

MAELAS code

User manual v1.0

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*MAELAS: MAGneto-ELAStic properties calculation via computational high-throughput approach*

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# Outline

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# WHAT IS MAGNETOSTRICTION?

Magnetostriction is a physical phenomenon in which the process of magnetization induces a change in shape or dimension of a magnetic material.

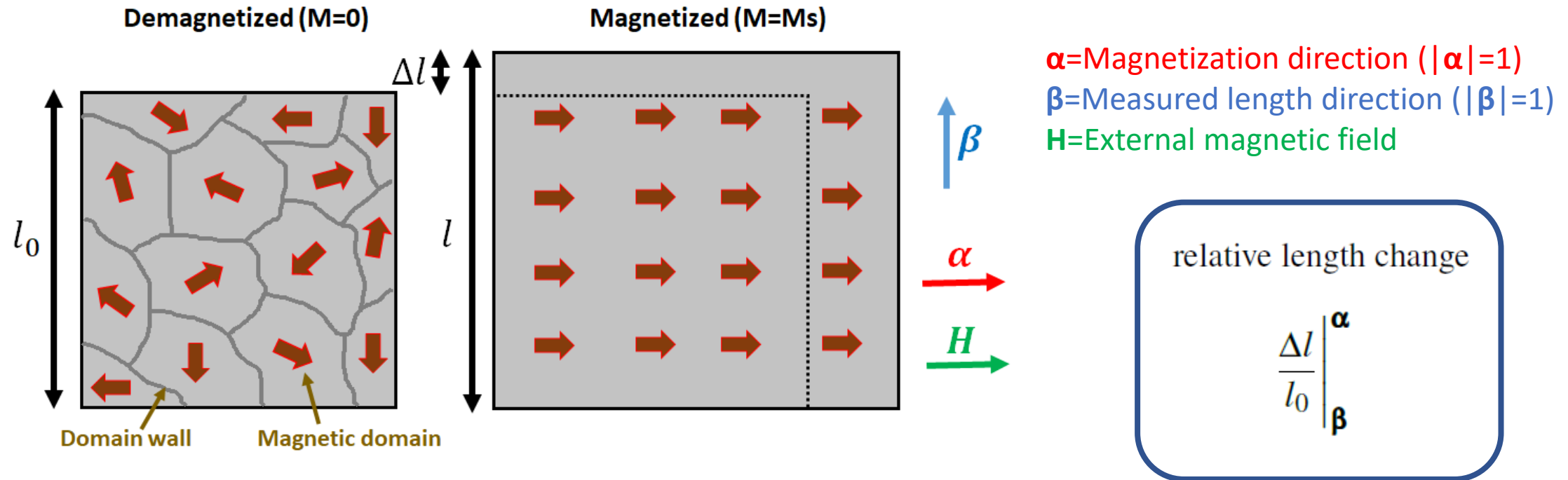


Figure 1: Magnetostriction of a single crystal under an external magnetic field ( $\alpha \parallel H$ ) perpendicular to the measured length direction ( $\beta \perp H$ ). Symbols  $M$  and  $M_s$  stand for macroscopic magnetization and saturation magnetization, respectively. Dash line on the right represents the original size of the demagnetized material. The magnetostriction effect has been magnified in order to help to visualize it easily, in real materials it is smaller ( $\Delta l/l_0 \sim 10^{-3} - 10^{-6}$ ).

# WHAT IS MAELAS CODE?

- MAELAS code is a software to calculate anisotropic magnetostrictive 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 magnetostrictive 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

The MAELAS code requires to have Python3( $\geq 3.6$ ). 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 python3 in your machine, you can type

```
sudo apt-get update  
sudo apt-get install python3
```

Note that in some HPC clusters you might need to load the Python module (ml Python). To install MAELAS code, download and extract the .zip file, go to the folder that contains the file setup.py and type

```
python3 setup.py install --user
```

This procedure will also install all required dependencies automatically

pymatgen( $\geq 2020.4.29$ ), scikit-learn( $\geq 0.23.1$ ), pyfiglet( $\geq 0.8.post0$ ), argparse( $\geq 1.4.0$ ), numpy( $\geq 1.18.4$ ), matplotlib( $\geq 3.2.1$ ), scipy( $\geq 1.4.1$ ), setuptools( $\geq 40.8.0$ )

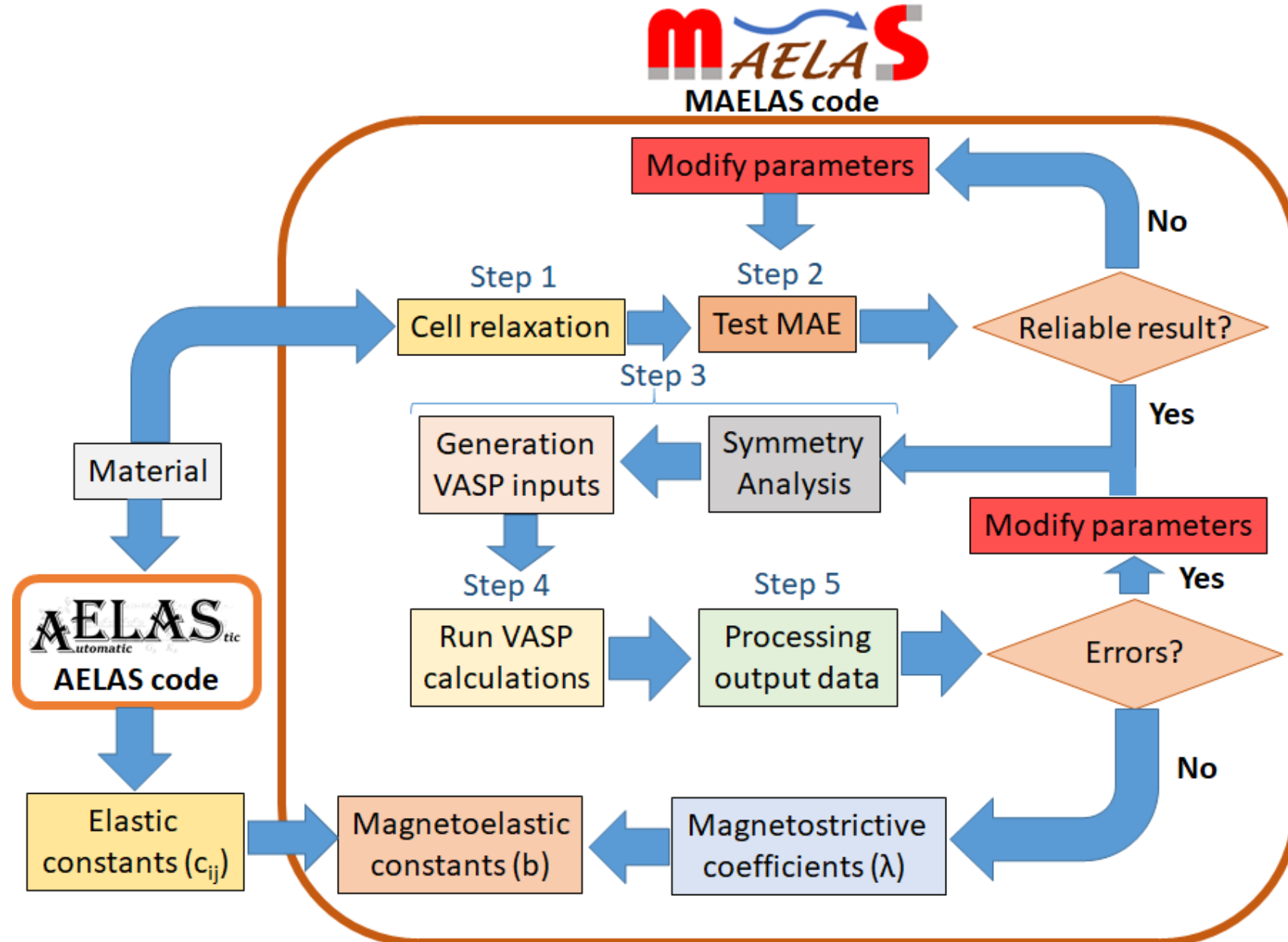
More available options for the installation can be found in the file INSTALL. By default, the executable file "maelas" is installed in the folder /home/\$USER/.local/bin/ where \$USER is the name of your username folder. This folder should be included to the PATH variable by adding in the file /home/\$USER/.bashrc the following line

```
export PATH=/home/$USER/.local/bin/:$PATH
```

Then you should close the terminal and open the terminal again. If you need to install pip3 in Ubuntu Linux, then type

```
sudo apt-get update  
sudo apt-get install python3-pip
```

# 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 magnetostrictive 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 in the same folder where you want to generate the input files for VASP, and after going to this folder then type

```
maelas -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,

```
maelas -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 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. Note that the user might need to modify vasp\_jsub\_rlx (it is in PBS Pro format) depending on the cluster or local computer batch scheduling. More options can be added in vasp\_jsub\_rlx file through the terminal command line, to see them just type

```
maelas -h
```

Note that generated INCAR and KPOINTS files contain standard setting for cell relaxation. The user might need to change these files in order to include more advanced settings. 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: Test MAE

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

```
maelas -m -i POSCAR_rlx -k 70 -s1 1 0 0 -s2 0 0 1
```

where -m indicates that you want to generate input VASP files for the calculation of MAE, -i POSCAR\_rlx is the initial relaxed POSCAR file (you can name it whatever you want), -k 70 is the length parameter that determines a regular mesh of k-points, -s1 1 0 0 is the first spin direction to calculate MAE: s1x s1y s1z and -s2 0 0 1 is the second spin direction to calculate MAE: s2x s2y s2z . It will generate the following files:

POSCAR\_0\_0 (it is the same POSCAR as )

INCAR\_0\_C (non-collinear calculation where C=1,2 is the spin orientation case)

INCAR\_std (collinear calculation to generate the WAVECAR and CHGCAR files to run non-collinear calculations)

KPOINTS (file for the kpoint generation of VASP)

vasp\_mae, vasp\_mae\_jsub and vasp\_mae\_0 (interconnected bash scripts to run VASP calculations automatically)

vasp\_mae\_cp\_oszicar (bash script to get the calculated OSZICAR\_0\_0\_C files after VASP calculation is finished)

The generated files vasp\_mae, vasp\_mae\_jsub and vasp\_mae\_0 are interconnected scripts to submit jobs in HPC facilities. One needs only to execute the file vasp\_mae in order to run all VASP jobs automatically. You can specify some job settings in these scripts by adding more tags in the command line. For instance,

```
maelas -m -i POSCAR_rlx -k 70 -s1 1 0 0 -s2 0 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. Note that the user might need to modify vasp\_mae\_jsub (it is in PBS Pro format) depending on the cluster or local computer batch scheduling. More options can be added in these script files through the terminal command line, to see them just type

```
maelas -h
```



# HOW TO USE MAELAS CODE

## Step 3: Generation of VASP files for the calculation of anisotropic magnetostrictive coefficients

Copy the relaxed POSCAR and POTCAR 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

```
maelas -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 anisotropic magnetostrictive coefficients, -i POSCAR\_rlx is the initial relaxed POSCAR file (you can name it whatever you want), -k 70 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)

KPOINTS

vasp\_maelas, vasp\_jsub and vasp\_0 (interconnected bash scripts to run VASP calculations automatically)

vasp\_cp\_oszicar (bash script to get the 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,

```
maelas -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 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. Note that the user might need to modify vasp\_jsub (it is in PBS Pro format) depending on the cluster or local computer batch scheduling. More options can be added in these script files through the terminal command line, to see them just type

```
maelas -h
```

# HOW TO USE MAELAS CODE

## Step 4: 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 (VASP executable “vasp\_std”) to generate WAVECAR and CHGCAR files, and two non-collinear (VASP executable “vasp\_nc”) 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. Note that the user might need to modify vasp\_jsub depending on the cluster or local computer queuing system.

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.

### VASP executables:

“vasp\_std” is the standard version of vasp without spin-orbit coupling (LNONCOLLINEAR = .FALSE., LSORBIT = .FALSE.)

“vasp\_nc” is for non-collinear calculations for instance to perform fully non-collinear magnetic structure calculations or to include spin-orbit interactions in the calculations (LSORBIT = .TRUE.)

# HOW TO USE MAELAS CODE

## Step 5: Derivation of anisotropic magnetostrictive coefficients and magnetoelastic constants

Finally, to derive the anisotropic magnetostrictive coefficients one needs to have in the same folder the following files:

POSCAR\_rlx (the relaxed POSCAR file used as input in step 3)

POSCAR\_A\_B (distorted POSCAR generated in step 3)

OSZICAR\_A\_B\_C (non-collinear OSZICAR files calculated in step 4 for each POSCAR\_A\_B and INCAR\_A\_C)

Next, in the terminal go to this folder and type

```
maelas -d -i POSCAR_rlx -n 7
```

where -d indicates that you want to derive the spin-dependent magnetostrictive coefficients from the calculated OSZICAR files, -i POSCAR\_rlx is the relaxed POSCAR file used as input in step 3 (you can name it whatever you want) and -n 7 is the number of distorted states for each magnetostriction mode used in step 3.

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

```
maelas -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

```
maelas -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 |

User can see all possible optional arguments by typing

```
maelas -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 value of the parameter epsilon for the strain tensor 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 magnetostrictive coefficients.
- d Derivation of magnetostrictive coefficients from the energy written in the OSZICAR files.
- r Generation of required VASP files for the cell relaxation
- m Generation of required VASP files to test MAE
- s1 s1x s1y s1z First spin direction to calculate MAE
- s2 s2x s2y s2z Second spin direction to calculate MAE
- b Calculation of the magnetoelastic constants from the calculated magnetostrictive 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)
- sg SGO Space group number 1-230. If it is equal to 0, then it will be determined by a symmetry analysis (default: 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)
- mp 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

```
maelas -r -i POSCAR0 -k 40
```

```
qsub vasp_jsub_rlx
```

### Step 2: Test MAE

```
maelas -m -i POSCAR_rlx -k 70 -s1 1 0 0 -s2 0 0 1
```

```
./vasp_mae
```

```
./vasp_mae_cp_oszicar
```

### Step 3: Generate VASP inputs for calculation of magnetostrictive coefficients

```
maelas -g -i POSCAR_rlx -k 70 -n 7 -s 0.1
```

### Step 4: Run VASP calculations

```
./vasp_maelas
```

```
./vasp_cp_oszicar
```

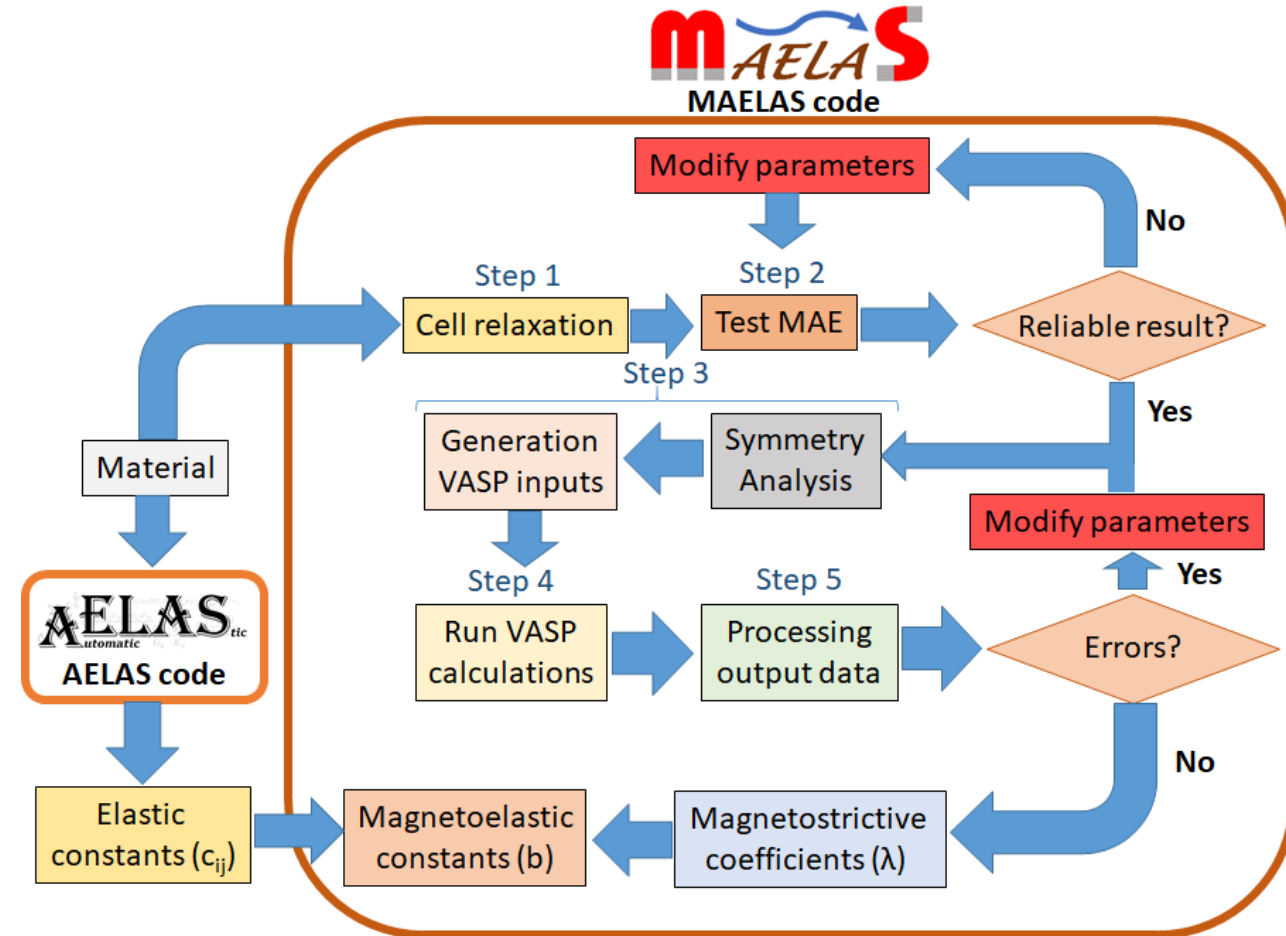
### Step 5: Derivation of anisotropic magnetostrictive coefficients

```
maelas -d -i POSCAR_rlx -n 7
```

### Step 5: Derivation of anisotropic magnetostrictive coefficients and magnetoelastic constants

```
maelas -d -i POSCAR_rlx -n 7 -b -e ELADAT
```

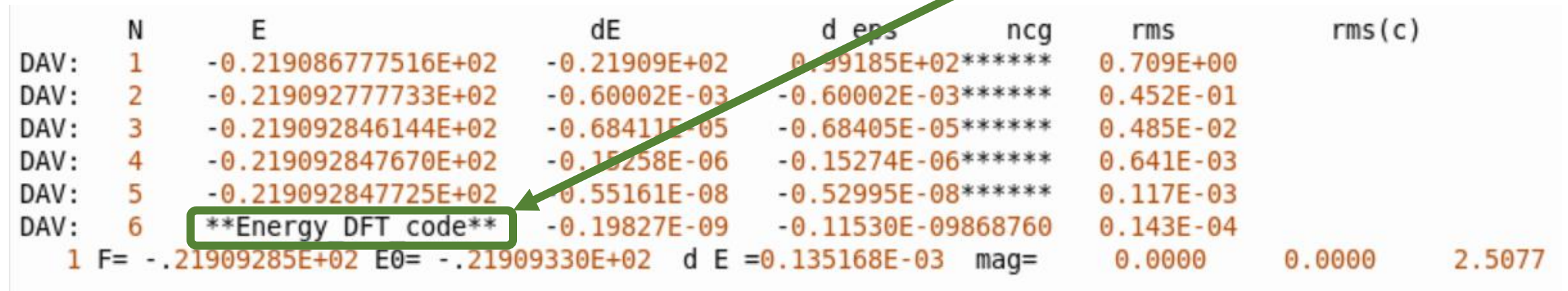
**See all optional arguments:** `maelas -h`



# HOW TO USE MAELAS CODE

## Using MAELAS with other DFT codes instead of VASP

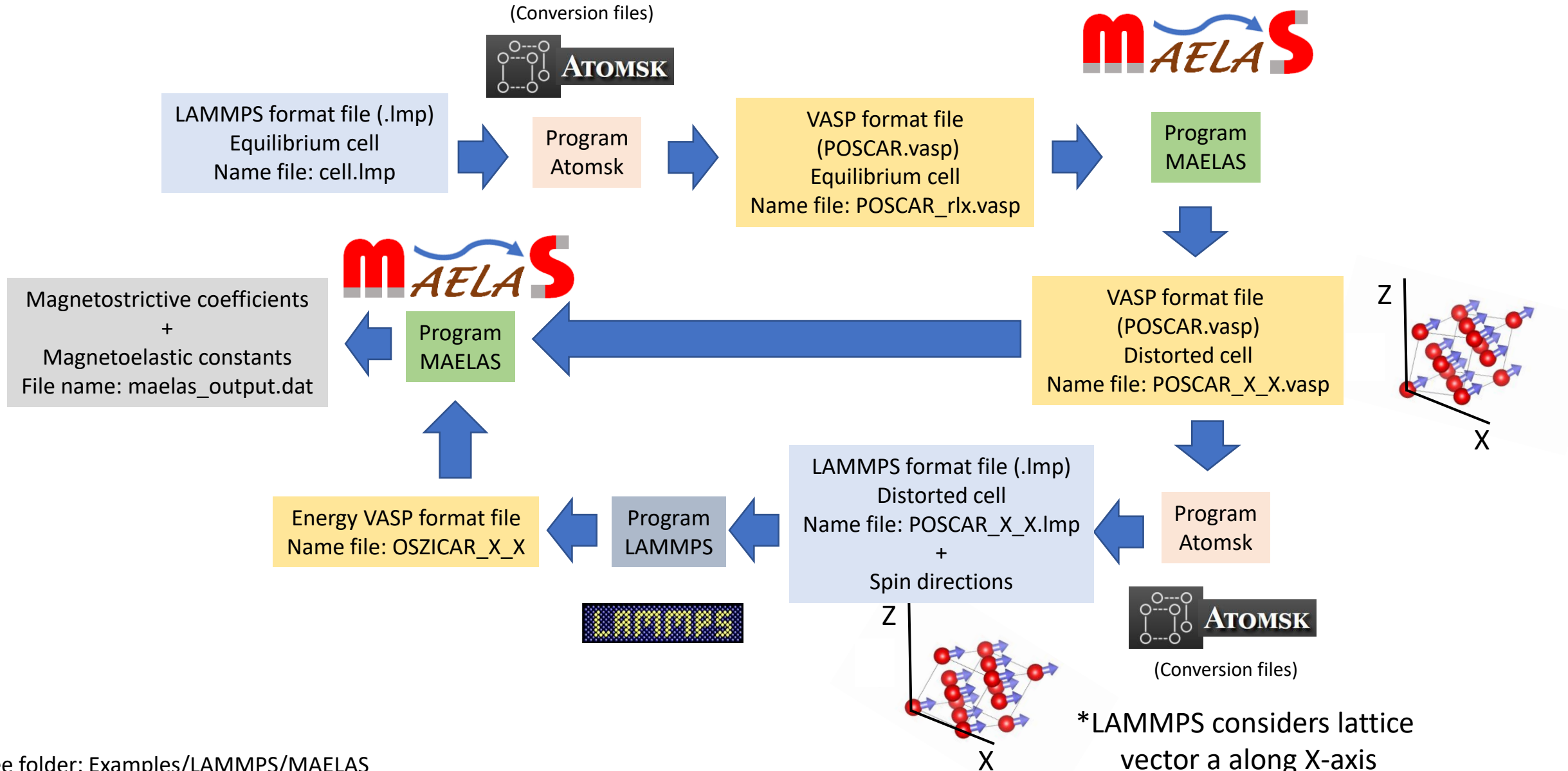
MAELAS has been designed to read and write files for VASP code automatically. However, it is possible to use MAELAS with other DFT codes instead of VASP, after file conversion to VASP format files. Although, this process might require some extra work for the user. Namely, converting initial and distorted 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-like file, one should write the calculated 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 | <b>**Energy DFT code**</b> | -0.19827E-09       | -0.11530E-09      | 8760  | 0.143E-04 |               |
| 1 F= |   | -.21909285E+02             | E0= -.21909330E+02 | d E =0.135168E-03 | mag=  | 0.0000    | 0.0000 2.5077 |

# HOW TO USE MAELAS CODE

## Interface between LAMMPS and MAELAS



See folder: Examples/LAMMPS/MAELAS

More details can be found in reference: P. Nieves et al. "Spin-lattice model for cubic crystals" arXiv:2012.05076 (2020)

# HOW TO USE MAELAS CODE

## Crystal systems supported by MAELAS v1.0

Table 1: Number of independent second-order elastic constants of each crystal system. Number of independent magnetoelastic and magnetostriction coefficients up to second-order of the direction cosine polynomial in the first-order magnetoelastic energy. In the last column we specify which crystal systems are supported by the current version of MAELAS.

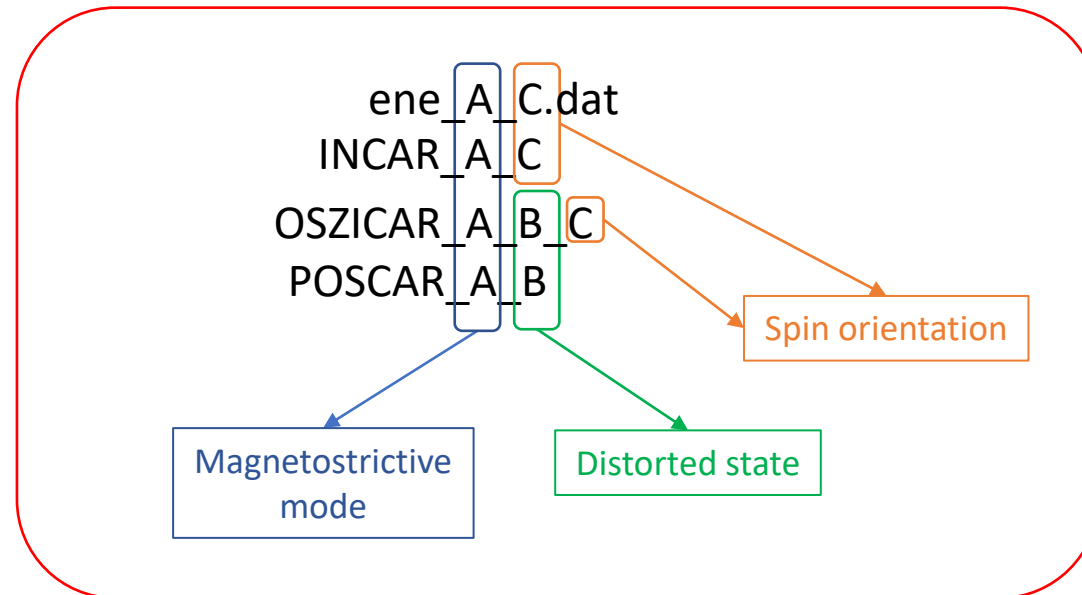
| Crystal system  | Point groups                 | Space groups | Elastic constants<br>( $c_{ij}$ ) | Magnetoelastic constants<br>( $b$ ) | Magnetostriction coefficients<br>( $\lambda$ ) | MAELAS |
|-----------------|------------------------------|--------------|-----------------------------------|-------------------------------------|--|--------|
| Triclinic       | $1, \bar{1}$                 | 1 – 2        | 21                                | 36                                  | 36   | No     |
| Monoclinic      | $2, m, 2/m$                  | 3 – 15       | 13                                | 20                                  | 20   | No     |
| Orthorhombic    | $222, 2mm, mmm$              | 16 – 74      | 9                                 | 12                                  | 12   | Yes    |
| Tetragonal (II) | $4, \bar{4}, 4/m$            | 75 – 88      | 7                                 | 10                                  | 10   | No     |
| Tetragonal (I)  | $4mm, 422, \bar{4}2m, 4/mmm$ | 89 – 142     | 6                                 | 7                                   | 7  | Yes    |
| Trigonal (II)   | $3, \bar{3}$                 | 143 – 148    | 7                                 | 12                                  | 12   | No     |
| Trigonal (I)    | $32, 3m, \bar{3}m$           | 149 – 167    | 6                                 | 8                                   | 8  | Yes    |
| Hexagonal(II)   | $6, \bar{6}, 6/m$            | 168 – 176    | 5                                 | 8                                   | 8  | No     |
| Hexagonal (I)   | $6mm, 622, \bar{6}2m, 6/mmm$ | 177 – 194    | 5                                 | 6                                   | 6  | Yes    |
| Cubic (II)      | $23, m\bar{3}$               | 195 – 206    | 3                                 | 4                                   | 4  | No     |
| Cubic (I)       | $432, \bar{4}3m, m\bar{3}m$  | 207 – 230    | 3                                 | 3                                   | 3  | Yes    |

The crystal systems not supported by MAELAS might be included in the new versions of the code



# HOW TO USE MAELAS CODE

## MAELAS file notation



# Methodology

$$\frac{\Delta l}{l_0} \left| \frac{\alpha_1^i}{\beta^i} - \frac{\Delta l}{l_0} \right| \frac{\alpha_2^i}{\beta^i} = \eta^i \lambda^i$$

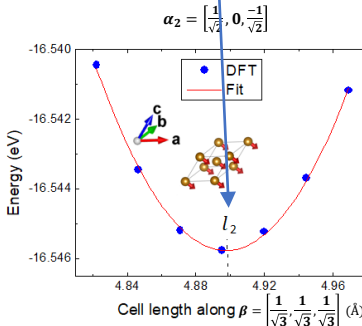
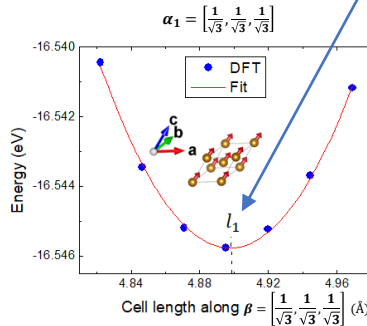
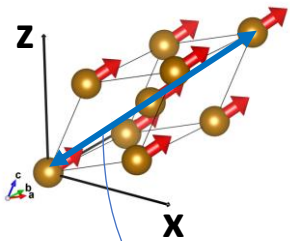
$$\begin{aligned} \frac{\Delta l}{l_0} \left| \frac{\alpha_1^i}{\beta^i} - \frac{\Delta l}{l_0} \right| \frac{\alpha_2^i}{\beta^i} &= \frac{l_1 - l_0}{l_0} - \frac{l_2 - l_0}{l_0} = \frac{2(l_1 - l_2)}{(l_1 + l_2) \left[ 1 - \frac{l_1 + l_2 - 2l_0}{l_1 + l_2} \right]} \\ &= \frac{2(l_1 - l_2)}{l_1 + l_2} \left[ 1 + \frac{l_1 + l_2 - 2l_0}{l_1 + l_2} + \dots \right] \approx \frac{2(l_1 - l_2)}{l_1 + l_2} \end{aligned}$$

$$\lambda^i = \frac{2(l_1 - l_2)}{\eta^i (l_1 + l_2)}$$

Fitting to a quadratic function

$$E(l) \Big|_{\beta} = A_j l^2 + B_j l + C_j, \quad j = 1, 2$$

$$\text{Minimum: } l_{1(2)} = -B_{1(2)} / (2A_{1(2)})$$



$$\text{Cell length along } \beta = \left[ \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right]$$

Table 2: Implemented distortion ( $\beta$ ) and spin directions ( $\alpha_1$ ,  $\alpha_2$ ) in MAELAS to calculate the anisotropic magnetostriction coefficients according to Eq.30. The second column presents the equation of the relative length change that we used in Eq.30 for each crystal system. In the last column we show the value of parameter  $\eta$  that is defined in Eq.30. The symbols  $a, b, c$  correspond to the lattice parameters of the relaxed (not distorted) unit cell.

| Crystal system | $\frac{\Delta l}{l_0}$ | Magnetostriction coefficient | $\beta$   | $\alpha_1$  | $\alpha_2$  | $\eta$  |
|----------------|------------------------|------------------------------|---|---|---|---|
| Cubic (I)      | Eq.10                  | $\lambda_{001}$              | (0, 0, 1)   | (0, 0, 1)   | (1, 0, 0)   | $\frac{3}{2}$   |
|                |                        | $\lambda_{111}$              | $\left( \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)$ | $\left( \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)$ | $\left( \frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right)$  | $\frac{3}{2}$   |
| Hexagonal (I)  | Eq.16                  | $\lambda^{\alpha 1,2}$       | (1, 0, 0)   | $\left( \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)$ | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$  | $\frac{1}{3}$   |
|                |                        | $\lambda^{\alpha 2,2}$       | (0, 0, 1)   | (0, 0, 1)   | (1, 0, 0)   | 1   |
|                |                        | $\lambda^{\gamma 2}$         | (1, 0, 0)   | (1, 0, 0)   | (0, 1, 0)   | 1   |
|                |                        | $\lambda^{\epsilon,2}$       | $\left( \frac{a,0,c}{\sqrt{a^2+c^2}} \right)$                               | $\left( \frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right)$                  | $\left( \frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right)$ | $\frac{2ac}{a^2+c^2}$   |
|                |                        | $\lambda^{\delta,2}$         | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$                  | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$                  | $\left( \frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$ | $\frac{2ac}{a^2+c^2}$   |
| Trigonal (I)   | Eq.20                  | $\lambda^{\alpha 1,2}$       | (1, 0, 0)   | (0, 0, 1)   | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$  | 1   |
|                |                        | $\lambda^{\alpha 2,2}$       | (0, 0, 1)   | (0, 0, 1)   | (1, 0, 0)   | 1   |
|                |                        | $\lambda^{\gamma 1}$         | (1, 0, 0)   | (1, 0, 0)   | (0, 1, 0)   | 1   |
|                |                        | $\lambda^{\gamma 2}$         | $\left( \frac{a,0,c}{\sqrt{a^2+c^2}} \right)$                               | $\left( \frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right)$                  | $\left( \frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}} \right)$ | $\frac{ac}{a^2+c^2}$  |
|                |                        | $\lambda_{12}$               | $\left( \frac{a,0,c}{\sqrt{a^2+c^2}} \right)$                               | $\left( 0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right)$                  | $\left( 0, \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}} \right)$ | $\frac{a^2}{2(a^2+c^2)}$  |
|                |                        | $\lambda_{21}$               | $\left( \frac{a,0,c}{\sqrt{a^2+c^2}} \right)$                               | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$                  | $\left( \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, 0 \right)$ | $\frac{ac}{a^2+c^2}$  |
|                |                        | $\lambda^{\delta,2}$         | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$                  | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$                  | $\left( \frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$ | $\frac{2ac}{a^2+c^2}$   |
| Tetragonal (I) | Eq.24                  | $\lambda^{\alpha 1,2}$       | (1, 0, 0)   | $\left( \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)$ | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$  | $\frac{1}{3}$   |
|                |                        | $\lambda^{\alpha 2,2}$       | (0, 0, 1)   | (0, 0, 1)   | (1, 0, 0)   | 1   |
|                |                        | $\lambda^{\gamma 2}$         | (1, 0, 0)   | (1, 0, 0)   | (0, 1, 0)   | 1   |
|                |                        | $\lambda^{\epsilon,2}$       | $\left( \frac{a,0,c}{\sqrt{a^2+c^2}} \right)$                               | $\left( \frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right)$                  | $\left( \frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right)$ | $\frac{2ac}{a^2+c^2}$   |
|                |                        | $\lambda^{\delta,2}$         | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$                  | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$                  | $\left( \frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$ | 1   |
|                |                        | $\lambda_1$                  | (1, 0, 0)   | (1, 0, 0)   | (0, 0, 1)   | 1   |
|                |                        | $\lambda_2$                  | (1, 0, 0)   | (0, 1, 0)   | (0, 0, 1)   | 1   |
| Orthorhombic   | Eq.27                  | $\lambda_3$                  | (0, 1, 0)   | (1, 0, 0)   | (0, 0, 1)   | 1   |
|                |                        | $\lambda_4$                  | (0, 1, 0)   | (0, 1, 0)   | (0, 0, 1)   | 1   |
|                |                        | $\lambda_5$                  | (0, 0, 1)   | (1, 0, 0)   | (0, 0, 1)   | 1   |
|                |                        | $\lambda_6$                  | (0, 0, 1)   | (0, 1, 0)   | (0, 0, 1)   | 1   |
|                |                        | $\lambda_7$                  | $\left( \frac{a,b,0}{\sqrt{a^2+b^2}} \right)$                               | $\left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$                  | (0, 0, 1)   | $\frac{(a-b)(a[\lambda_1+\lambda_2]-b[\lambda_3+\lambda_4])+4ab\lambda_7}{2(a^2+b^2)\lambda_7}$ |
|                |                        | $\lambda_8$                  | $\left( \frac{a,0,c}{\sqrt{a^2+c^2}} \right)$                               | $\left( \frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right)$                  | (0, 0, 1)   | $\frac{(a-c)(a\lambda_1-c\lambda_5)+4ac\lambda_8}{2(a^2+c^2)\lambda_8}$                         |
|                |                        | $\lambda_9$                  | $\left( \frac{0,b,c}{\sqrt{b^2+c^2}} \right)$                               | $\left( 0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right)$                  | (0, 0, 1)   | $\frac{(b-c)(b\lambda_4-c\lambda_6)+4bc\lambda_9}{2(b^2+c^2)\lambda_9}$                         |

# Workflow

## CUBIC (I)

SG 207-230

# Cubic (I)

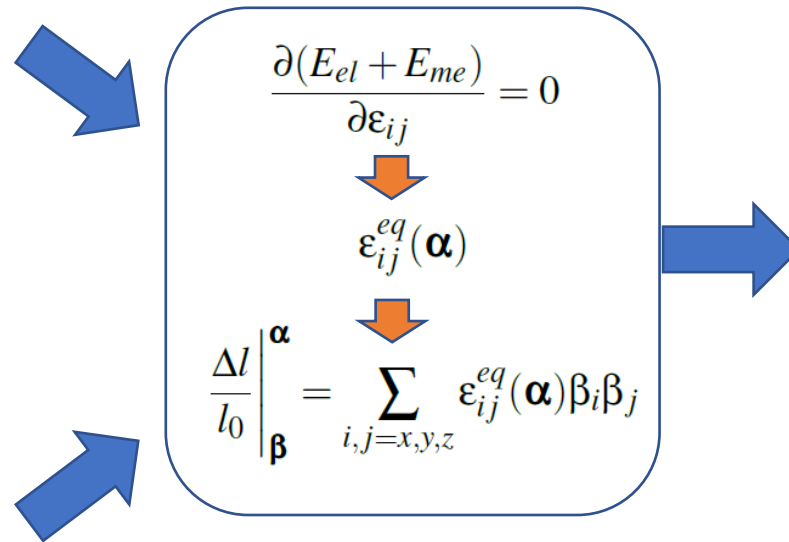
## Workflow

Elastic energy

$$E_{el}^{cub} = \frac{c_{11}}{2}(\epsilon_{xx}^2 + \epsilon_{yy}^2 + \epsilon_{zz}^2) + c_{12}(\epsilon_{xx}\epsilon_{yy} + \epsilon_{xx}\epsilon_{zz} + \epsilon_{yy}\epsilon_{zz}) + \frac{c_{44}}{2}(\epsilon_{xy}^2 + \epsilon_{yz}^2 + \epsilon_{xz}^2)$$

Magnetoelastic energy

$$E_{me}^{cub(I)} = b_0(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) + b_1(\alpha_x^2\epsilon_{xx} + \alpha_y^2\epsilon_{yy} + \alpha_z^2\epsilon_{zz}) + b_2(\alpha_x\alpha_y\epsilon_{xy} + \alpha_x\alpha_z\epsilon_{xz} + \alpha_y\alpha_z\epsilon_{yz})$$



$$\left. \frac{\Delta l}{l_0} \right|_{\beta}^{\alpha} = \lambda^{\alpha} + \frac{3}{2}\lambda_{001} \left( \alpha_x^2\beta_x^2 + \alpha_y^2\beta_y^2 + \alpha_z^2\beta_z^2 - \frac{1}{3} \right) + 3\lambda_{111}(\alpha_x\alpha_y\beta_x\beta_y + \alpha_y\alpha_z\beta_y\beta_z + \alpha_x\alpha_z\beta_x\beta_z)$$

$$\lambda^{\alpha} = \frac{-b_0 - \frac{1}{3}b_1}{c_{11} + 2c_{12}},$$

$$\lambda_{001} = \frac{-2b_1}{3(c_{11} - c_{12})},$$

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

# Workflow

$$\left. \frac{\Delta l}{l_0} \right|_{\beta}^{\alpha} = \lambda^{\alpha} + \frac{3}{2} \lambda_{001} \left( \alpha_x^2 \beta_x^2 + \alpha_y^2 \beta_y^2 + \alpha_z^2 \beta_z^2 - \frac{1}{3} \right) + 3 \lambda_{111} (\alpha_x \alpha_y \beta_x \beta_y + \alpha_y \alpha_z \beta_y \beta_z + \alpha_x \alpha_z \beta_x \beta_z)$$

POSCAR → Symmetry analysis

Space group: 207-230

Cubic (I)

$\lambda_{001}$

$\lambda_{111}$

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

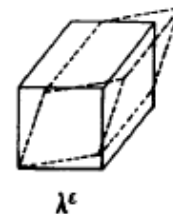
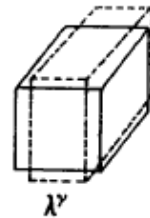
OSZICAR\_2\_X\_1  
 OSZICAR\_2\_X\_2

cell length along  $\beta$

Fitting:  $E(l) = Al^2 + Bl + C$   
 Minimum:  $l_{1(2)} = -B_{1(2)}/(2A_{1(2)})$

$$\lambda^i = \frac{2(l_1 - l_2)}{\eta^i(l_1 + l_2)}$$

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



$$\left. \epsilon \right|_{\beta=(0,0,1)}^{\lambda_{001}} = \begin{pmatrix} \frac{1}{\sqrt{1+\epsilon}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\epsilon}} & 0 \\ 0 & 0 & 1+\epsilon \end{pmatrix}, \quad \left. \epsilon \right|_{\beta=(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})}^{\lambda_{111}} = \zeta \begin{pmatrix} 1 & \frac{\epsilon}{2} & \frac{\epsilon}{2} \\ \frac{\epsilon}{2} & 1 & \frac{\epsilon}{2} \\ \frac{\epsilon}{2} & \frac{\epsilon}{2} & 1 \end{pmatrix}$$

$$\zeta = \sqrt[3]{4/(4 - 3\epsilon^2 + \epsilon^3)}$$

The maximum value of  $\epsilon$  is set with tag-s

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

# Workflow

## HEXAGONAL (I)

SG 177-194

# Hexagonal (I)

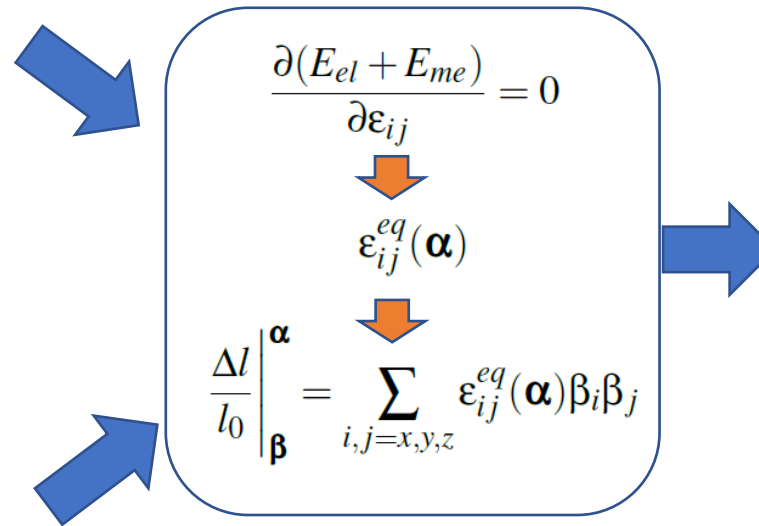
## Workflow

### Elastic energy

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

### Magnetoelastic energy

$$E_{me}^{hex(I)} = b_{11}(\epsilon_{xx} + \epsilon_{yy}) + b_{12}\epsilon_{zz} + b_{21}\left(\alpha_z^2 - \frac{1}{3}\right)(\epsilon_{xx} + \epsilon_{yy}) + b_{22}\left(\alpha_z^2 - \frac{1}{3}\right)\epsilon_{zz} \\ + \frac{1}{2}b_3[(\alpha_x^2 - \alpha_y^2)(\epsilon_{xx} - \epsilon_{yy}) + 2\alpha_x\alpha_y\epsilon_{xy}] + b_4(\alpha_x\alpha_z\epsilon_{xz} + \alpha_y\alpha_z\epsilon_{yz}).$$

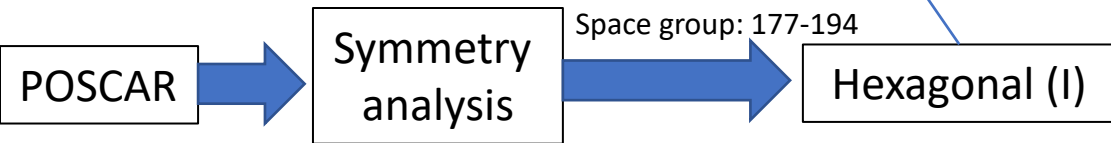
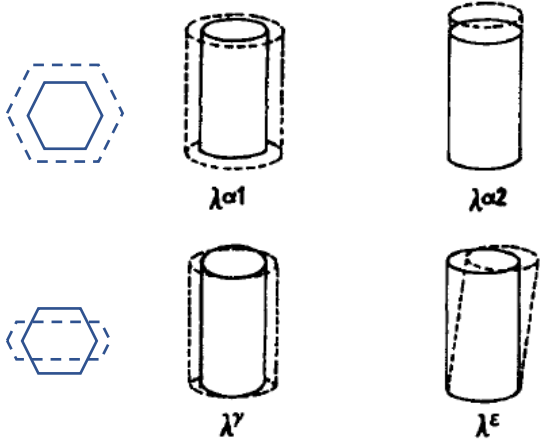


$$\frac{\Delta l}{l_0} \Big|_{\beta}^{\alpha} = \lambda^{\alpha 1,0}(\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0}\beta_z^2 + \lambda^{\alpha 1,2}\left(\alpha_z^2 - \frac{1}{3}\right)(\beta_x^2 + \beta_y^2) \\ + \lambda^{\alpha 2,2}\left(\alpha_z^2 - \frac{1}{3}\right)\beta_z^2 + \lambda^{\gamma,2}\left[\frac{1}{2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + 2\alpha_x\alpha_y\beta_x\beta_y\right] \\ + 2\lambda^{\epsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z),$$

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

# Workflow

$$\left. \frac{\Delta l}{l_0} \right|_{\beta}^{\alpha} = \lambda^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0} \beta_z^2 + \lambda^{\alpha 1,2} \left( \alpha_z^2 - \frac{1}{3} \right) (\beta_x^2 + \beta_y^2) \\ + \lambda^{\alpha 2,2} \left( \alpha_z^2 - \frac{1}{3} \right) \beta_z^2 + \lambda^{\gamma,2} \left[ \frac{1}{2} (\alpha_x^2 - \alpha_y^2) (\beta_x^2 - \beta_y^2) + 2\alpha_x \alpha_y \beta_x \beta_y \right] \\ + 2\lambda^{\varepsilon,2} (\alpha_x \alpha_z \beta_x \beta_z + \alpha_y \alpha_z \beta_y \beta_z),$$



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

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

$$\lambda^i = \frac{2(l_1 - l_2)}{\eta^i(l_1 + l_2)}$$

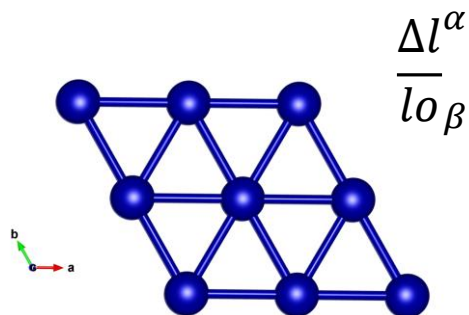
Fitting:  $E(l) = Al^2 + Bl + C$   
 Minimum:  $l_{1(2)} = -B_{1(2)}/(2A_{1(2)})$

cell length along  $\beta$



Hexagonal (I)

# Distorted states



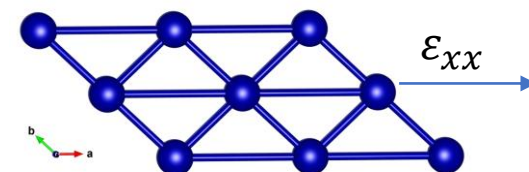
$$\frac{\Delta l^\alpha}{l o_\beta}$$

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

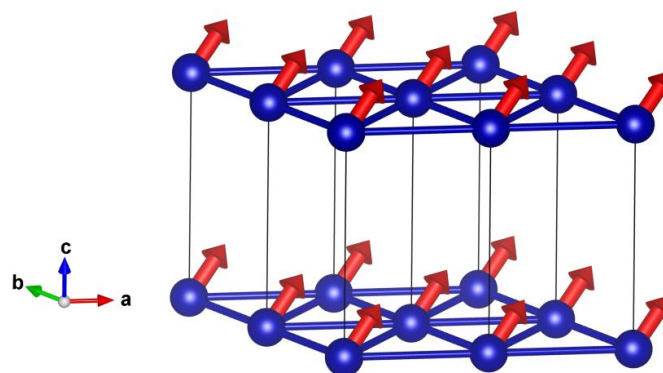
strain along x-axis:  $\beta = (1,0,0)$

$$\epsilon_{\beta=(1,0,0)}^{\lambda^{\alpha 1,2}} = \begin{pmatrix} 1+\epsilon & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\epsilon}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+\epsilon}} \end{pmatrix}$$

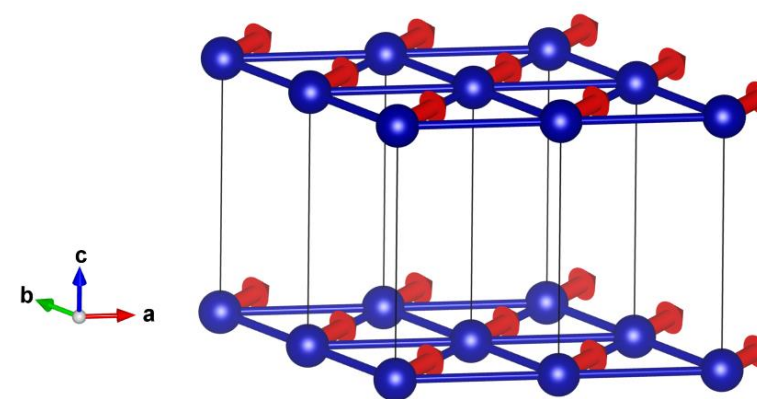
$$\lambda^{\alpha 1,2}$$



volume-conserving

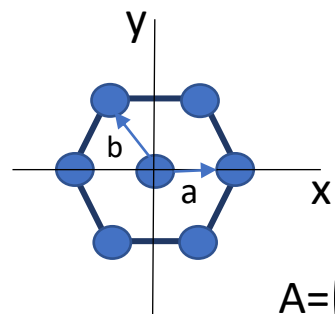


$$S=(1,1,1)$$



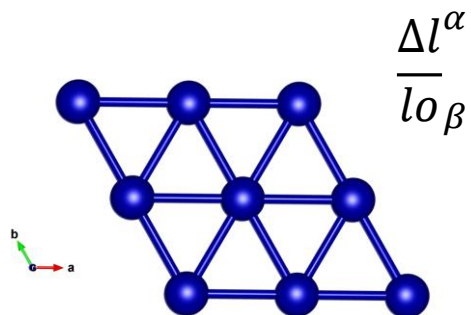
$$S=(1,1,0)$$

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



Hexagonal (I)

# Distorted states



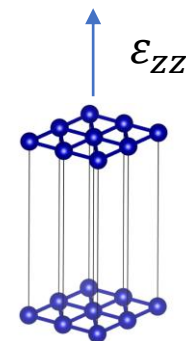
$$\frac{\Delta l^\alpha}{l o_\beta}$$

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

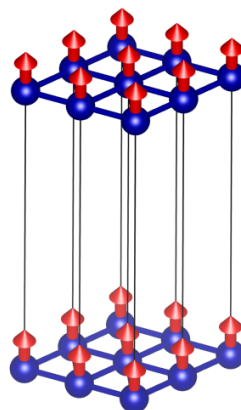
strain along z-axis:  $\beta = (0,0,1)$

$$\epsilon \Big|_{\beta=(0,0,1)}^{\lambda^{\alpha 2,2}} = \begin{pmatrix} \frac{1}{\sqrt{1+\epsilon}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\epsilon}} & 0 \\ 0 & 0 & 1+\epsilon \end{pmatrix}$$

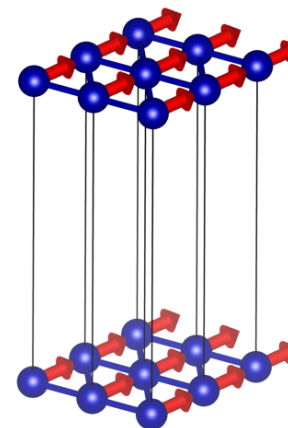
$$\lambda^{\alpha 2,2}$$



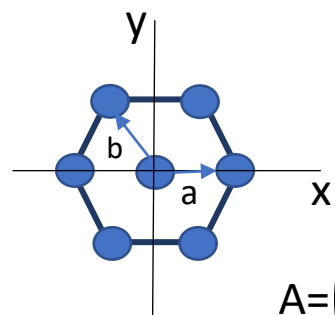
volume-conserving



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



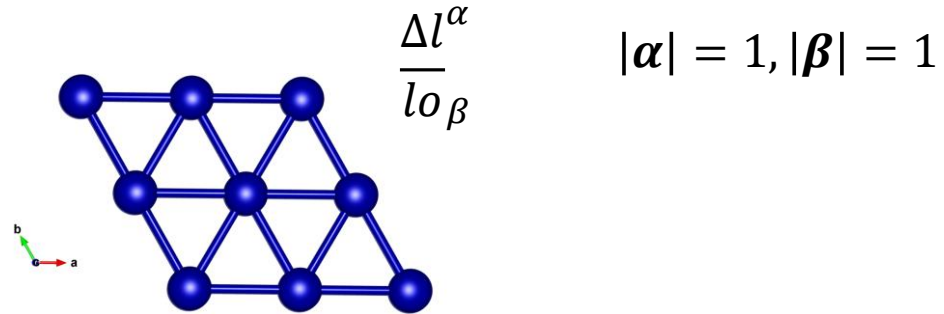
$$S=(1,0,0)$$



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

Hexagonal (I)

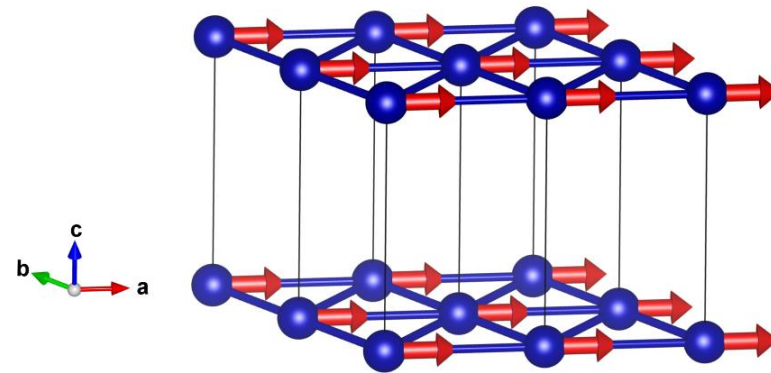
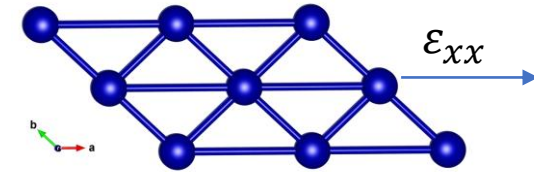
# Distorted states



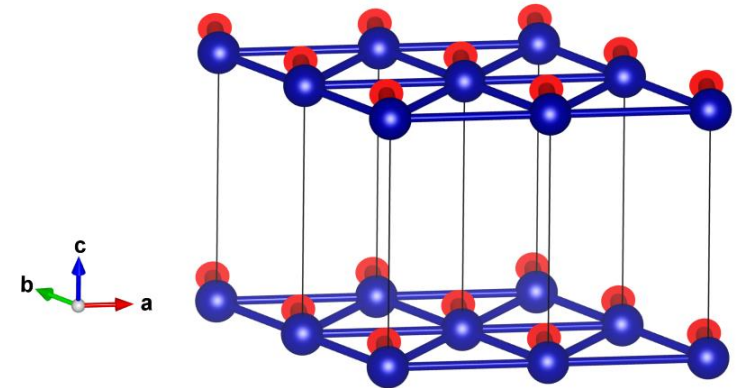
$$\epsilon_{\beta=(1,0,0)}^{\lambda\gamma,2} = \begin{pmatrix} 1+\epsilon & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\epsilon}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+\epsilon}} \end{pmatrix}$$

volume-conserving

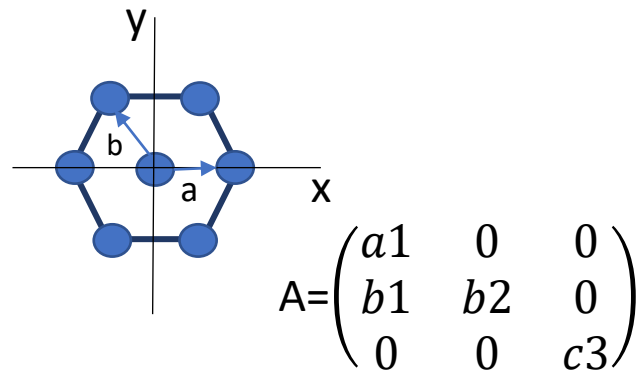
$\lambda\gamma,2$



$S=(1,0,0)$



$S=(0,1,0)$

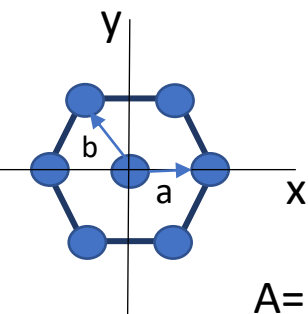
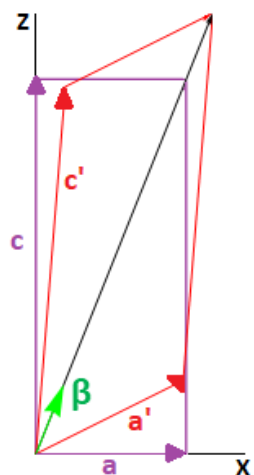


# Hexagonal (I)

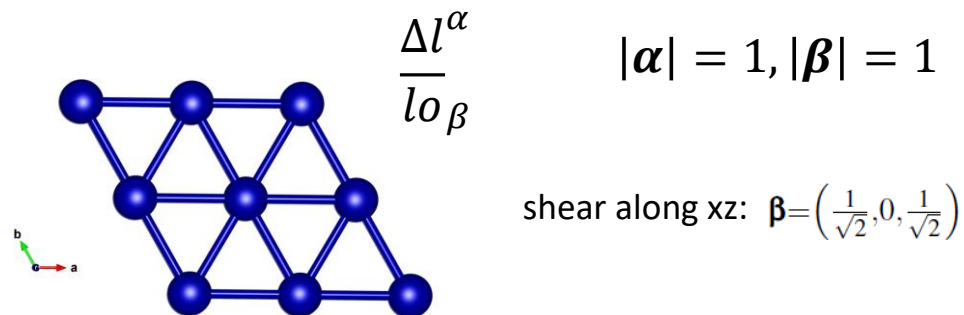
# Distorted states

$a$  and  $c$  are the lattice parameters of the relaxed (not distorted) unit cell

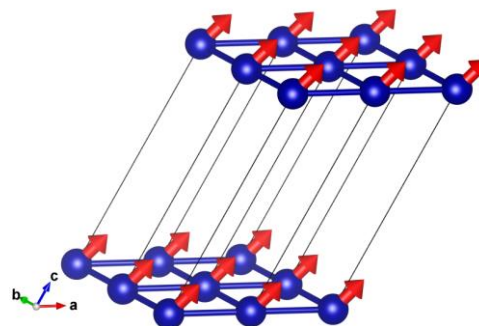
$$\beta = \frac{a+c}{|a+c|} = \frac{a'+c'}{|a'+c'|}$$



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

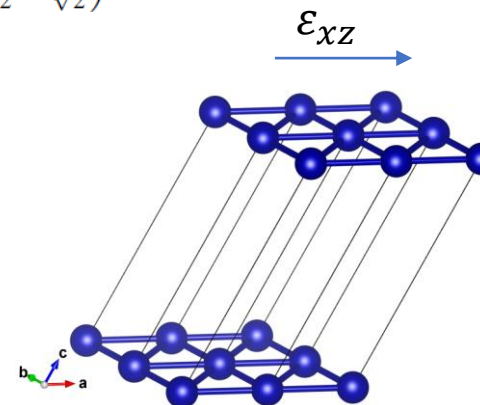


$$\lambda^{\epsilon,2}$$



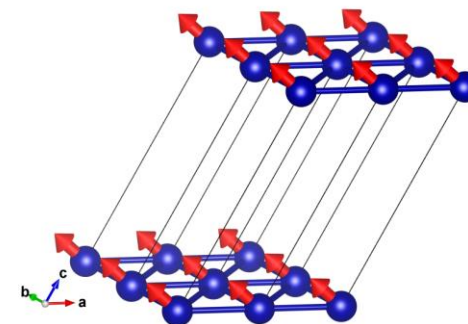
$$S=(1,0,1)$$

$$\underline{\epsilon} \Big|_{\beta = \frac{(a,0,c)}{\sqrt{a^2+c^2}}}^{\lambda^{\epsilon,2}} = \omega \begin{pmatrix} 1 & 0 & \frac{\epsilon c}{2a} \\ 0 & 1 & 0 \\ \frac{\epsilon a}{2c} & 0 & 1 \end{pmatrix}$$



$$\omega = \sqrt[3]{4/(4-\epsilon^2)}$$

volume-conserving



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

# 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

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

| Gauge direction |           |               | Magnetization direction |   |               |               |   |               | Magnetostriiction coefficients    |   |   |
|-----------------|-----------|---------------|-------------------------|---|---------------|---------------|---|---------------|-----------------------------------|---|---|
| $\beta_x$       | $\beta_y$ | $\beta_z$     | Initial                 |   |               | Final         |   |               | $\lambda(x,y)_0 - \lambda(x,y)_f$ | Eq. (3)   | Birss <sup>b</sup>  |
| 1               | 0         | 0             | 1                       | 0 | 0             | 0             | 1 | 0             | $\lambda(a,a) - \lambda(b,a)$     | $\lambda_A - \lambda_B$                                 | $Q_8$   |
| 0               | 0         | 1             | 0                       | 0 | 1             | 1             | 0 | 0             | $\lambda(c,c) - \lambda(a,c)$     | $-\lambda_C$  | $-Q_2 - Q_4$  |
| 1               | 0         | 0             | 1                       | 0 | 0             | 0             | 0 | 1             | $\lambda(a,a) - \lambda(c,a)$     | $\lambda_A$   | $-Q_2$  |
| $\sqrt{2}$      |           | $\sqrt{2}$    | $\sqrt{2}$              |   | $\sqrt{2}$    | $\sqrt{2}$    |   | $\sqrt{2}$    | $\lambda(d,d) - \lambda(e,d)$     | $-\lambda_1^{\alpha,2} + \frac{1}{2}\lambda^{\gamma,2}$ | $-\frac{1}{2}Q_6$   |
| $\frac{1}{2}$   | 0         | $\frac{1}{2}$ | $\frac{1}{2}$           | 0 | $\frac{1}{2}$ | $\frac{1}{2}$ | 0 | $\frac{1}{2}$ |                                   | $\lambda^{\epsilon,2}$                                  | $-\frac{1}{2}\lambda_A - \frac{1}{2}\lambda_C + 2\lambda_D$ |

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

MAELAS notation

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

# Workflow

## TRIGONAL (I)

SG 149-167

# Trigonal (I)

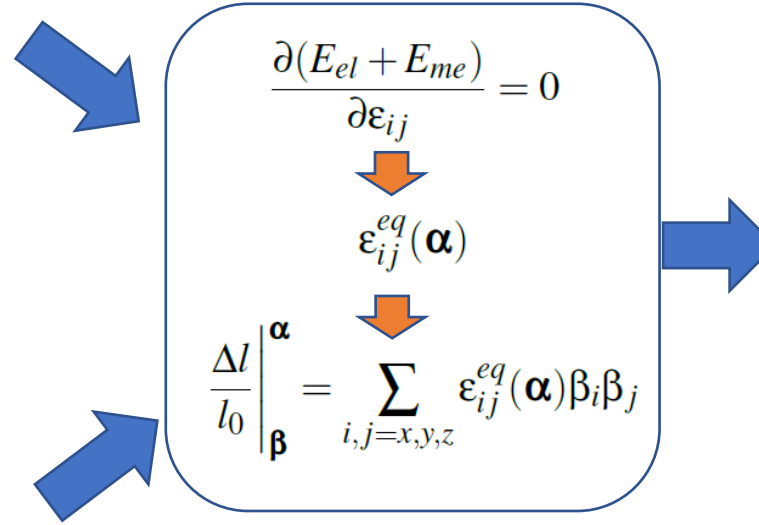
## Workflow

Elastic energy

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

Magnetoelastic energy

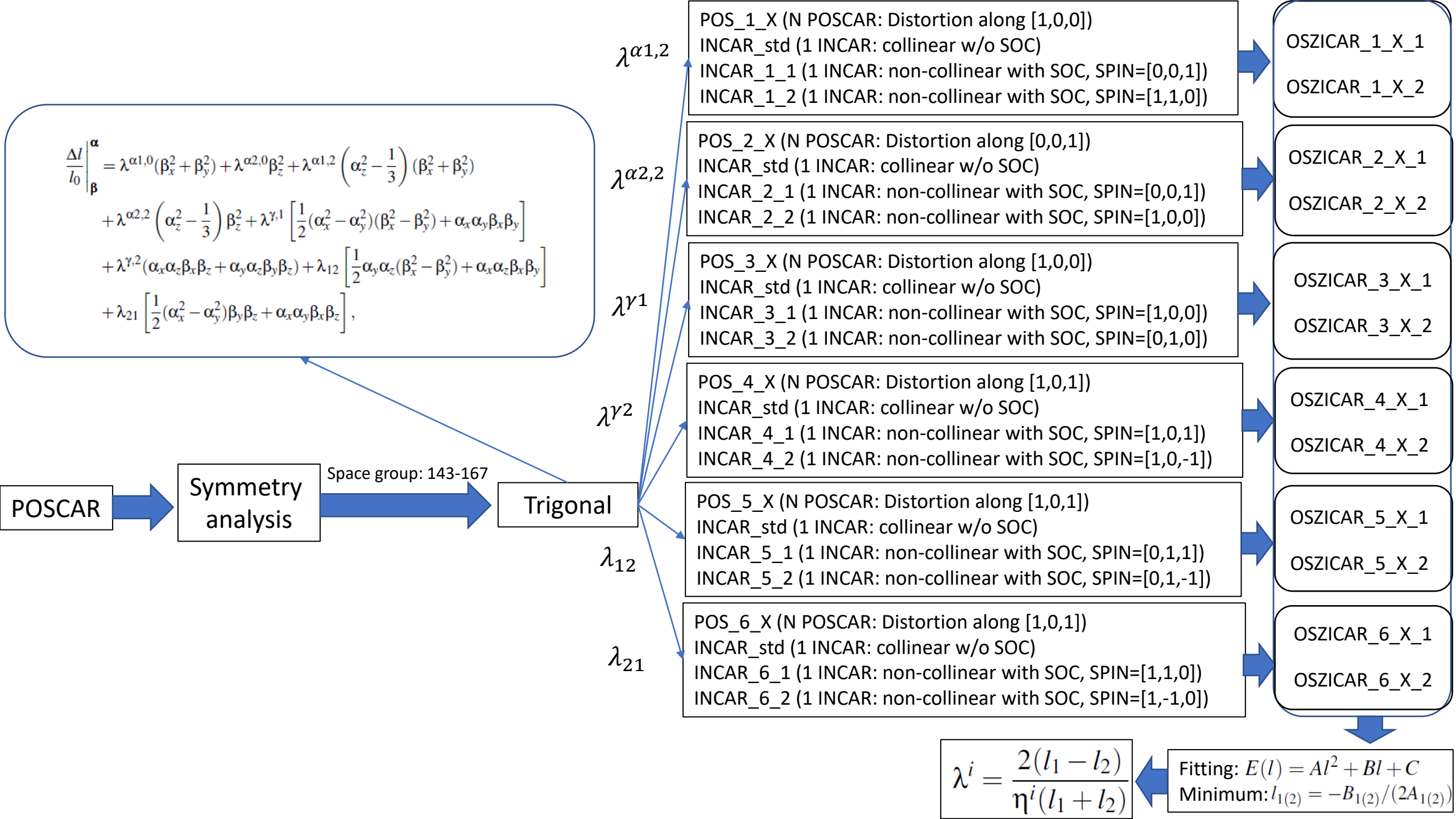
$$E_{me}^{trig(I)} = b_{11}(\epsilon_{xx} + \epsilon_{yy}) + b_{12}\epsilon_{zz} + b_{21}\left(\alpha_z^2 - \frac{1}{3}\right)(\epsilon_{xx} + \epsilon_{yy}) + b_{22}\left(\alpha_z^2 - \frac{1}{3}\right)\epsilon_{zz} \\ + \frac{1}{2}b_3[(\alpha_x^2 - \alpha_y^2)(\epsilon_{xx} - \epsilon_{yy}) + 2\alpha_x\alpha_y] + b_4(\alpha_x\alpha_z\epsilon_{xz} + \alpha_y\alpha_z\epsilon_{yz}) \\ + b_{14}\left[\frac{1}{2}(\alpha_x^2 - \alpha_y^2)\epsilon_{yz} + \alpha_x\alpha_y\epsilon_{xz}\right] + b_{34}\left[\frac{1}{2}\alpha_y\alpha_z(\epsilon_{xx} - \epsilon_{yy}) + \alpha_x\alpha_z\epsilon_{xy}\right].$$



$$\frac{\Delta l}{l_0} \Big|_{\beta}^{\alpha} = \lambda^{\alpha 1,0}(\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0}\beta_z^2 + \lambda^{\alpha 1,2}\left(\alpha_z^2 - \frac{1}{3}\right)(\beta_x^2 + \beta_y^2) \\ + \lambda^{\alpha 2,2}\left(\alpha_z^2 - \frac{1}{3}\right)\beta_z^2 + \lambda^{\gamma,1}\left[\frac{1}{2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + \alpha_x\alpha_y\beta_x\beta_y\right] \\ + \lambda^{\gamma,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z) + \lambda_{12}\left[\frac{1}{2}\alpha_y\alpha_z(\beta_x^2 - \beta_y^2) + \alpha_x\alpha_z\beta_x\beta_y\right] \\ + \lambda_{21}\left[\frac{1}{2}(\alpha_x^2 - \alpha_y^2)\beta_y\beta_z + \alpha_x\alpha_y\beta_x\beta_z\right],$$

$$\lambda^{\alpha 1,0} = \frac{b_{11}c_{33} + b_{12}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 2,0} = \frac{2b_{11}c_{13} - b_{12}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 1,2} = \frac{-b_{21}c_{33} + b_{22}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 2,2} = \frac{2b_{21}c_{13} - b_{22}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\gamma,1} = \frac{c_{14}b_{14} - c_{44}b_3}{\frac{1}{2}c_{44}(c_{11} - c_{12}) - c_{14}^2}, \\ \lambda^{\gamma,2} = \frac{\frac{1}{2}b_4(c_{11} - c_{12}) - b_{34}c_{14}}{\frac{1}{2}c_{44}(c_{11} - c_{12}) - c_{14}^2}, \\ \lambda_{12} = \frac{c_{14}b_4 - c_{44}b_{34}}{\frac{1}{2}c_{44}(c_{11} - c_{12}) - c_{14}^2}, \\ \lambda_{21} = \frac{\frac{1}{2}b_{14}(c_{11} - c_{12}) - b_{34}c_{14}}{\frac{1}{2}c_{44}(c_{11} - c_{12}) - c_{14}^2}.$$







# Workflow

## TETRAGONAL (I)

SG 89-142

# Workflow

Tetragonal (I)

Elastic energy

$$E_{el}^{tet} = \frac{1}{2}c_{11}(\epsilon_{xx}^2 + \epsilon_{yy}^2) + c_{12}\epsilon_{xx}\epsilon_{yy} + c_{13}(\epsilon_{xx} + \epsilon_{yy})\epsilon_{zz} + \frac{1}{2}c_{33}\epsilon_{zz}^2 \\ + \frac{1}{2}c_{44}(\epsilon_{xz}^2 + \epsilon_{yz}^2) + \frac{1}{2}c_{66}\epsilon_{xy}^2.$$

Magnetoelastic energy

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

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



$$\epsilon_{ij}^{eq}(\alpha)$$



$$\left.\frac{\Delta l}{l_0}\right|_{\beta}^{\alpha} = \sum_{i,j=x,y,z} \epsilon_{ij}^{eq}(\alpha) \beta_i \beta_j$$

$$\left.\frac{\Delta l}{l_0}\right|_{\beta}^{\alpha} = \lambda^{\alpha 1,0}(\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0}\beta_z^2 + \lambda^{\alpha 1,2}\left(\alpha_z^2 - \frac{1}{3}\right)(\beta_x^2 + \beta_y^2) \\ + \lambda^{\alpha 2,2}\left(\alpha_z^2 - \frac{1}{3}\right)\beta_z^2 + \frac{1}{2}\lambda^{\gamma,2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + 2\lambda^{\delta,2}\alpha_x\alpha_y\beta_x\beta_y \\ + 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z),$$

$$\lambda^{\alpha 1,0} = \frac{b_{11}c_{33} + b_{12}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$

$$\lambda^{\alpha 2,0} = \frac{2b_{11}c_{13} - b_{12}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$

$$\lambda^{\alpha 1,2} = \frac{-b_{21}c_{33} + b_{22}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$

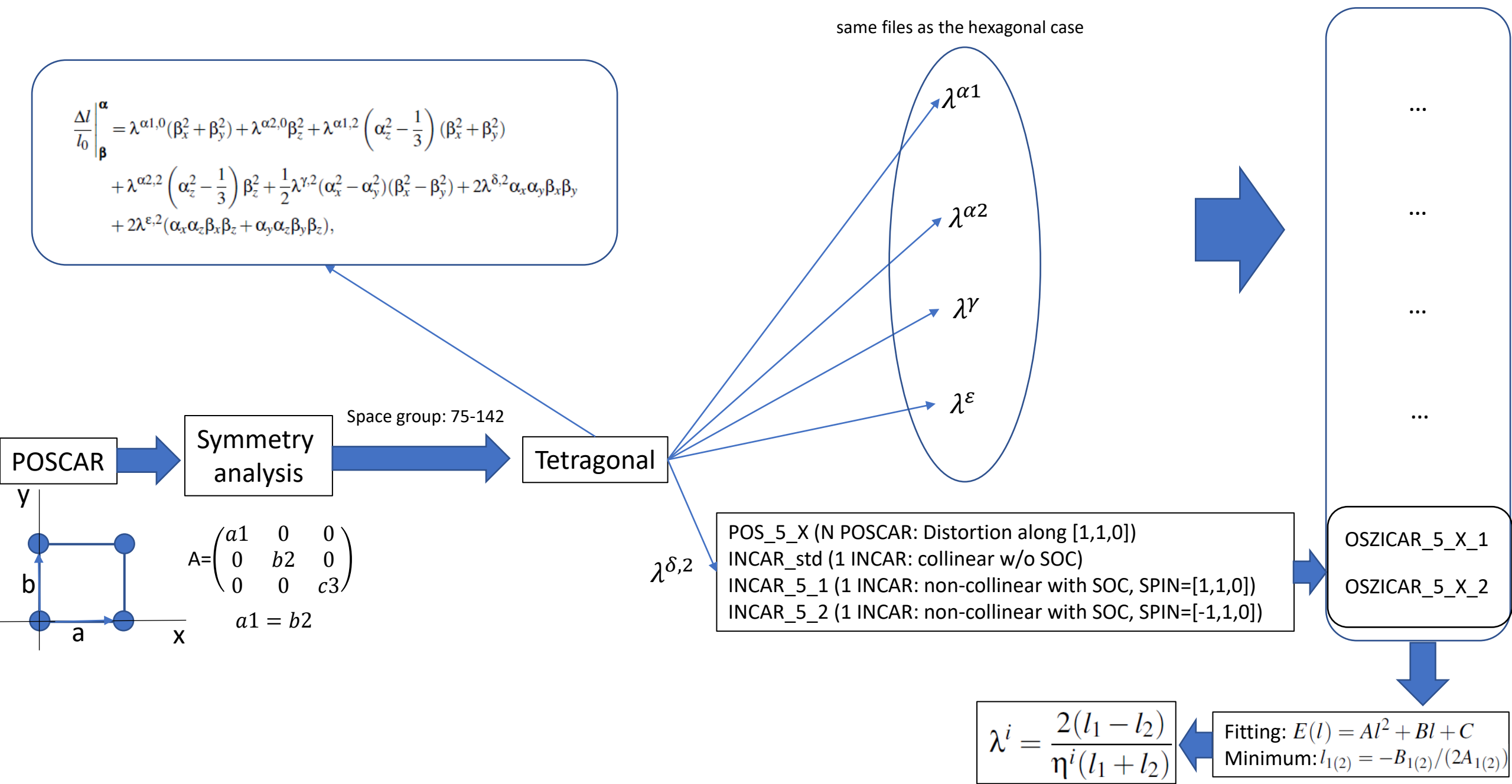
$$\lambda^{\alpha 2,2} = \frac{2b_{21}c_{13} - b_{22}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$

$$\lambda^{\gamma,2} = \frac{-b_3}{c_{11} - c_{12}},$$

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

$$\lambda^{\varepsilon,2} = \frac{-b_4}{2c_{44}}.$$

# Workflow



# Relation between different notations

## Tetragonal (I)

Cullen

Mason

$$\left. \frac{\Delta I}{I_0} \right|_{\beta}^{\alpha} = \lambda^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0} \beta_z^2 + \lambda^{\alpha 1,2} \left( \alpha_z^2 - \frac{1}{3} \right) (\beta_x^2 + \beta_y^2) \\ + \lambda^{\alpha 2,2} \left( \alpha_z^2 - \frac{1}{3} \right) \beta_z^2 + \frac{1}{2} \lambda^{\gamma,2} (\alpha_x^2 - \alpha_y^2) (\beta_x^2 - \beta_y^2) + 2 \lambda^{\delta,2} \alpha_x \alpha_y \beta_x \beta_y \\ + 2 \lambda^{\epsilon,2} (\alpha_x \alpha_z \beta_x \beta_z + \alpha_y \alpha_z \beta_y \beta_z),$$



$$\left. \frac{\Delta I}{I_0} \right|_{\beta}^{\alpha} = \lambda_{Mason}^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda_{Mason}^{\alpha 2,0} \beta_z^2 + \frac{1}{2} \lambda_1 [(\alpha_x \beta_x - \alpha_y \beta_y)^2 - (\alpha_x \beta_y + \alpha_y \beta_x)^2] \\ + (1 - \beta_z^2)(1 - \alpha_z^2) - 2 \alpha_z \beta_z (\alpha_x \beta_x + \alpha_y \beta_y) + 4 \lambda_2 \alpha_z \beta_z (\alpha_x \beta_x + \alpha_y \beta_y) \\ + 4 \lambda_3 \alpha_x \alpha_y \beta_x \beta_y + \lambda_4 [\beta_z^2 (1 - \alpha_z^2) - \alpha_z \beta_z (\alpha_x \beta_x + \alpha_y \beta_y)] \\ + \frac{1}{2} \lambda_5 [(\alpha_x \beta_y - \alpha_y \beta_x)^2 - (\alpha_x \beta_x + \alpha_y \beta_y)^2 + (1 - \beta_z^2)(1 - \alpha_z^2)].$$

$$\lambda_{Mason}^{\alpha 1,0} = \lambda^{\alpha 1,0} + \frac{2}{3} \lambda^{\alpha 1,2}$$

$$\lambda_{Mason}^{\alpha 2,0} = \lambda^{\alpha 2,0} + \frac{2}{3} \lambda^{\alpha 2,2}$$

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

$$\lambda_2 = \frac{1}{2} \lambda^{\epsilon,2} - \frac{1}{4} \lambda^{\alpha 2,2} - \frac{1}{4} \lambda^{\alpha 1,2} + \frac{1}{8} \lambda^{\gamma,2}$$

$$\lambda_3 = \frac{1}{2} \lambda^{\delta,2} - \lambda^{\alpha 1,2}$$

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

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

# Workflow

ORTHORHOMBIC

SG 16-74

# Orthorhombic

# Workflow

## Elastic energy

$$E_{el}^{ortho} = \frac{1}{2}c_{11}\epsilon_{xx}^2 + \frac{1}{2}c_{22}\epsilon_{yy}^2 + c_{12}\epsilon_{xx}\epsilon_{yy} + c_{13}\epsilon_{xx}\epsilon_{zz} + c_{23}\epsilon_{yy}\epsilon_{zz} + \frac{1}{2}c_{33}\epsilon_{zz}^2 \\ + \frac{1}{2}c_{44}\epsilon_{yz}^2 + \frac{1}{2}c_{55}\epsilon_{xz}^2 + \frac{1}{2}c_{66}\epsilon_{xy}^2.$$

## Magnetoelastic energy

$$E_{me}^{ortho} = b_{01}\epsilon_{xx} + b_{02}\epsilon_{yy} + b_{03}\epsilon_{zz} + b_1\alpha_x^2\epsilon_{xx} + b_2\alpha_y^2\epsilon_{xx} + b_3\alpha_x^2\epsilon_{yy} + b_4\alpha_y^2\epsilon_{yy} \\ + b_5\alpha_x^2\epsilon_{zz} + b_6\alpha_y^2\epsilon_{zz} + b_7\alpha_x\alpha_y\epsilon_{xy} + b_8\alpha_x\alpha_z\epsilon_{xz} + b_9\alpha_y\alpha_z\epsilon_{yz},$$

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



$$\epsilon_{ij}^{eq}(\alpha)$$



$$\left. \frac{\Delta l}{l_0} \right|_{\beta}^{\alpha} = \sum_{i,j=x,y,z} \epsilon_{ij}^{eq}(\alpha) \beta_i \beta_j$$

$$\left. \frac{\Delta l}{l_0} \right|_{\beta}^{\alpha} = \lambda^{\alpha 1,0} \beta_x^2 + \lambda^{\alpha 2,0} \beta_y^2 + \lambda^{\alpha 3,0} \beta_z^2 + \lambda_1 (\alpha_x^2 \beta_x^2 - \alpha_x \alpha_y \beta_x \beta_y - \alpha_x \alpha_z \beta_x \beta_z) \\ + \lambda_2 (\alpha_y^2 \beta_x^2 - \alpha_x \alpha_y \beta_x \beta_y) + \lambda_3 (\alpha_x^2 \beta_y^2 - \alpha_x \alpha_y \beta_x \beta_y) \\ + \lambda_4 (\alpha_y^2 \beta_y^2 - \alpha_x \alpha_y \beta_x \beta_y - \alpha_y \alpha_z \beta_y \beta_z) + \lambda_5 (\alpha_x^2 \beta_z^2 - \alpha_x \alpha_z \beta_x \beta_z) \\ + \lambda_6 (\alpha_y^2 \beta_z^2 - \alpha_y \alpha_z \beta_y \beta_z) + 4\lambda_7 \alpha_x \alpha_y \beta_x \beta_y + 4\lambda_8 \alpha_x \alpha_z \beta_x \beta_z + 4\lambda_9 \alpha_y \alpha_z \beta_y \beta_z.$$

$$b_{01} = -c_{11}\lambda^{\alpha 1,0} - c_{12}\lambda^{\alpha 2,0} - c_{13}\lambda^{\alpha 3,0}$$

$$b_{02} = -c_{12}\lambda^{\alpha 1,0} - c_{22}\lambda^{\alpha 2,0} - c_{23}\lambda^{\alpha 3,0}$$

$$b_{03} = -c_{13}\lambda^{\alpha 1,0} - c_{23}\lambda^{\alpha 2,0} - c_{33}\lambda^{\alpha 3,0}$$

$$b_1 = -c_{11}\lambda_1 - c_{12}\lambda_3 - c_{13}\lambda_5$$

$$b_2 = -c_{11}\lambda_2 - c_{12}\lambda_4 - c_{13}\lambda_6$$

$$b_3 = -c_{12}\lambda_1 - c_{22}\lambda_3 - c_{23}\lambda_5$$

$$b_4 = -c_{12}\lambda_2 - c_{22}\lambda_4 - c_{23}\lambda_6$$

$$b_5 = -c_{13}\lambda_1 - c_{23}\lambda_3 - c_{33}\lambda_5$$

$$b_6 = -c_{13}\lambda_2 - c_{23}\lambda_4 - c_{33}\lambda_6$$

$$b_7 = c_{66}(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 - 4\lambda_7)$$

$$b_8 = c_{55}(\lambda_1 + \lambda_5 - 4\lambda_8)$$

$$b_9 = c_{44}(\lambda_4 + \lambda_6 - 4\lambda_9).$$

$$\left. \frac{\Delta I}{I_0} \right|_{\mathbf{\beta}}^{\mathbf{\alpha}} = \lambda^{\alpha 1,0} \beta_x^2 + \lambda^{\alpha 2,0} \beta_y^2 + \lambda^{\alpha 3,0} \beta_z^2 + \lambda_1 (\alpha_x^2 \beta_x^2 - \alpha_x \alpha_y \beta_x \beta_y - \alpha_x \alpha_z \beta_x \beta_z) \\ + \lambda_2 (\alpha_y^2 \beta_x^2 - \alpha_x \alpha_y \beta_x \beta_y) + \lambda_3 (\alpha_x^2 \beta_y^2 - \alpha_x \alpha_y \beta_x \beta_y) \\ + \lambda_4 (\alpha_y^2 \beta_y^2 - \alpha_x \alpha_y \beta_x \beta_y - \alpha_y \alpha_z \beta_y \beta_z) + \lambda_5 (\alpha_x^2 \beta_z^2 - \alpha_x \alpha_z \beta_x \beta_z) \\ + \lambda_6 (\alpha_y^2 \beta_z^2 - \alpha_y \alpha_z \beta_y \beta_z) + 4\lambda_7 \alpha_x \alpha_y \beta_x \beta_y + 4\lambda_8 \alpha_x \alpha_z \beta_x \beta_z + 4\lambda_9 \alpha_y \alpha_z \beta_y \beta_z.$$

POSCAR

Symmetry  
analysis

SG: 16-74

Orthorhombic

MAELAS uses the same lattice convention as AELAS code:

$$c < a < b$$

$\lambda_1$

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])

$\lambda_2$

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])

$\lambda_3$

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])

$\lambda_4$

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])

$\lambda_5$

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])

$\lambda_6$

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])

$\lambda_7$

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])

$\lambda_8$

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])

$\lambda_9$

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])

$$\lambda^i = \frac{2(l_1 - l_2)}{\eta^i(l_1 + l_2)}$$

Fitting:  $E(l) = Al^2 + Bl + C$   
Minimum:  $l_{1(2)} = -B_{1(2)}/(2A_{1(2)})$

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

BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

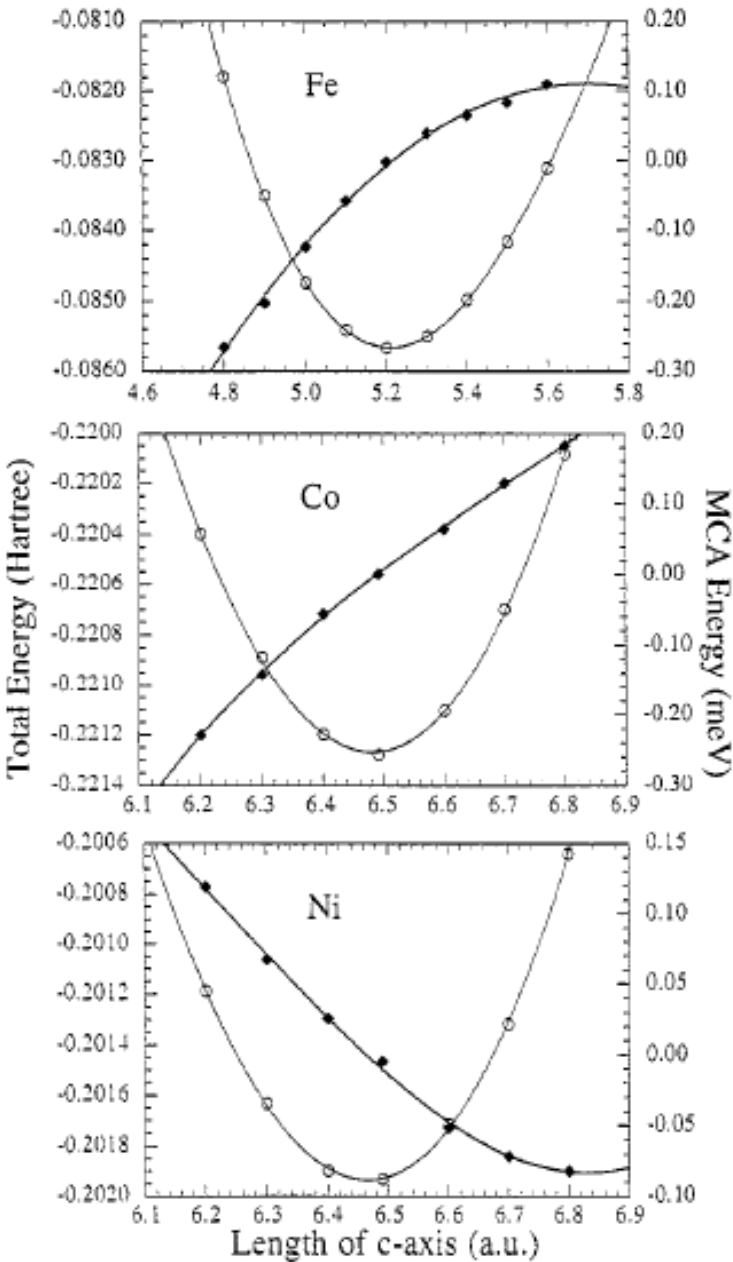
Cubic systems: Itenerant magnets

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

|        | a (a.u.) | $\sigma$ | $M_s(\mu_B)$ | $M_L(\mu_B)$ | $\lambda_{001}(10^{-6})$ |
|--------|----------|----------|--------------|--------------|--------------------------|
| 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                      |

R. C. O'Handley,  
Modern magnetic materials,  
Wiley, 2000.

|   | T = 4.2 K                      |                                | Room Temperature               |                                |                         |
|---|--------------------------------|--------------------------------|--------------------------------|--------------------------------|-------------------------|
|   | $\lambda_{100}(\lambda^{r,2})$ | $\lambda_{111}(\lambda^{r,2})$ | $\lambda_{100}(\lambda^{r,2})$ | $\lambda_{111}(\lambda^{r,2})$ | Polycrystal $\lambda_s$ |
| 3d Metals   |                                |                                |                                |                                |                         |
| BCC-Fe  | 26                             | -30                            | 21                             | -21                            | -7                      |
| HCP-Co <sup>u</sup>                                 | (-150)                         | (45)                           | (-140)                         | (50)                           | (-62)                   |
| FCC-Ni  | -60                            | -35                            | -46                            | -24                            | -34                     |
| BCC-FeCo  | —                              | —                              | 140                            | 30                             | —                       |
| a-Fe <sub>80</sub> B <sub>20</sub>                  | 48 (isotropic)                 | —                              | —                              | —                              | +32                     |
| a-Fe <sub>40</sub> Ni <sub>40</sub> B <sub>20</sub> | +20                            | —                              | —                              | —                              | +14                     |
| a-Cos <sub>80</sub> B <sub>20</sub>                 | -4                             | —                              | —                              | —                              | -4                      |

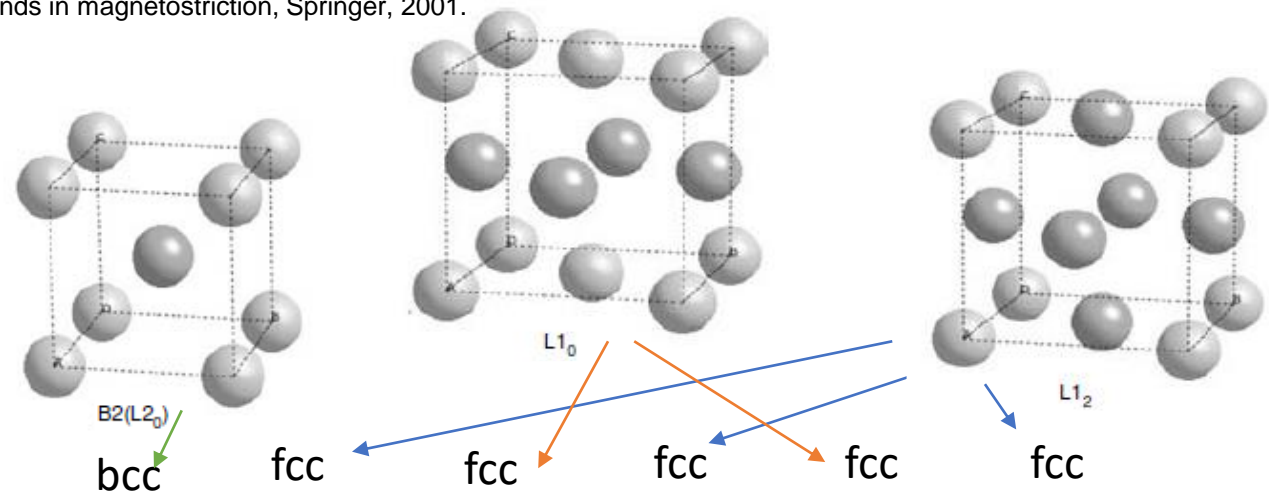




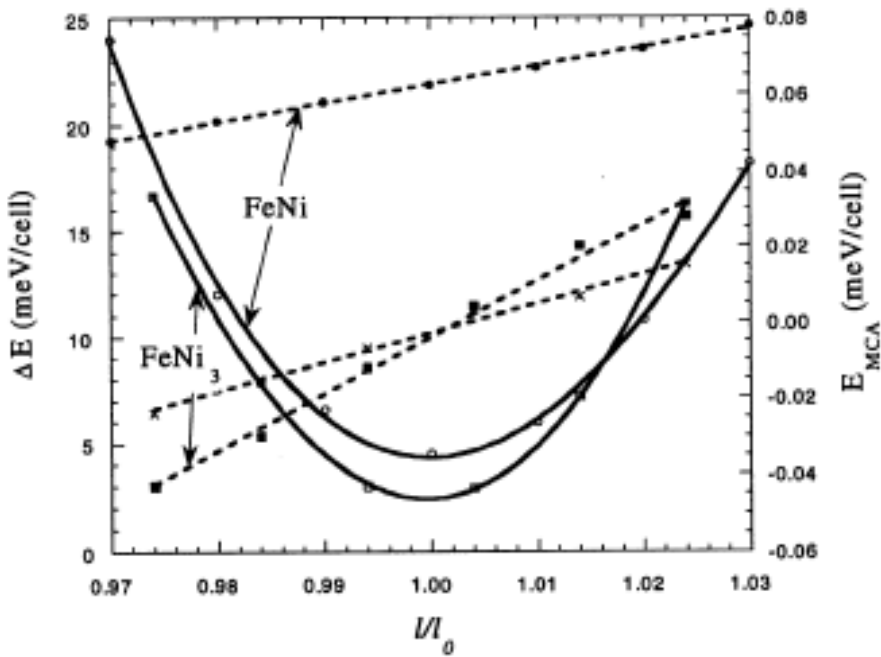
# BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

## Cubic systems: Itenerant magnets

M. Gibbs, Modern trends in magnetostriction, Springer, 2001.



|                           | FeCo           | FeCo <sub>3</sub> | FeNi           | FeNi <sub>3</sub> | CoNi           | CoNi <sub>3</sub> |
|---------------------------|----------------|-------------------|----------------|-------------------|----------------|-------------------|
| a (a.u.)                  | 5.38<br>(5.39) | 6.70              | 6.76<br>(6.76) | 6.70<br>(6.71)    | 6.62<br>(6.67) | 6.66<br>(6.65)    |
| c (a.u.)                  | 5.38<br>(5.39) | 6.70              | 6.76<br>(6.76) | 6.70<br>(6.71)    | 6.78<br>(6.67) | 6.66<br>(6.65)    |
| $E_{MCA}(\mu eV)$         | 0              | 0                 | 63             | 0                 | 143            | 0                 |
| $\sigma$                  | -0.35          | -0.36             | -0.33          | -0.35             | -0.34          | -0.36             |
| $\lambda_{001} (10^{-6})$ | 83<br>(125)    | -68               | 10<br>(12)     | 27<br>(13)        | 42<br>(42-100) | 33                |



# BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

G. Engdahl, Handbook of giant magnetostrictive materials, Academic Press, 1999

## Cubic systems: Rare-Earth magnets

M. Gibbs, Modern trends in magnetostriction, Springer, 2001.

### C15 cubic Laves phase

|                                      | Theory | Experiment |
|--------------------------------------|--------|------------|
| $\lambda_{001}$ (GdCo <sub>2</sub> ) | -407   | -1200      |
| $\lambda_{111}$ (GdCo <sub>2</sub> ) | 19     | < 10       |
| $\lambda_{001}$ (SmCo <sub>2</sub> ) | -290   | ---        |
| $\lambda_{001}$ (ErCo <sub>2</sub> ) | -516   | -1000      |
| $\lambda_{001}$ (GdFe <sub>2</sub> ) | 44     | 39         |

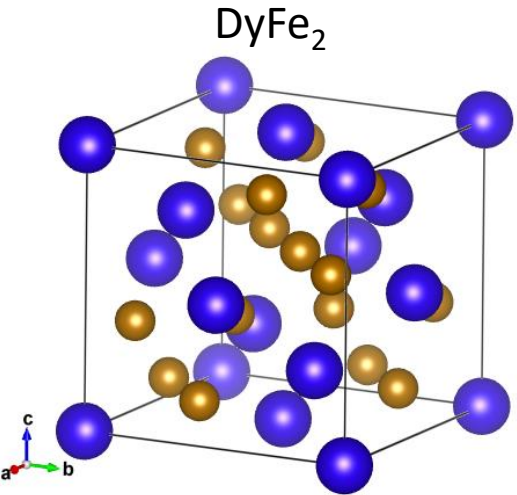
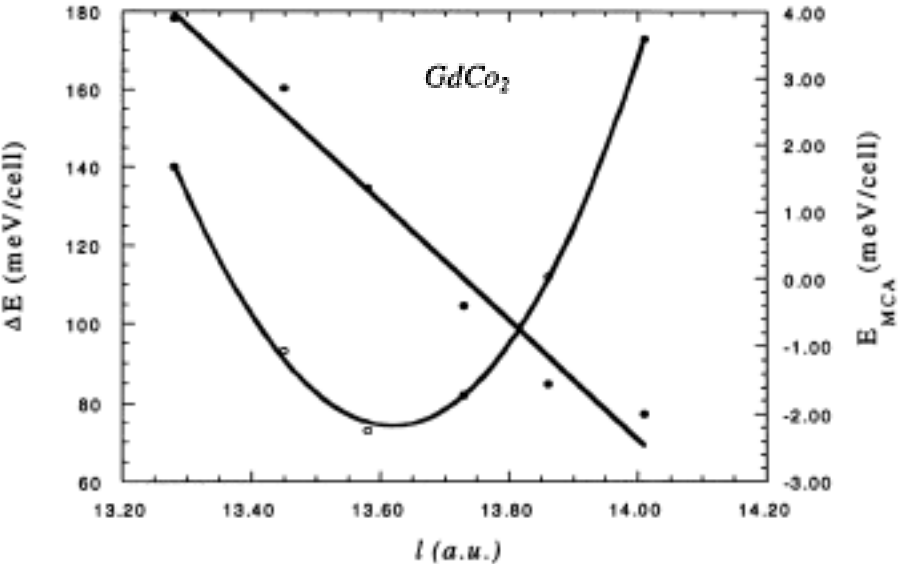


Table 16-10. Low-temperature magnetostriction constants for RCo<sub>2</sub> crystals [from Levitin and Markosyan (1990) unless otherwise noted].

| R in RCo <sub>2</sub> | 10 <sup>6</sup> $\lambda_{111}$ | 10 <sup>6</sup> $\lambda_{100}$ | T <sub>c</sub> (K) <sup>a</sup> |
|-----------------------|---------------------------------|---------------------------------|---------------------------------|
| Gd                    | < 10 <sup>-5</sup>              | -1200                           | 409                             |
| Tb                    | 4500                            | -1200 <sup>b</sup>              | 256                             |
| Dy                    | 5000 <sup>b, c</sup>            | -2000 <sup>d</sup>              | 159                             |
|                       |                                 | -1300 <sup>e</sup>              |                                 |
| Ho                    | 300, 600 <sup>c</sup>           | -2000                           | 85                              |
| Er                    | -2500                           | -1000                           | 36                              |
| Tm                    | -4100 <sup>b</sup>              | 750 <sup>c</sup>                | 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 <sub>c</sub> (K) |
|-------------------|--------------------------|--------------------------|--------------------|
| NdAl <sub>2</sub> | —                        | -700                     | 61                 |
| TbAl <sub>2</sub> | -3000                    | —                        | 114                |
| DyAl <sub>2</sub> | —                        | -1700                    | 68                 |
| TbMn <sub>2</sub> | -3000                    | —                        | 40                 |
| TbFe <sub>2</sub> | 4000, 4500               | —                        | 711                |
| DyFe <sub>2</sub> | —                        | -70                      | 635                |
| HoFe <sub>2</sub> | —                        | -750                     | 612                |
| TmFe <sub>2</sub> | -3500, -2600             | —                        | 610                |
| TbCo <sub>2</sub> | 4400                     | —                        | 256                |
| DyCo <sub>2</sub> | —                        | -2000                    | 159                |
| HoCo <sub>2</sub> | —                        | -2200                    | 85                 |
| ErCo <sub>2</sub> | -2500                    | —                        | 36                 |
| TbNi <sub>2</sub> | 1500                     | —                        | 45                 |
| DyNi <sub>2</sub> | —                        | -1300                    | 30                 |
| HoNi <sub>2</sub> | —                        | -1000                    | 22                 |

Table 1.7. Magnitudes of Single-Crystal Magnetostriction in Rare Earth-Fe<sub>2</sub> Compounds

| Compound          | $\frac{2}{3}\lambda_{111}(10^{-6})$<br>(calculated at 0 K) | $\frac{2}{3}\lambda_{111}(10^{-6})$<br>(measured at room temperature) | T <sub>c</sub> |
|-------------------|--|---|----------------|
| SmFe <sub>2</sub> | -4800  | -3150   | 676            |
| TbFe <sub>2</sub> | 6600   | 3690  | 697, 711       |
| DyFe <sub>2</sub> | 6300   | 1890  | 635            |
| HoFe <sub>2</sub> | 2400   | 288   | 606            |
| ErFe <sub>2</sub> | -2250  | -450  | 590, 597       |
| TmFe <sub>2</sub> | -5550  | -315  | 560            |

BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

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

| 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 <sup>a)</sup> | 0.14               | -0.13             | 0.11                 | 0.02                   | -  | -  | -                    |
| Terbium <sup>b)</sup>    | -2.6 <sup>c)</sup> | 9.0 <sup>c)</sup> | 8.7                  | 15.0 <sup>c)</sup>     | -0.8   | 4.3  | -2.1                 |
| Dysprosium <sup>b)</sup> | -                  | -                 | 9.4                  | 5.5                    | -2.0   | 7.3  | 1.5                  |
| Holmium <sup>b)</sup>    | -                  | -                 | 2.5 <sup>c)</sup>    | -                      | -3.9   | 7.1  | -                    |
| Erbium <sup>b)</sup>     | -                  | -                 | -5.1 <sup>c)</sup>   | -                      | +0.3   | 6.2  | -                    |

<sup>a)</sup> After Mishima et al. (1976).  
<sup>b)</sup> After Rhyne (1972).  
<sup>c)</sup> Extrapolated from paramagnetic range using single-ion theory.

|                           | $T = 4.2 \text{ K}$                 |                                       | Room Temperature                    |                                       |                         |
|---------------------------|-------------------------------------|---------------------------------------|-------------------------------------|---------------------------------------|-------------------------|
|                           | $\lambda_{100}(\lambda^{\gamma,2})$ | $\lambda_{111}(\lambda^{\epsilon,2})$ | $\lambda_{100}(\lambda^{\gamma,2})$ | $\lambda_{111}(\lambda^{\epsilon,2})$ | Polycrystal $\lambda_s$ |
| <i>Spinel Ferrites</i>    |                                     |                                       |                                     |                                       |                         |
| $\text{Fe}_3\text{O}_4$   | 0                                   | 50                                    | -15                                 | 56                                    | +40                     |
| $\text{MnFe}_2\text{O}_4$ | —                                   | —                                     | (-54)                               | (10)                                  | —                       |
| $\text{CoFe}_2\text{O}_4$ | —                                   | —                                     | -670                                | 120                                   | -110                    |
| <i>Garnets</i>            |                                     |                                       |                                     |                                       |                         |
| YIG                       | -0.6                                | -2.5                                  | -1.4                                | -1.6                                  | -2                      |

R. C. O'Handley,  
Modern magnetic materials,  
Wiley, 2000.

Oxide magnets

# MAELAS TESTS

Table 3: Anisotropic magnetostrictive coefficients and MAE calculated using the program MAELAS and measured in experiment ( $T \approx 0$  K) for a set of magnetic materials. In parenthesis we show the magnetostrictive coefficients with Mason's definitions obtained using the relations given by Eq. A.2.

| Material | Crystal system           | DFT method | Magnetostriction coefficient   | MAELAS ( $\times 10^{-6}$ ) | Expt. ( $\times 10^{-6}$ )       | MAE               | MAELAS ( $\mu\text{eV}/\text{atom}$ ) | Expt. ( $\mu\text{eV}/\text{atom}$ ) |                  |
|----------|--------------------------|------------|--|-----------------------------|----------------------------------|-------------------|---------------------------------------|--------------------------------------|------------------|
| BCC Fe   | Cubic (I)<br>SG 229      | GGA        | $\lambda_{001}$  | 23                          | 26 <sup>a</sup>                  | $E(110) - E(001)$ | 0.1                                   | 1.0 <sup>b</sup>                     |                  |
|          |                          |            | $\lambda_{111}$  | 19                          | -30 <sup>a</sup>                 | $E(111) - E(001)$ | 0.21                                  | 1.3 <sup>b</sup>                     |                  |
| HCP Co   | Hexagonal (I)<br>SG 194  | SCAN       | $\lambda^{\alpha 1,2} (\lambda_A)$   | 85 (-78)                    | 95 (-66) <sup>c</sup>            | $E(100) - E(001)$ | 53                                    | 61 <sup>b</sup>                      |                  |
|          |                          |            | $\lambda^{\alpha 2,2} (\lambda_B)$   | -115 (-92)                  | -126 (-123) <sup>c</sup>         |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\gamma,2} (\lambda_C)$   | 15 (115)                    | 57 (126) <sup>c</sup>            |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\varepsilon,2} (\lambda_D)$  | -19 (-1)                    | -286 (-128) <sup>c</sup>         |                   |                                       |                                      |                  |
| YCo5     | Hexagonal (I)<br>SG 191  | LSDA+U     | $\lambda^{\alpha 1,2}$   | -90                         | $ \lambda^{\alpha 1,2}  < 100^d$ | $E(100) - E(001)$ | 365                                   | 567 <sup>e</sup>                     |                  |
|          |                          |            | $\lambda^{\alpha 2,2}$   | 115                         | $ \lambda^{\alpha 2,2}  < 100^d$ |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\gamma,2}$   | 76                          |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\varepsilon,2}$  | 141                         |                                  |                   |                                       |                                      |                  |
| Fe2Si    | Trigonal (I)<br>SG 164   | GGA        | $\lambda^{\alpha 1,2}$   | -9                          |                                  | $E(100) - E(001)$ | -38                                   |                                      |                  |
|          |                          |            | $\lambda^{\alpha 2,2}$   | 15                          |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\gamma,1}$   | 8                           |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\gamma,2}$   | 28                          |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda_{12}$   | -3                          |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda_{21}$   | -13                         |                                  |                   |                                       |                                      |                  |
| Li0 FePd | Tetragonal (I)<br>SG 123 | GGA        | $\lambda^{\alpha 1,2}$   | -21                         |                                  | $E(100) - E(001)$ | 106                                   | 181 <sup>f</sup>                     |                  |
|          |                          |            | $\lambda^{\alpha 2,2}$   | 79                          |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\gamma,2}$   | 31                          |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\varepsilon,2}$  | 28                          |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\delta,2}$   | 106                         |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda^{\alpha 1,0} - \frac{\lambda^{\alpha 1,2}}{3} + \frac{\lambda^{\gamma,2}}{2}$ |                             |                                  |                   |                                       |                                      | 100 <sup>g</sup> |
| YCo      | Orthorhombic<br>SG 63    | LSDA+U     | $\lambda_1$  | -11                         |                                  | $E(100) - E(001)$ | 22                                    |                                      |                  |
|          |                          |            | $\lambda_2$  | 32                          |                                  | $E(010) - E(001)$ | -23                                   |                                      |                  |
|          |                          |            | $\lambda_3$  | 70                          |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda_4$  | -74                         |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda_5$  | -30                         |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda_6$  | 7                           |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda_7$  | 36                          |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda_8$  | -20                         |                                  |                   |                                       |                                      |                  |
|          |                          |            | $\lambda_9$  | 35                          |                                  |                   |                                       |                                      |                  |

More details can be found in P. Nieves, S. Arapan, S.H. Zhang, A.P. Kądziaława, R.F. Zhang and D. Legut, "MAELAS: MAGneto-ELAStic properties calculation via computational high-throughput approach", 2020, arXiv:2009.01638

# MAELAS TESTS

Table 4: Elastic and magnetoelastic constants calculated using the interface between AELAS and MAELAS codes. The third column shows the DFT method used to compute the elastic constants. The experimental elastic constants of BCC Fe and HCP Co were measured at  $T \approx 0$  K and  $T \approx 300$  K, respectively. The experimental magnetoelastic constants were estimated using the experimental elastic constants (seventh column) and the experimental magnetostrictive coefficients in Table 3 via the relations given in Section 2. The sixth column presents calculations of the elastic constants available in the Materials Project database [49, 50].

| Material         | Crystal system          | DFT method | Elastic constant   | AELAS (GPa)                     | Mat.Proj. (GPa)   | Expt. (GPa)   | Magnetoelastic constant                | MAELAS (MPa)                   | Expt. (MPa)                   |
|------------------|-------------------------|------------|--|---------------------------------|---|---|--|--------------------------------|-------------------------------|
| BCC Fe           | Cubic (I)<br>SG 229     | GGA        | $c_{11}$<br>$c_{12}$<br>$c_{44}$                         | 286<br>152<br>103               | 247 <sup>a</sup><br>150 <sup>a</sup><br>97 <sup>a</sup>   | 243 <sup>b</sup><br>138 <sup>b</sup><br>122 <sup>b</sup>  | $b_1$<br>$b_2$                         | -4.6<br>-5.9                   | -4.1<br>10.9                  |
| HCP Co           | Hexagonal (I)<br>SG 194 | GGA        | $c_{11}$<br>$c_{12}$<br>$c_{13}$<br>$c_{33}$<br>$c_{44}$ | 459<br>179<br>132<br>487<br>118 | 358 <sup>c</sup><br>165 <sup>c</sup><br>114 <sup>c</sup><br>409 <sup>c</sup><br>95 <sup>c</sup> | 307 <sup>d</sup><br>165 <sup>d</sup><br>103 <sup>d</sup><br>358 <sup>d</sup><br>75 <sup>d</sup> | $b_{21}$<br>$b_{22}$<br>$b_3$<br>$b_4$ | -39.1<br>33.6<br>-4.2<br>4.5   | -31.9<br>25.5<br>-8.1<br>42.9 |
|                  |                         | SCAN       | $c_{11}$<br>$c_{12}$<br>$c_{13}$<br>$c_{33}$<br>$c_{44}$ | 648<br>212<br>189<br>633<br>239 |   |   | $b_{21}$<br>$b_{22}$<br>$b_3$<br>$b_4$ | -51.3<br>40.5<br>6.4<br>8.9    |                               |
| YCo <sub>5</sub> | Hexagonal (I)<br>SG 191 | GGA        | $c_{11}$<br>$c_{12}$<br>$c_{13}$<br>$c_{33}$<br>$c_{44}$ | 208<br>103<br>114<br>270<br>49  | 192 <sup>e</sup><br>123 <sup>e</sup><br>113 <sup>e</sup><br>262 <sup>e</sup><br>48 <sup>e</sup> |   | $b_{21}$<br>$b_{22}$<br>$b_3$<br>$b_4$ | 14.9<br>-10.4<br>-8.0<br>-13.6 |                               |
|                  |                         | LSDA+U     | $c_{11}$<br>$c_{12}$<br>$c_{13}$<br>$c_{33}$<br>$c_{44}$ | -63<br>363<br>115<br>249<br>44  |   |   | $b_{21}$<br>$b_{22}$<br>$b_3$<br>$b_4$ | 13.9<br>-7.9<br>32.5<br>-12.4  |                               |

Table 5: Elastic and magnetoelastic constants calculated using the interface between AELAS and MAELAS codes. The third column shows the DFT method used to compute the elastic constants. The experimental elastic constants of L1<sub>0</sub> FePd were measured at  $T \approx 300$  K. The sixth column presents calculations of the elastic constants available in the Materials Project database [49, 50].

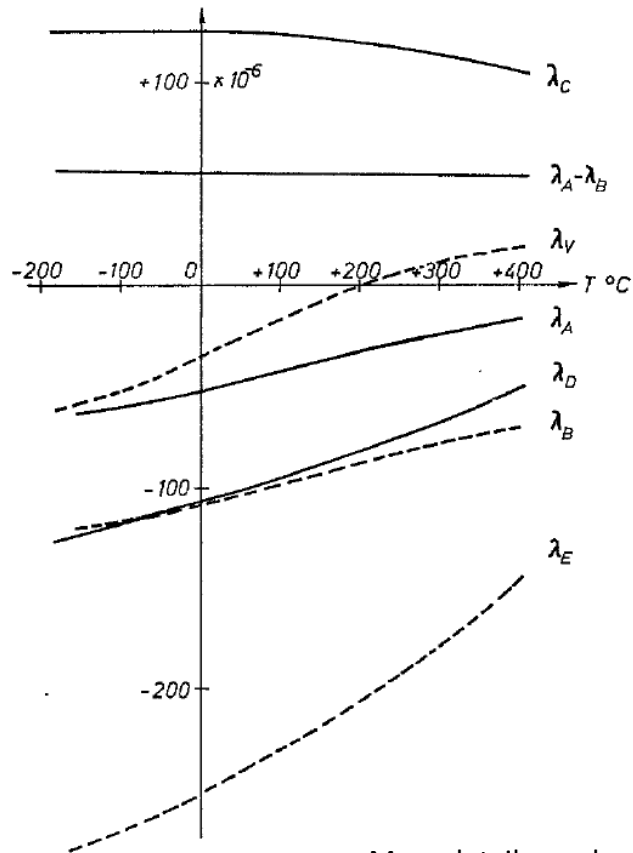
| Material             | Crystal system           | DFT method | Elastic constant   | AELAS (GPa)  | Mat.Proj. (GPa)  | Expt. (GPa)  | Magnetoelastic constant   | MAELAS (MPa)   | Expt. (MPa) |
|----------------------|--------------------------|------------|--|--|--|--|---|--|-------------|
| Fe <sub>2</sub> Si   | Trigonal (I)<br>SG 164   | GGA        | $c_{11}$<br>$c_{12}$<br>$c_{13}$<br>$c_{14}$<br>$c_{33}$<br>$c_{44}$                                     | 428<br>164<br>133<br>-27<br>434<br>118               | 415 <sup>a</sup><br>169 <sup>a</sup><br>133 <sup>a</sup><br>-25 <sup>a</sup><br>428 <sup>a</sup><br>107 <sup>a</sup>   |  | $b_{21}$<br>$b_{22}$<br>$b_3$<br>$b_4$<br>$b_{14}$<br>$b_{34}$                | 3.1<br>-4.2<br>-0.7<br>3.3<br>-1.4<br>-0.4                       |             |
| L1 <sub>0</sub> FePd | Tetragonal (I)<br>SG 123 | GGA        | $c_{11}$<br>$c_{12}$<br>$c_{13}$<br>$c_{33}$<br>$c_{44}$<br>$c_{66}$                                     | 324<br>67<br>133<br>264<br>101<br>37                 | 293 <sup>b</sup><br>62 <sup>b</sup><br>125 <sup>b</sup><br>254 <sup>b</sup><br>99 <sup>b</sup><br>38 <sup>b</sup>  | 214 <sup>c</sup><br>143 <sup>c</sup><br>143 <sup>c</sup><br>227 <sup>c</sup><br>92 <sup>c</sup><br>93 <sup>c</sup> | $b_{21}$<br>$b_{22}$<br>$b_3$<br>$b'_3$<br>$b_4$                              | -2.4<br>-15.2<br>-7.9<br>-7.9<br>-5.6                            |             |
| YCo                  | Orthorhombic<br>SG 63    | GGA        | $c_{11}$<br>$c_{12}$<br>$c_{13}$<br>$c_{22}$<br>$c_{23}$<br>$c_{33}$<br>$c_{44}$<br>$c_{55}$<br>$c_{66}$ | 76<br>45<br>48<br>102<br>55<br>141<br>40<br>27<br>39 | 94 <sup>d</sup><br>61 <sup>d</sup><br>44 <sup>d</sup><br>93 <sup>d</sup><br>56 <sup>d</sup><br>121 <sup>d</sup><br>38 <sup>d</sup><br>29 <sup>d</sup><br>41 <sup>d</sup> |  | $b_1$<br>$b_2$<br>$b_3$<br>$b_4$<br>$b_5$<br>$b_6$<br>$b_7$<br>$b_8$<br>$b_9$ | -0.9<br>0.6<br>-5.0<br>5.7<br>0.9<br>1.5<br>-5.0<br>1.1<br>-8.2  |             |
|                      |                          | LSDA+U     | $c_{11}$<br>$c_{12}$<br>$c_{13}$<br>$c_{22}$<br>$c_{23}$<br>$c_{33}$<br>$c_{44}$<br>$c_{55}$<br>$c_{66}$ | 101<br>65<br>58<br>94<br>70<br>138<br>42<br>29<br>35 |  |  | $b_1$<br>$b_2$<br>$b_3$<br>$b_4$<br>$b_5$<br>$b_6$<br>$b_7$<br>$b_8$<br>$b_9$ | -1.7<br>1.2<br>-3.8<br>4.3<br>-0.1<br>2.3<br>-4.4<br>1.1<br>-8.7 |             |

More details can be found in P. Nieves, S. Arapan, S.H. Zhang, A.P. Kądziaława, R.F. Zhang and D. Legut, “MAELAS: MAGneto-ELAStic properties calculation via computational high-throughput approach”, 2020, arXiv:2009.01638

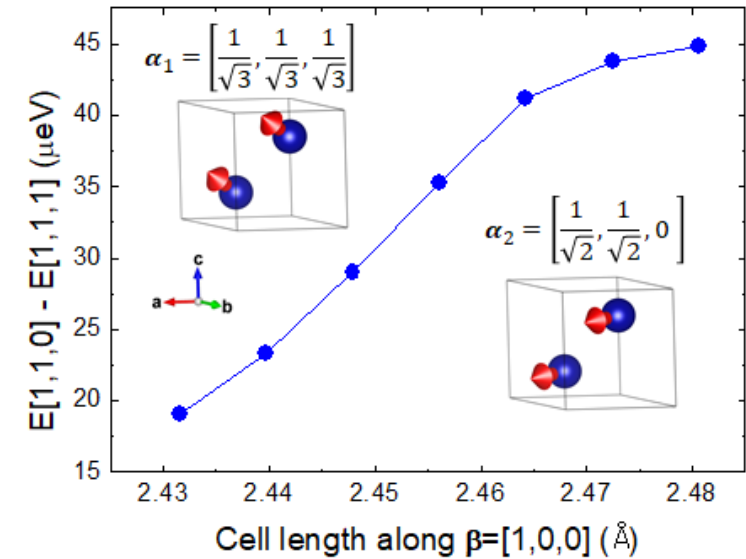
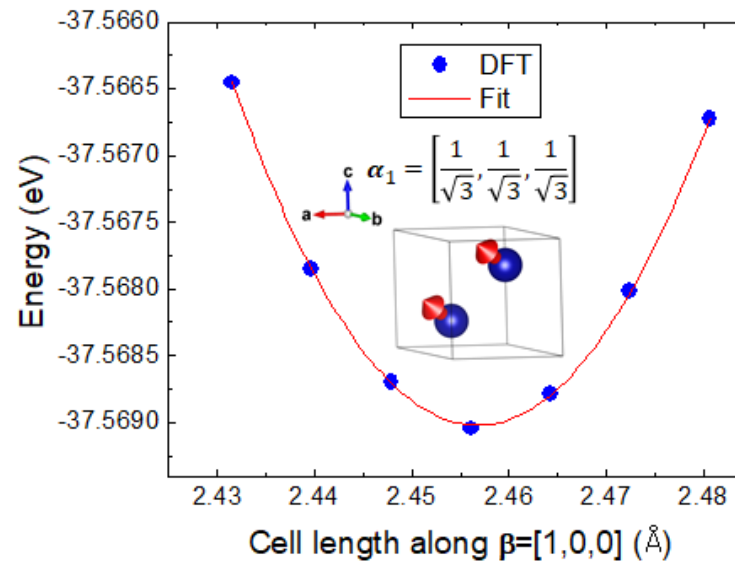
# MAELAS TESTS: HCP Co

## Experimental results

Z. Physik 224, 148—155 (1969)



## Calculation of $\lambda^{\alpha_{1,2}}$ for HCP Co using MAELAS



More details can be found in P. Nieves, S. Arapan, S.H. Zhang, A.P. Kądziaława, R.F. Zhang and D. Legut, "MAELAS: MAGneto-ELAStic properties calculation via computational high-throughput approach", 2020, arXiv:2009.01638



# Visualization tool MAELASviewer

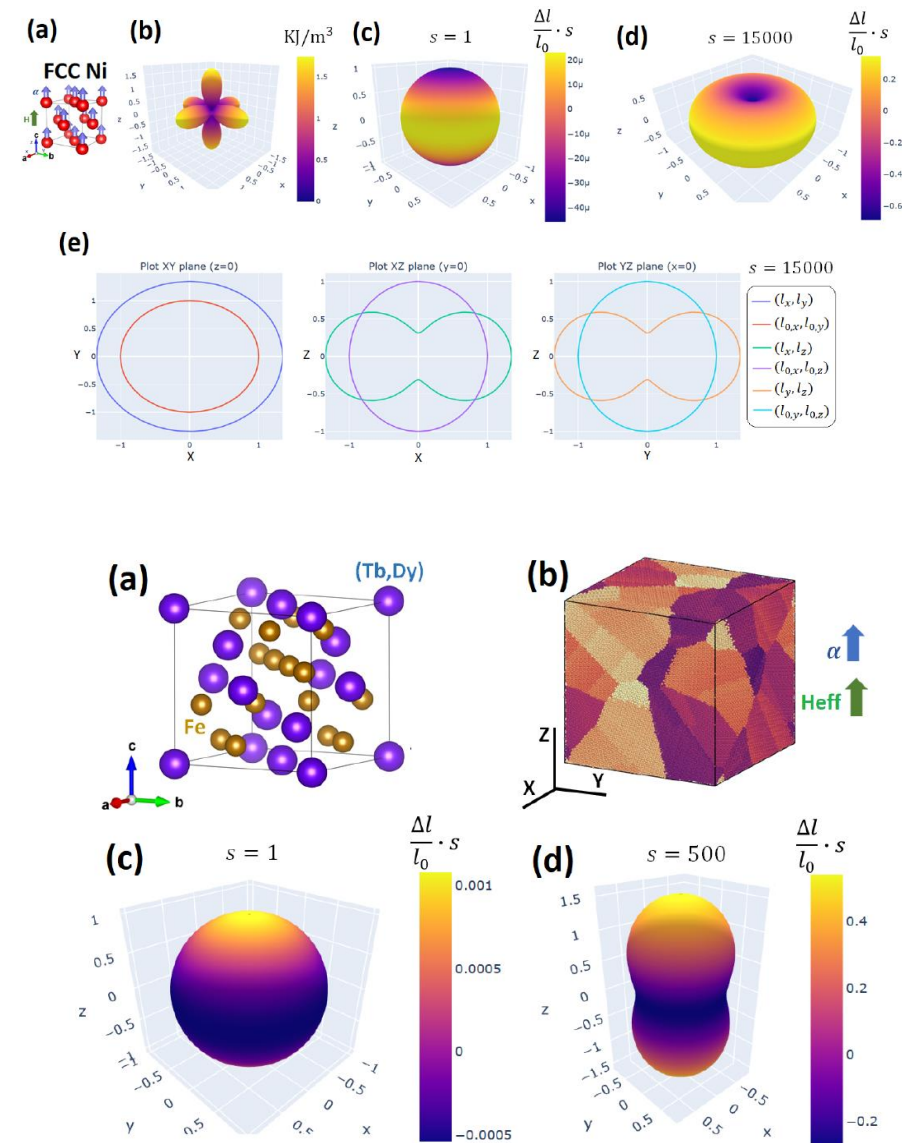
We have also developed an online visualization tool called MAELASviewer that is available at

<https://maelasviewer.herokuapp.com>

This interactive applet shows the magnetostriction for the supported crystal systems of MAELAS. Users can simulate the Joule and Wiedemann effects.

More details of this application can be found in:

Nieves, P.; Arapan, S.; Kądziaława, A.P.; Legut, D. MAELASviewer: An Online Tool to Visualize Magnetostriction. Sensors 2020, 20, 6436.



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