	$\lambda_2^{a,0} - \frac{1}{3}\lambda_2^{a,2}$	$\lambda^{\gamma,4}$
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).

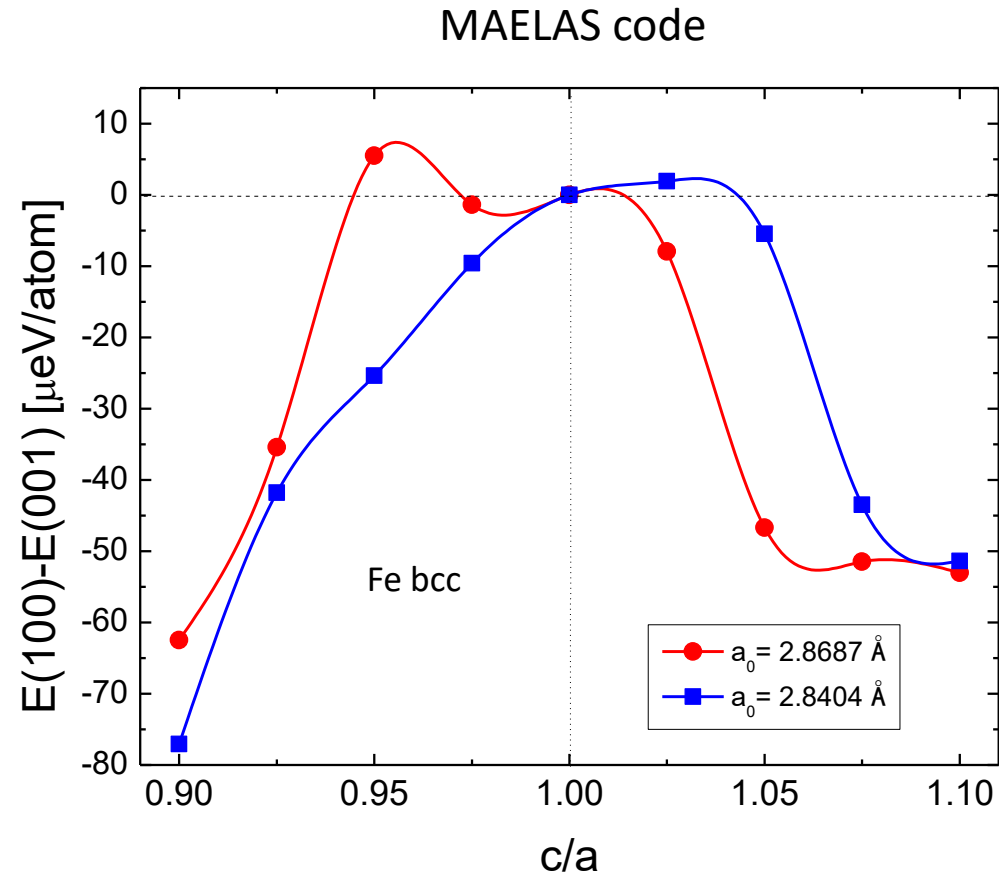
^{c)} Extrapolated from paramagnetic range using single-ion theory.

Oxide magnets

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

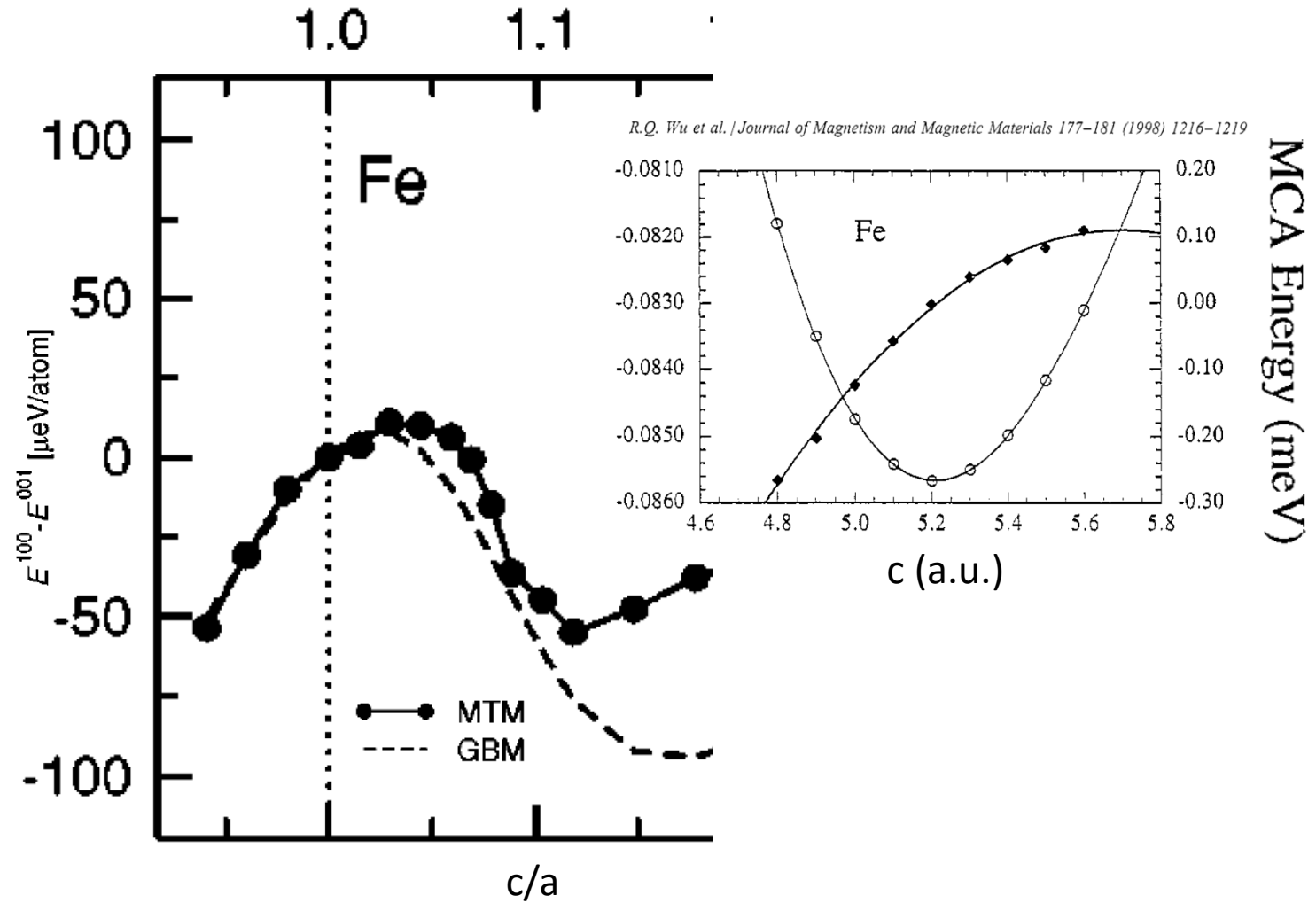
MAELAS TESTS: Fe bcc

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



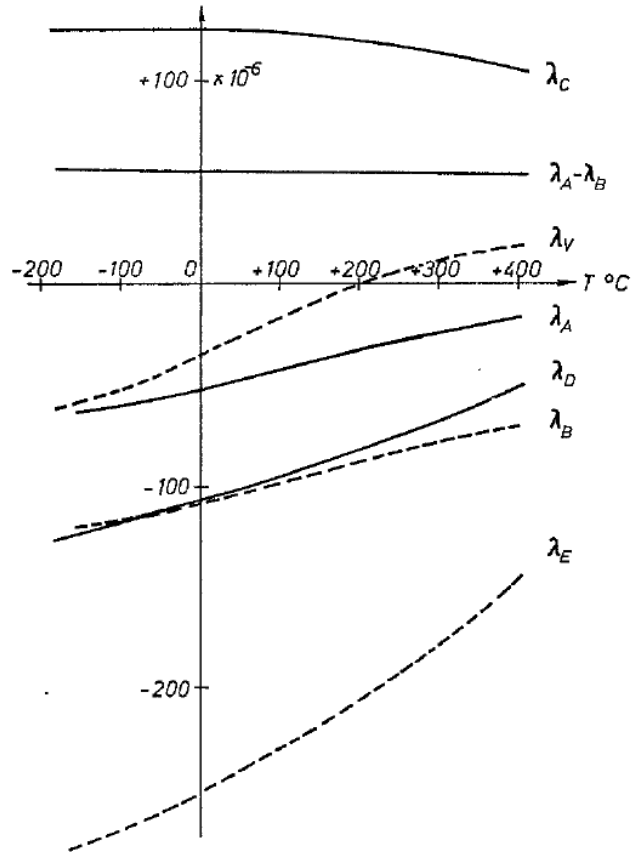
MAELAS (kp=185) $\lambda_{001} = 13 \cdot 10^{-6}$

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

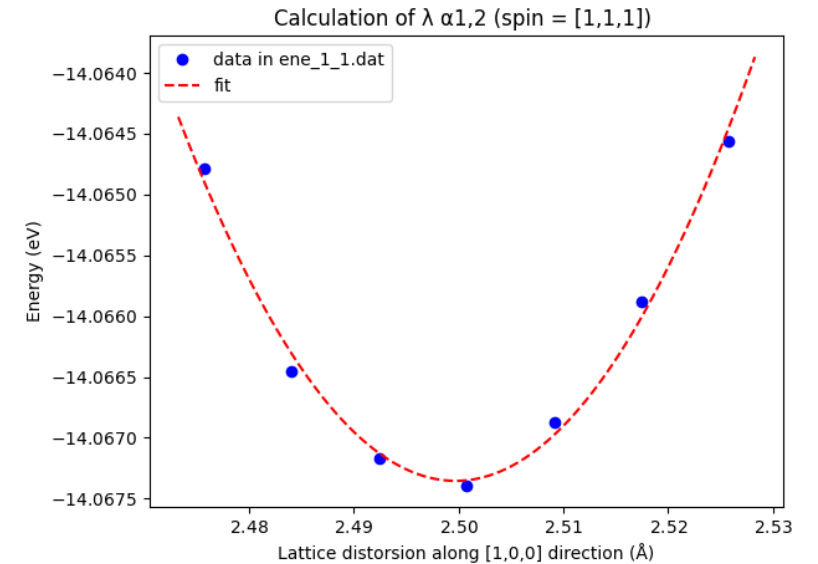
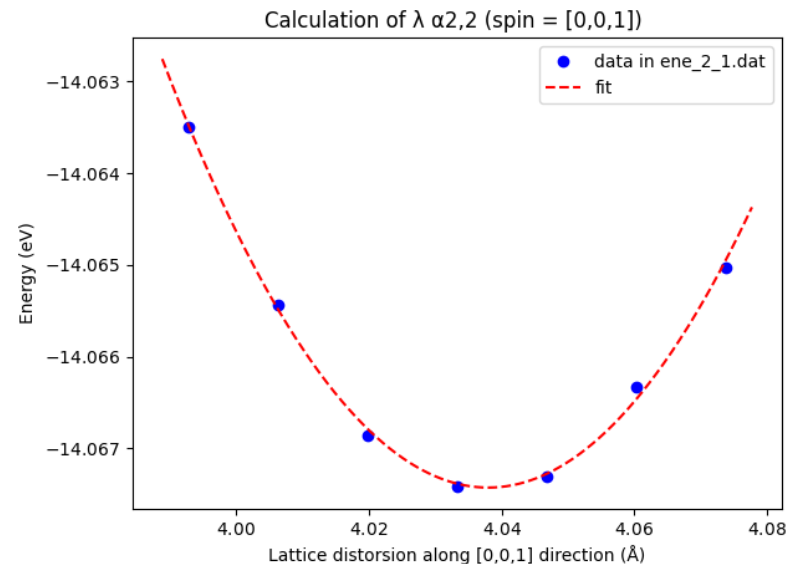


MAELAS TESTS: Co hcp

Z. Physik 224, 148—155 (1969)



	Experiment ($\times 10^{-6}$)	MAELAS $k_p=70$ ($\times 10^{-6}$)
λ_A	-66	-10
λ_B	-123	-26
λ_C	126	25
λ_D	-128	-11

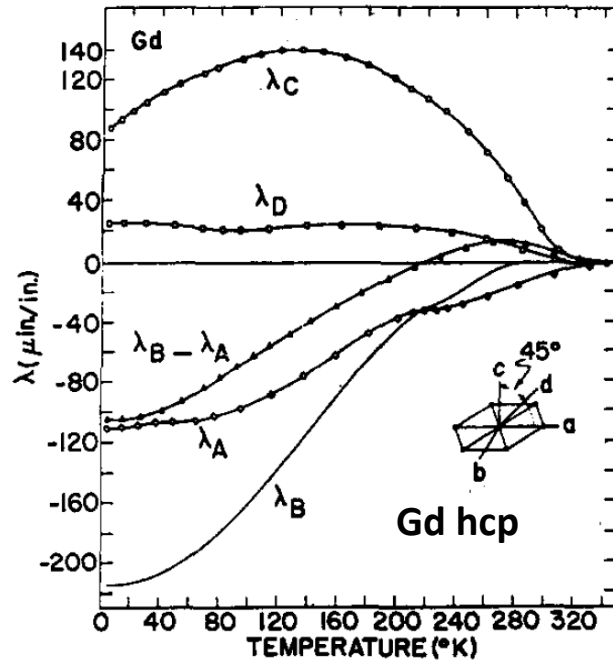


Magnetocrystalline anisotropy energy ratio for the relaxed structure: $K1 \text{ exp.} / K1 \text{ theory} = 0.7 / 0.13 = 5.38$

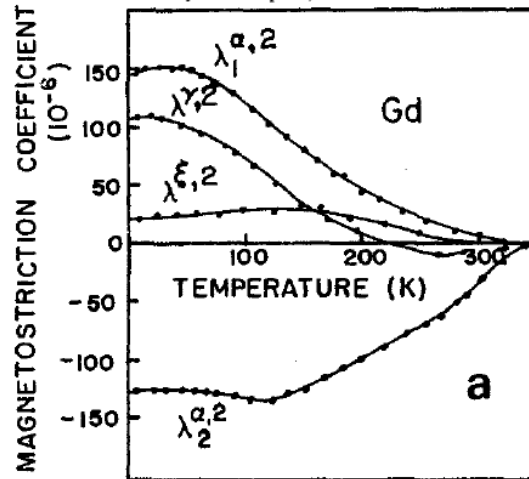
MAELAS TESTS: Gd hcp

Experiments

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



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

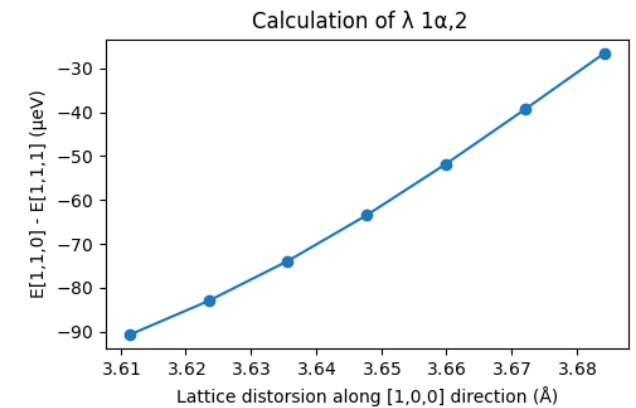
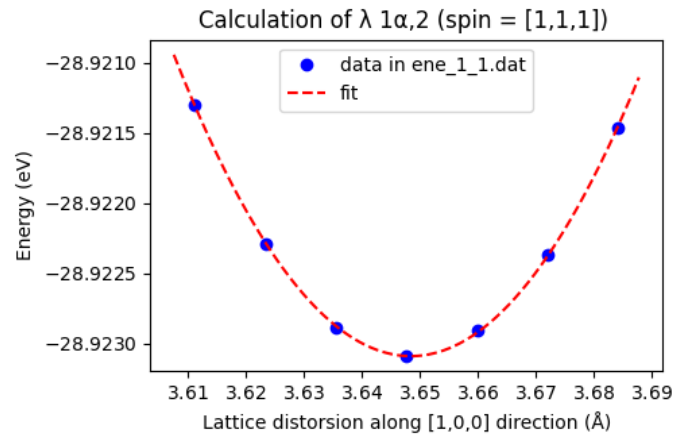


	Experiment ($\times 10^{-6}$)	MAELAS ($\times 10^{-6}$)
λ_A	-110	-262
λ_B	-215	-305
λ_C	85	521
λ_D	22	22

LDAUU=6.7

LDAUJ=0.7

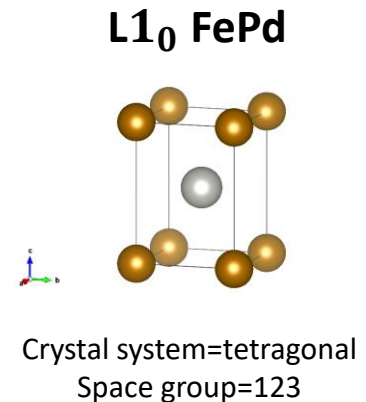
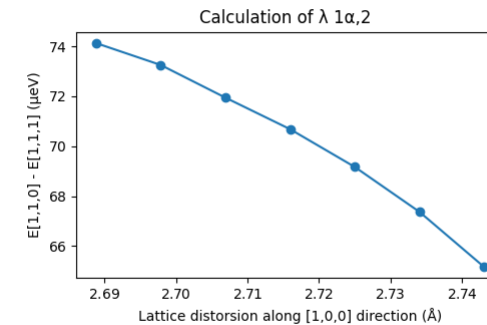
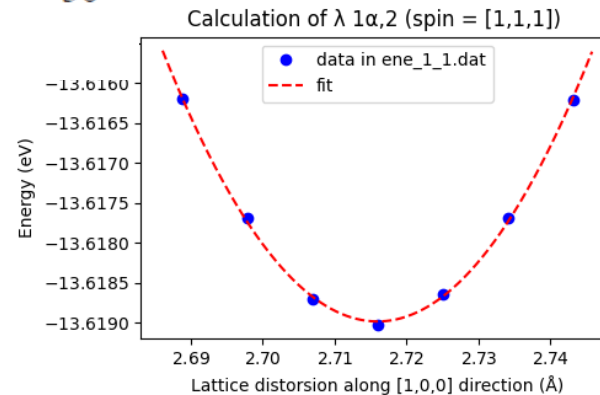
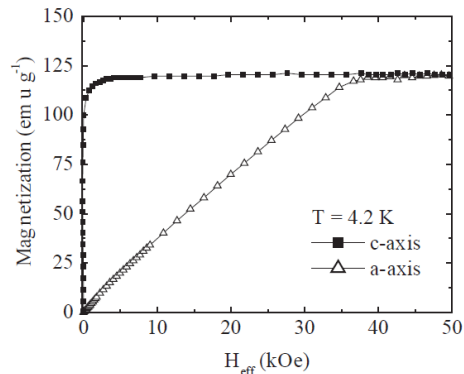
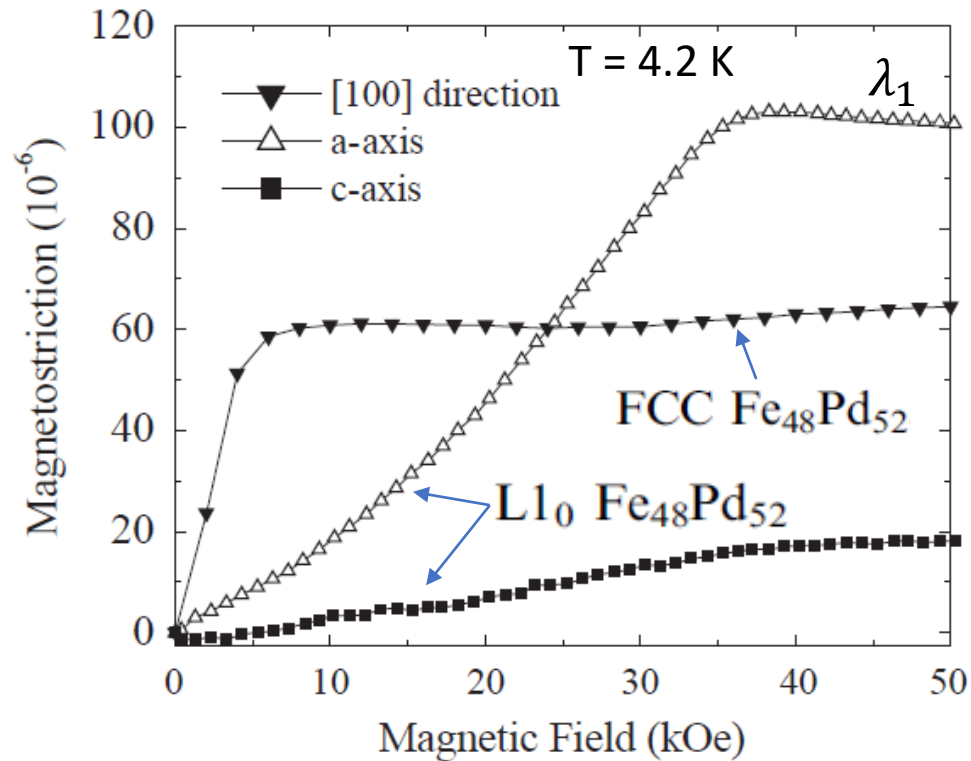
kpoints 22x22x11



MAELAS TESTS: L1₀ 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)
λ ₁	100	28
λ ₂	-	-10
λ ₃	-	83
λ ₄	-	-75
λ ₅	-	20

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

Bibliography

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