

# MAELAS code

User manual v3.0.0

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*MAELAS: MAgneto-ELASTic properties calculation via computational high-throughput approach*

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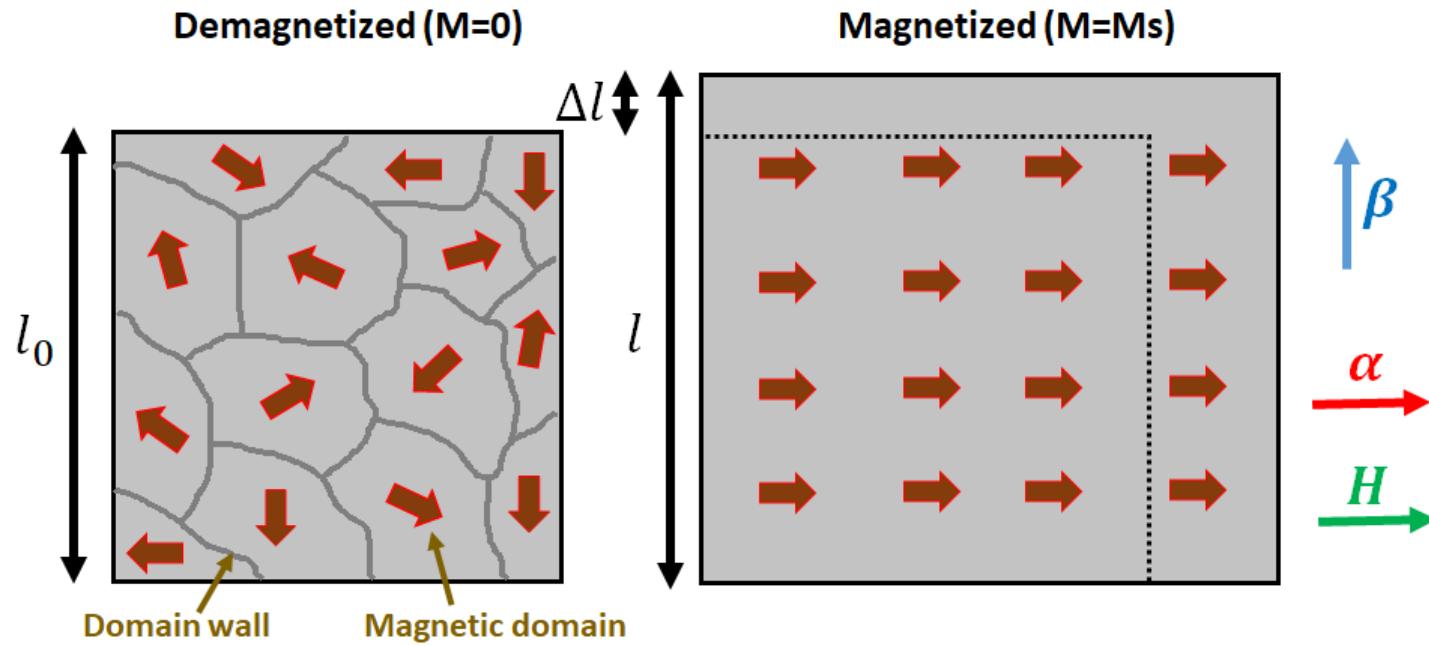
<http://www.md-esg.eu/>

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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.



$\alpha$ =Magnetization direction ( $|\alpha|=1$ )  
 $\beta$ =Measured length direction ( $|\beta|=1$ )  
 $H$ =External magnetic field

relative length change

$$\frac{\Delta l}{l_0} \Bigg|_{\beta}^{\alpha}$$

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 magnetostrictive coefficients and magnetoelastic constants up to second order. There are 3 modes:
- In -mode 1, it generates the required input files for VASP code to perform Density Functional Theory calculations, and it deduces the value of anisotropic magnetostrictive coefficients ( $\lambda^{ani}$ ) from the calculated energies given by VASP. If the elastic tensor is provided, then it can also calculate the anisotropic magnetoelastic constants ( $b^{ani}$ ). It requires spin-polarized calculations with SOC.
- In -mode 2, it generates the required input files for VASP code to perform Density Functional Theory calculations, and it deduces the value of anisotropic magnetoelastic constants ( $b^{ani}$ ) from the calculated energies given by VASP. If the elastic tensor is provided, then it can also calculate the anisotropic magnetostrictive coefficients ( $\lambda^{ani}$ ). It requires spin-polarized calculations with SOC.
- In -mode 3, it generates the required input files for VASP code to perform Density Functional Theory calculations, and it deduces the value of isotropic magnetoelastic constants ( $b^{iso}$ ) from the calculated energies given by VASP. If the elastic tensor is provided, then it can also calculate the isotropic magnetostrictive coefficients ( $\lambda^{iso}$ ) and spontaneous volume magnetostriiction ( $\omega_S$ ). It requires spin-polarized calculations without SOC (exchange magnetostriction).
- MAELAS can also be used with other DFT codes instead of VASP, after file conversion to VASP format files.

# UPDATE HISTORY FOR MAELAS

## Date: August 24, 2022 (version 3.0.0)

- New methodology to calculate the isotropic magnetoelastic constants through a cubic fitting of the energy versus strain. This new method can be executed by adding tag -mode 3 in the command line. If the elastic tensor is provided, then it also calculates the isotropic magnetostrictive coefficients.
- The isotropic and anisotropic contributions to spontaneous volume magnetostriction are also calculated.
- The results are also printed using the universal notation proposed by E. du Tremolet de Lacheisserie [E. D. T. de Lacheisserie, Magnetostriction: Theory and Application of Magnetoelasticity (CRC Press, Boca Raton, FL, 1993)] which is valid for any crystal symmetry.

## Date: September 15, 2021 (version 2.0.1)

We included the calculation of saturation magnetostriction for polycrystals with tetragonal (I), trigonal (I) and orthorhombic symmetries.

## Date: June 7, 2021 (version 2.0.0)

(1) New methodology derived from the magnetoelastic energy for direct calculation of magnetoelastic constants through a linear fitting of the energy versus strain. This new method can be executed by adding tag -mode 2 in the command line.

The method implemented in version 1.0 (based on the quadratic fitting of the energy versus length) is also available in version 2.0, and it can be executed using tag -mode 1. The new method -mode 2 is more accurate than -mode 1, especially for non-cubic crystals.

(2) We fixed some issues related to the trigonal (I) symmetry in version 1.0:

- The deformation gradient  $F$  and measuring length direction  $\beta$  for  $\lambda_{12}$  in trigonal (I) symmetry has been changed.
- We also corrected the theoretical relations between  $\lambda^{Y,1}$ ,  $\lambda^{Y,2}$  and  $\lambda_{21}$  with the magnetoelastic and elastic constants in trigonal (I) symmetry.

## Date: September 3, 2020 (version 1.0.0)

Implementation of the method based on the length optimization of the unit cell proposed by Wu and Freeman [R. Wu, A. J. Freeman, Journal of Applied Physics 79, 6209–6212 (1996)] to calculate the anisotropic magnetostrictive coefficients. This method can be executed by adding tag ``-mode 1`` in the command line. If the elastic tensor is provided, then it also calculates the anisotropic magnetoelastic constants.

# INSTALLATION

The MAELAS code requires to have Python3(>=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(>=2020.4.29), scikit-learn(>=0.23.1), pyfiglet(>=0.8.post0), argparse(>=1.4.0), numpy(>=1.18.4), matplotlib(>=3.2.1), scipy(>=1.4.1), setuptools(>=40.8.0)
```

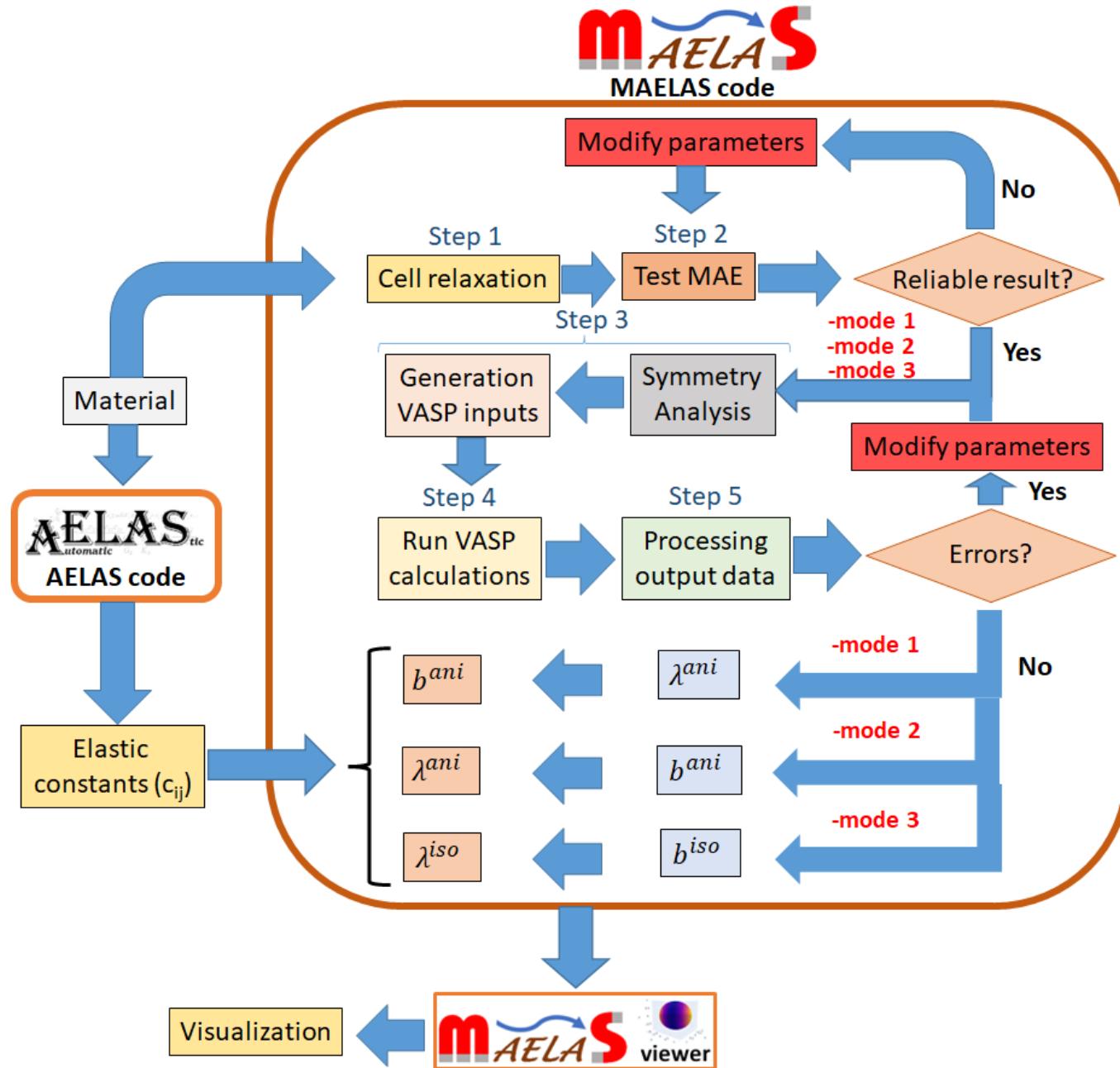
More available options for the installation can be found in the file INSTALL. By default, the executable file "maelas" is installed in the folder /home/\$USER/.local/bin/ where \$USER is the name of your username folder. This folder should be included to the PATH variable by adding in the file /home/\$USER/.bashrc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

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

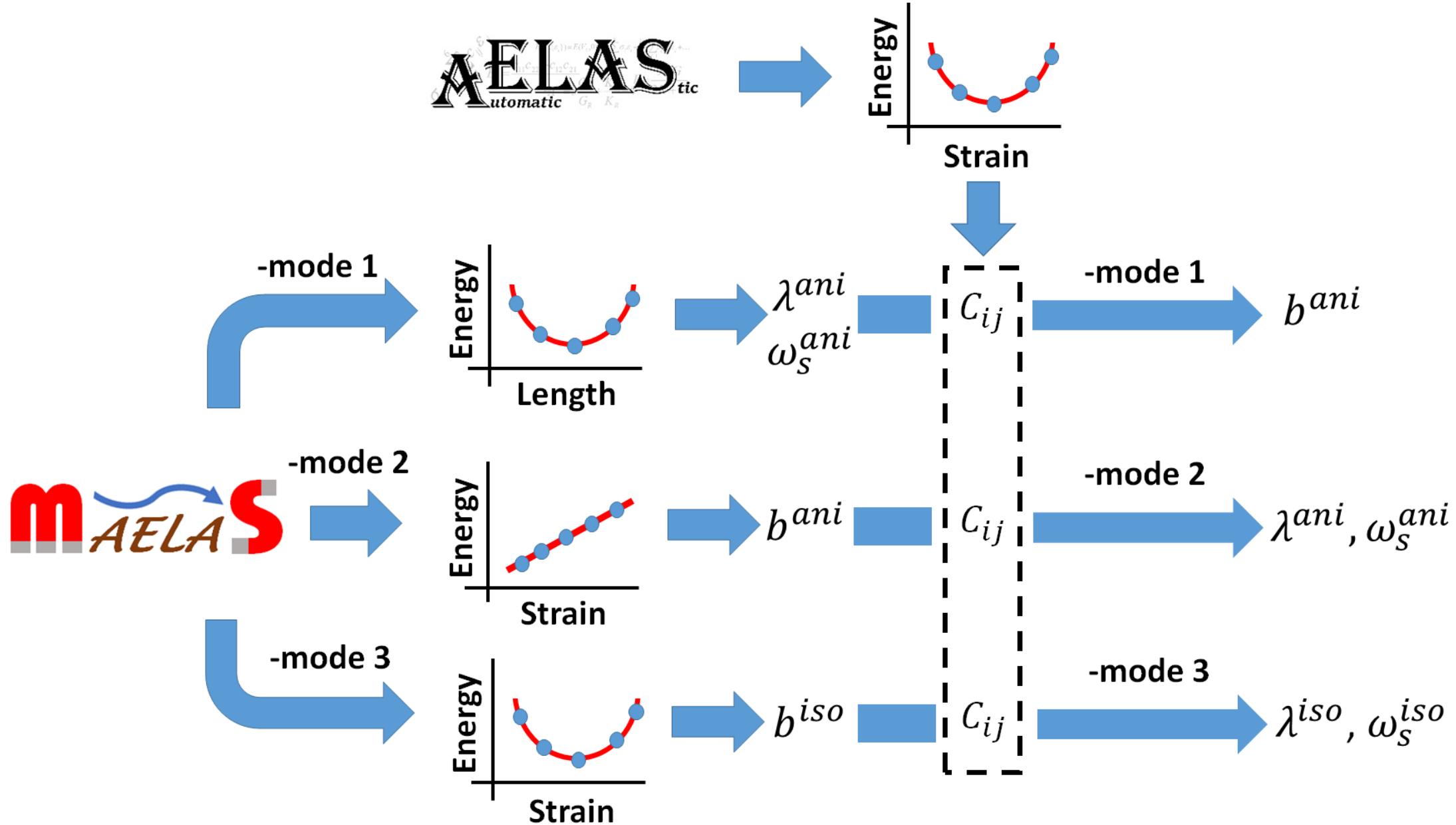
Then you should close the terminal and open the terminal again. If you need to install pip3 in Ubuntu Linux, then type

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

# HOW TO USE MAELAS CODE



# HOW TO USE MAELAS CODE



# 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 vaspx\_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 vaspx\_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 vaspx\_jsub\_rlx file, so one can submit this VASP job immediately in HPC facilities by typing

```
qsub vaspx_jsub_rlx
```

This procedure might be helpful for high-throughput routines. Note that the user might need to modify vaspx\_jsub\_rlx (it is in PBS Pro format) depending on the cluster or local computer batch scheduling. More options can be added in vaspx\_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 input files (mode1, mode 2 and mode 3)

Copy the relaxed POSCAR and POTCAR 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 -mode 1 -i POSCAR_rlx -k 70 -n 7 -s 0.01
```

or

```
maelas -g -mode 2 -i POSCAR_rlx -k 70 -n 7 -s 0.01
```

or

```
maelas -g -mode 3 -i POSCAR_rlx -k 70 -n 7 -s 0.01
```

where -g jointly with -mode 1 indicates that you want to generate input VASP files for the calculation of anisotropic magnetostrictive coefficients, while -g jointly with -mode 2 or -mode 3 indicate that you want to generate input VASP files for the calculation of anisotropic or isotropic magnetoelastic constants, respectively. -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 magnetostrictive coefficient and -s 0.01 is the maximum value of the parameter s for the deformation gradient  $F_{ij}(s)$  to generate the distorted POSCAR files. It will generate the following files:

- POSCAR\_A\_B (distorted cell where A=magnetostrictive coefficient (-mode 1) or magnetoelastic constant (-mode 2 and -mode 3), B=1,...,n distorted cell for each magnetostrictive coefficient or magnetoelastic constant)
- INCAR\_A\_C (non-collinear calculation where A=magnetostrictive coefficient (-mode 1) or magnetoelastic constant (-mode 2), C=1,2 is the spin orientation case, in -mode 3 these files are not generated because it only requires collinear calculations)
- INCAR\_std (collinear calculation to generate the WAVECAR and CHGCAR files to run non-collinear calculations in -mode 1 and -mode 2)
- KPOINTS
- vasp\_maelas, vasp\_jsub, and vasp\_0 (interconnected bash scripts to run VASP calculations automatically)
- vasp\_cp\_oszicar (bash script to get calculated OSZICAR\_A\_B\_C files after VASP calculation finish)

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# HOW TO USE MAELAS CODE

## Step 3: Generation of VASP input files (mode1, mode 2 and mode 3)

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. 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. 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 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 `/scratch/example_mag` is the folder where you want to run VASP calculations. This procedure might be helpful for high-throughput routines. More options can be added in these script files through the terminal command line, to see them just type

```
maelas -h
```

Note that generated `INCAR_std`, `INCAR_A_C`, and `KPOINTS` files contain standard settings for collinear and non-collinear calculations with VASP. The user can modify these files in order to add more advanced settings.

By default, `-mode 3` assumes spin-polarized calculations without SOC (only isotropic magnetic interactions), so that these generated files are suitable for this kind of calculation. In case you want also to include anisotropic magnetic interactions in the calculation of the isotropic magnetoelastic constants (`-mode 3`), then you need to add the flag `-ani`

```
maelas -g -mode 3 -ani -i POSCAR_rlx -k 70 -n 7 -s 0.01
```

Now, it should generate the following files: `POSCAR_A_B` ( $A=1, B=1,\dots,7$ ), `INCAR_std`, `INCAR_A_C` ( $C=1$ ), `KPOINTS`, `vasp_0`, `vasp_jsub`, `vasp_maelas`, `vasp_cp_oszicar` and `output.dat`. These generated files are suitable for spin-polarized calculations with SOC in `-mode 3`.

# HOW TO USE MAELAS CODE

## Step 4: Run VASP calculations

In -mode 1 and 2, 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. In -mode 3, for each generated POSCAR\_A\_B one should run only a collinear calculation. 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\_ncl”) 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 vaspmjsub 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\_ncl” 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 (-mode 1), anisotropic magnetoelastic constants (-mode 2) or isotropic magnetoelastic constants (-mode 3) from the energy written in the OSZICAR files**

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 a type

```
maelas -d -mode 1 -i POSCAR_rlx -n 7
```

or

```
maelas -d -mode 2 -i POSCAR_rlx -n 7 -s 0.01
```

or

```
maelas -d -mode 3 -i POSCAR_rlx -n 7 -s 0.01
```

where -d jointly with -mode 1 means that you want to derive the anisotropic magnetostrictive coefficients from the calculated OSZICAR files, while -d jointly with -mode 2 or 3 will derive the anisotropic or isotropic magnetoelastic constants, respectively, 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 magnetostrictive coefficient (-mode 1) or magnetoelastic constant (-mode 2 or 3) used in step 3. For -mode 2 and 3 it is also necessary to write the maximum applied strain in step 3 -s 0.01.

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# HOW TO USE MAELAS CODE

**Step 5: Derivation of anisotropic magnetostrictive coefficients (-mode 1), anisotropic magnetoelastic constants (-mode 2) or isotropic magnetoelastic constants (-mode 3) from the energy written in the OSZICAR files**

It will derive and print the calculated spin-dependent magnetostrictive coefficients (-mode 1) or magnetoelastic constants (-mode 2 or 3) in the terminal. If you want to print it in a file (for example, results.out), then you can type

```
maelas -d -mode 1 -i POSCAR_rlx -n 7 > results.out
```

or

```
maelas -d -mode 2 -i POSCAR_rlx -n 7 -s 0.01 > results.out
```

or

```
maelas -d -mode 3 -i POSCAR_rlx -n 7 -s 0.01 > results.out
```

In -mode 1, 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 magnetostrictive coefficient are shown in Fig. dE\_A.png.

In -mode 2, the energy values extracted from OSZICAR\_A\_B\_C files are shown in generated files ene\_A\_C.dat. The energy difference between the two spin configurations and linear fitting for each magnetoelastic constant are shown in Fig. dE\_A.png.

In -mode 3, 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. In case you want also to include anisotropic magnetic interactions in the calculation of the isotropic magnetoelastic constants (-mode 3), then you need to add the flag -ani

```
maelas -d -mode 3 -ani -i POSCAR_rlx -n 7 -s 0.01
```

Note that here you also need to copy the file called MAGANI generated in step 5 of -mode 2 which contains the data of the anisotropic magnetoelastic constants.

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# HOW TO USE MAELAS CODE

**Step 5: Derivation of anisotropic magnetostrictive coefficients (-mode 1), anisotropic magnetoelastic constants (-mode 2) or isotropic magnetoelastic constants (-mode 3) from the energy written in the OSZICAR files**

If the elastic tensor is provided as input, then MAELAS can also calculate the magnetoelastic constants -mode 1 or magnetostrictive coefficients -mode 2 or 3. 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 written by AELAS code (file ELADAT). You can check this format in the Examples folder. Hence, you could type

```
maelas -d -mode 1 -i POSCAR_rlx -n 7 -b -e ELADAT
```

or

```
maelas -d -mode 2 -i POSCAR_rlx -n 7 -s 0.01 -b -e ELADAT
```

or

```
maelas -d -mode 3 -i POSCAR_rlx -n 7 -s 0.01 -b -e ELADAT
```

or

```
maelas -d -mode 3 -ani -i POSCAR_rlx -n 7 -s 0.01 -b -e ELADAT
```

Format of the  
elastic tensor file

Elastic tensor:

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

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

# HOW TO USE MAELAS CODE

## Summary: In a nutshell (-mode 1)

### 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_ozsicar
```

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

```
maelas -g -mode 1 -i POSCAR_rlx -k 70 -n 7 -s 0.01
```

### Step 4: Run VASP calculations

```
./vasp_maelas
```

```
./vasp_cp_ozsicar
```

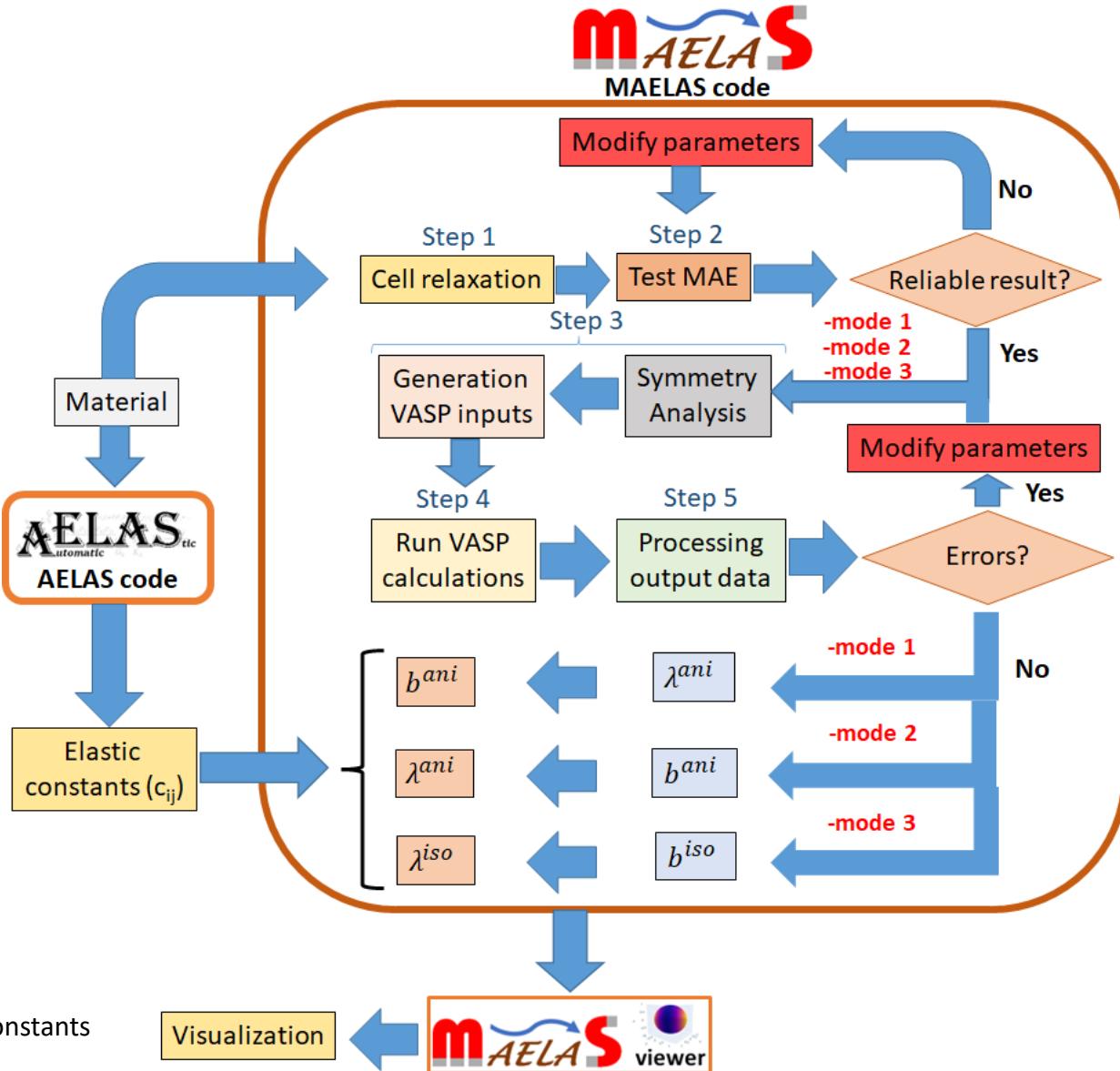
### Step 5a: Derivation of anisotropic magnetostrictive coefficients

```
maelas -d -mode 1 -i POSCAR_rlx -n 7
```

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

```
maelas -d -mode 1 -i POSCAR_rlx -n 7 -b -e ELADAT
```

See all optional arguments: maelas -h



# HOW TO USE MAELAS CODE

## Summary: In a nutshell (-mode 2)

### 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\_ozsicar

### Step 3: Generate VASP inputs for the calculation of anisotropic magnetoelastic constants

maelas -g -mode 2 -i POSCAR\_rlx -k 70 -n 7 -s 0.01

### Step 4: Run VASP calculations

./vasp\_maelas

./vasp\_cp\_ozsicar

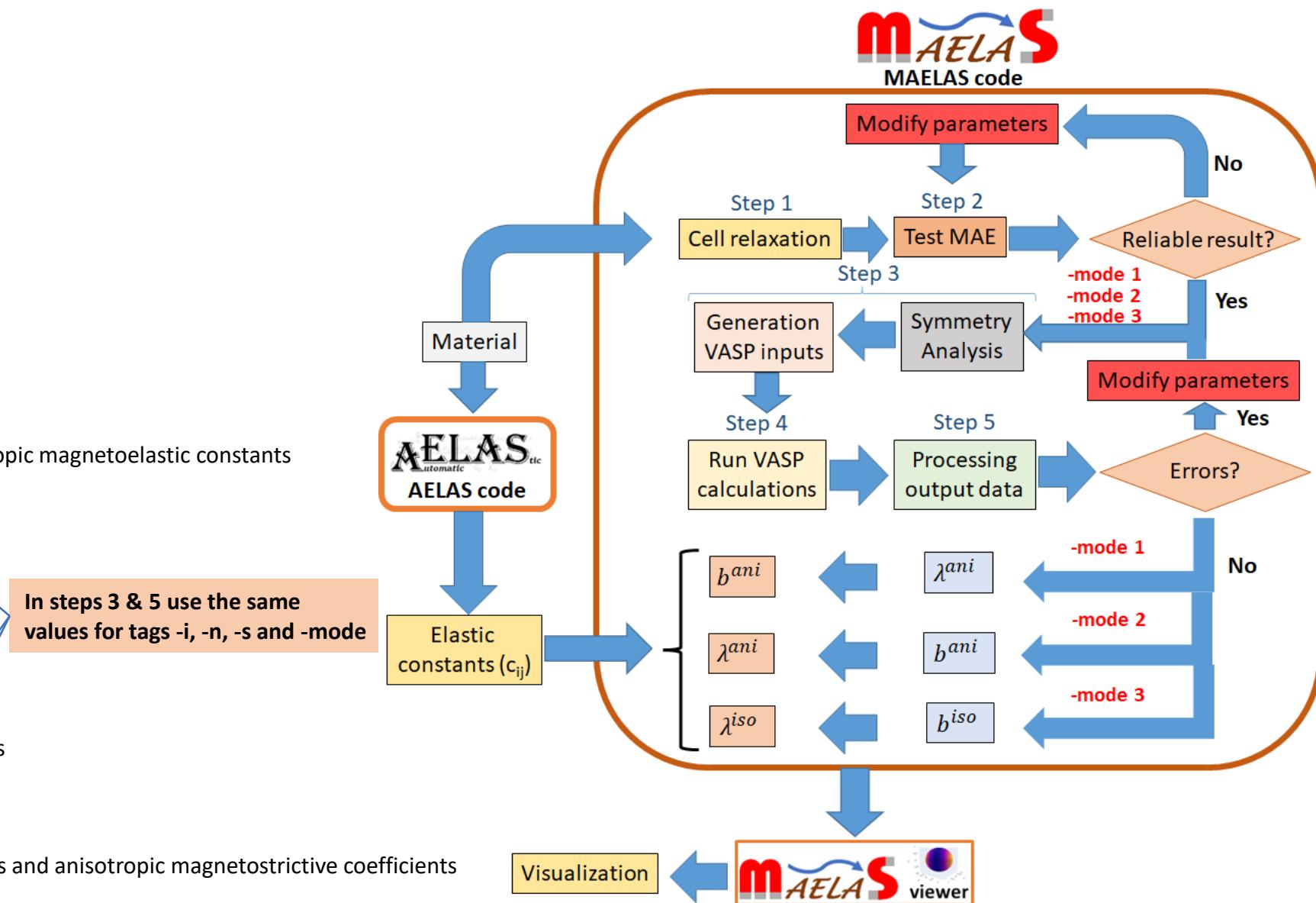
### Step 5a: Derivation of anisotropic magnetoelastic constants

maelas -d -mode 2 -i POSCAR\_rlx -n 7 -s 0.01

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

maelas -d -mode 2 -i POSCAR\_rlx -n 7 -s 0.01 -b -e ELADAT

See all optional arguments: maelas -h



# HOW TO USE MAELAS CODE

## Summary: In a nutshell (-mode 3)

### Step 1: Cell relaxation

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

```
qsub vasp_jsub_rlx
```

### Step 2: Test MAE (it does not require in this mode since SOC is not used)

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

```
./vasp_mae
```

```
./vasp_mae_cp_ozcifar
```

### Step 3: Generate VASP inputs for the calculation of isotropic magnetoelastic constants

```
maelas -g -mode 3 -i POSCAR_rlx -k 70 -n 7 -s 0.01
```

### Step 4: Run VASP calculations

```
./vasp_maelas
```

```
./vasp_cp_ozcifar
```

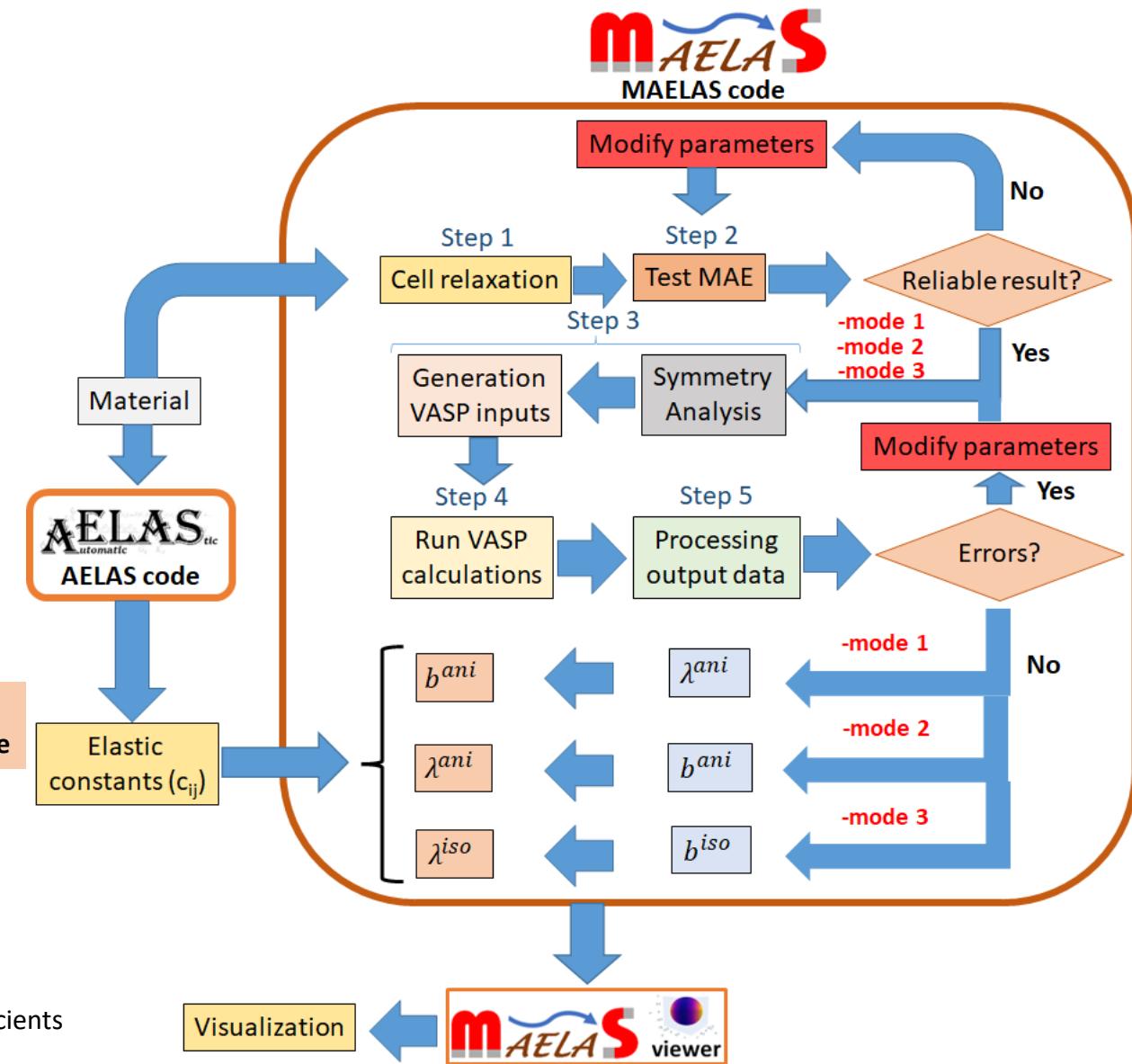
### Step 5a: Derivation of isotropic magnetoelastic constants

```
maelas -d -mode 3 -i POSCAR_rlx -n 7 -s 0.01
```

### Step 5b: Derivation of isotropic magnetoelastic constants and isotropic magnetostrictive coefficients

```
maelas -d -mode 3 -i POSCAR_rlx -n 7 -s 0.01 -b -e ELADAT
```

In steps 3 & 5 use the same values for tags -i, -n, -s and -mode



See all optional arguments: maelas -h

# HOW TO USE MAELAS CODE

**Summary: In a nutshell (-mode 3 including anisotropic magnetic interactions)**

**Step 1:** Cell relaxation

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

```
qsub vasp_jsub_rlx
```

**Step 2:** Test MAE (it does not require in this mode since SOC is not used)

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

```
./vasp_mae
```

```
./vasp_mae_cp_ozcifar
```

**Step 3:** Generate VASP inputs for the calculation of isotropic magnetoelastic constants

```
maelas -g -mode 3 -ani -i POSCAR_rlx -k 70 -n 7 -s 0.01
```

**Step 4:** Run VASP calculations

```
./vasp_maelas
```

```
./vasp_cp_ozcifar
```

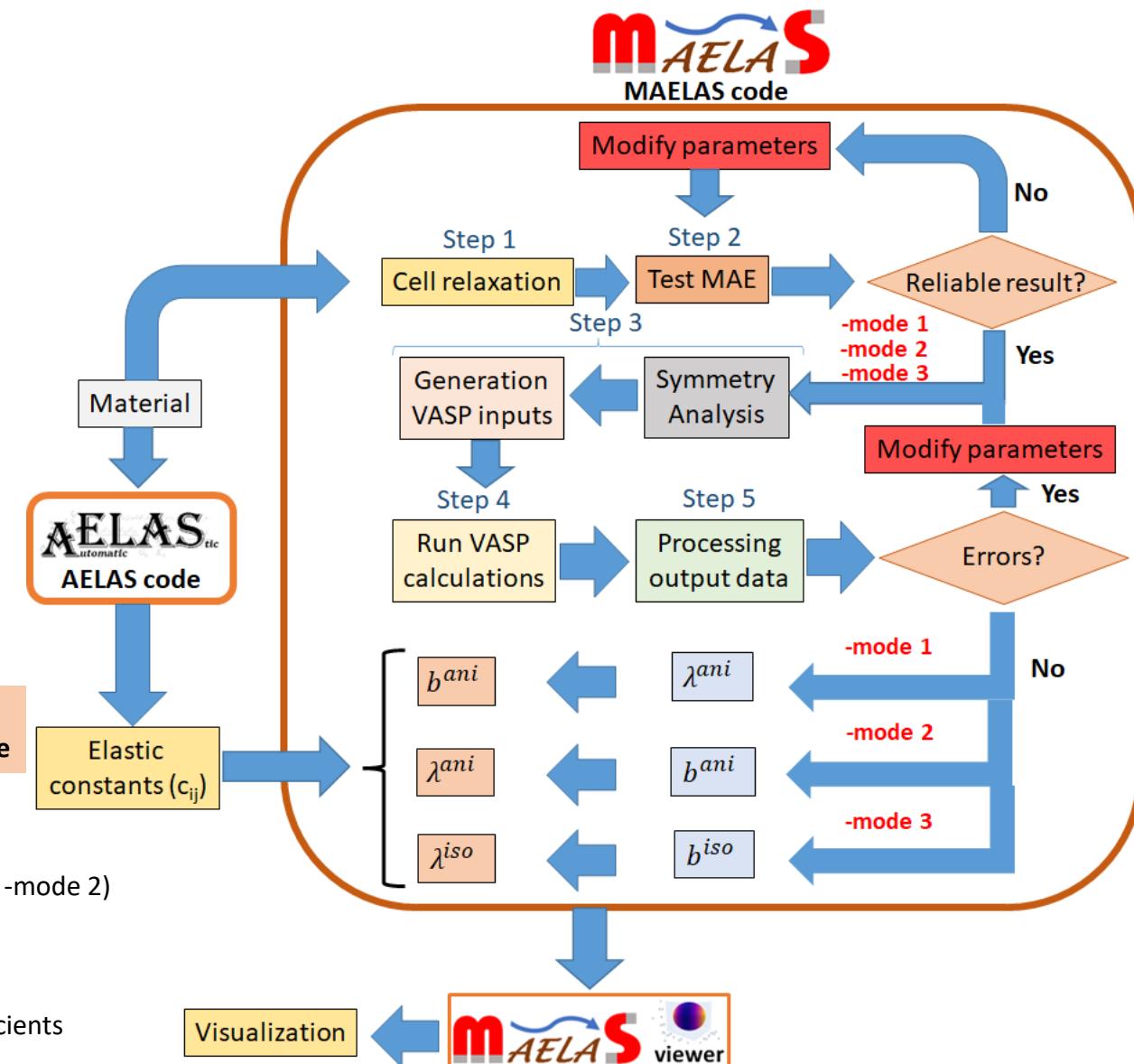
**Step 5a:** Derivation of isotropic magnetoelastic constants (it requires file MAGANI generated in -mode 2)

```
maelas -d -mode 3 -ani -i POSCAR_rlx -n 7 -s 0.01
```

**Step 5b:** Derivation of isotropic magnetoelastic constants and isotropic magnetostrictive coefficients

```
maelas -d -mode 3 -ani -i POSCAR_rlx -n 7 -s 0.01 -b -e ELADAT
```

See all optional arguments: maelas -h



## Full list of arguments in MAELAS code

User can see all possible optional arguments by typing

maelas -h

The optional arguments are the following:

HOW TO USE MAELAS CODE	
-h, --help	Show this help message and exit
-mode MODE	-mode 1: Scheme for the direct calculation of the anisotropic magnetostrictive coefficients. -mode 2: Scheme for the direct calculation of the anisotropic magnetoelastic constants -mode 3: Scheme for the direct calculation of the isotropic magnetoelastic constants (default: 2)
-i POS	Name of the initial non-distorted POSCAR file (default: POSCAR)
-n NDIST	Number of distorted states for the calculation of each magnetostrictive coefficient (-mode 1) or magnetoelastic constant (-mode 2 or 3) (default: 7)
-s STRAIN	Maximum value of the parameter s for the deformation gradient Fij(s) 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 (-mode 1) or magnetoelastic constants (-mode 2 or 3).
-d	Derivation of magnetostrictive coefficients (-mode 1) or magnetoelastic constants (-mode 2 or 3) 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 (-mode 1) or calculation of the magnetostrictive coefficients from the calculated magnetoelastic constants (-mode 2 or 3) 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 SG0	Space group number 1-230. If it is equal to 0, then it will be determined by a symmetry analysis (default: 0)
-nc	If this flag is used, then it does not apply a conventional transformation to the provided POSCAR (keep original size), useful for supercells and quasi-random structures.
-ani	It includes anisotropic magnetic interactions in -mode 3. It requires the file MAGANI created in -mode 2 that contains the values of the calculated anisotropic magnetoelastic constants.
-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

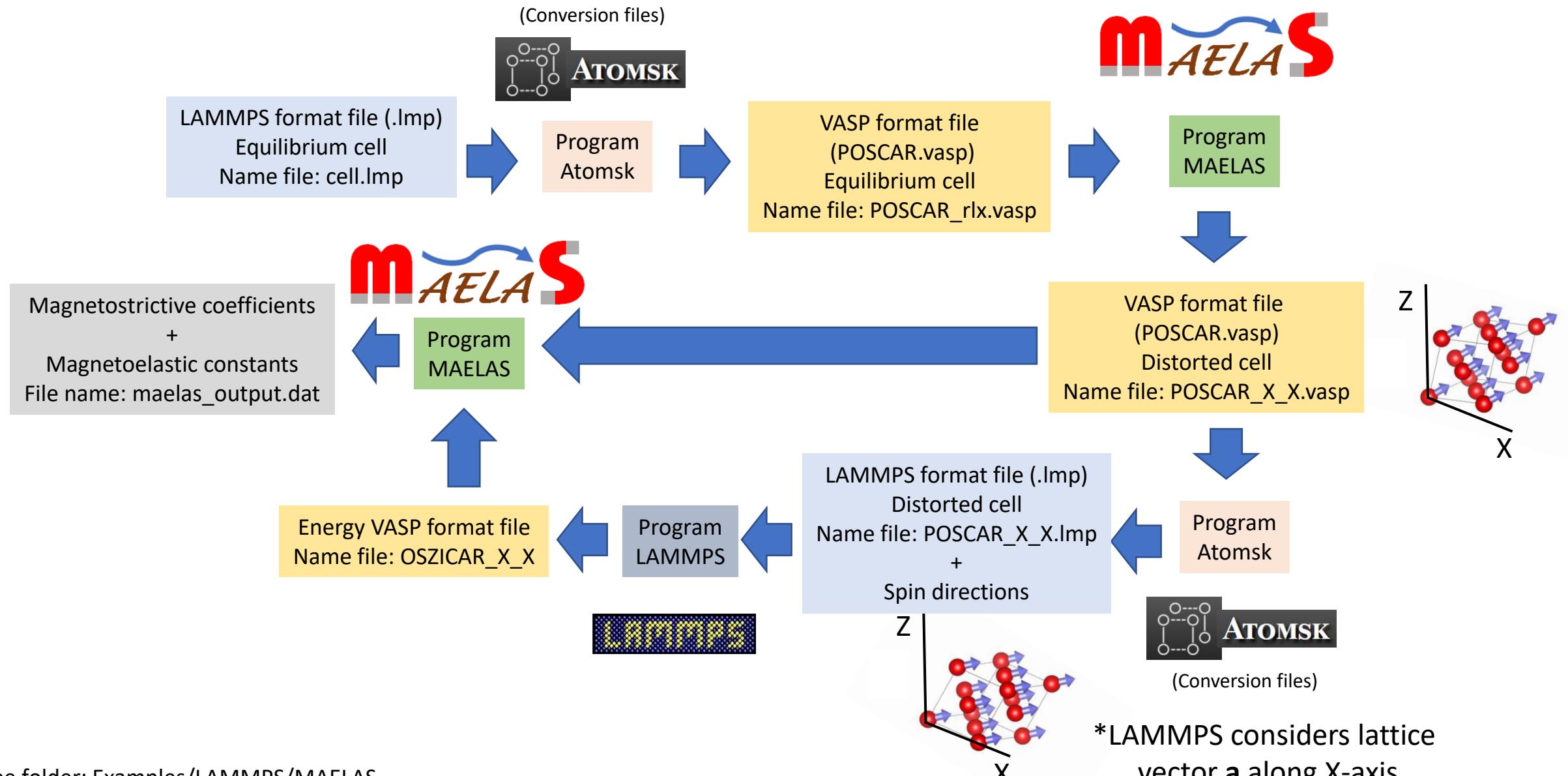
## Using MAELAS with other codes instead of VASP

MAELAS has been designed to read and write files for VASP code automatically. However, it is possible to use MAELAS with other 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 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	**Energy DFT code**	-0.19827E-09	-0.11530E-09868760	0.143E-04		
	1	F= -0.21909285E+02 E0= -0.21909330E+02	d E =0.135168E-03	mag= 0.0000	0.0000	2.5077	

# HOW TO USE MAELAS CODE

## 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

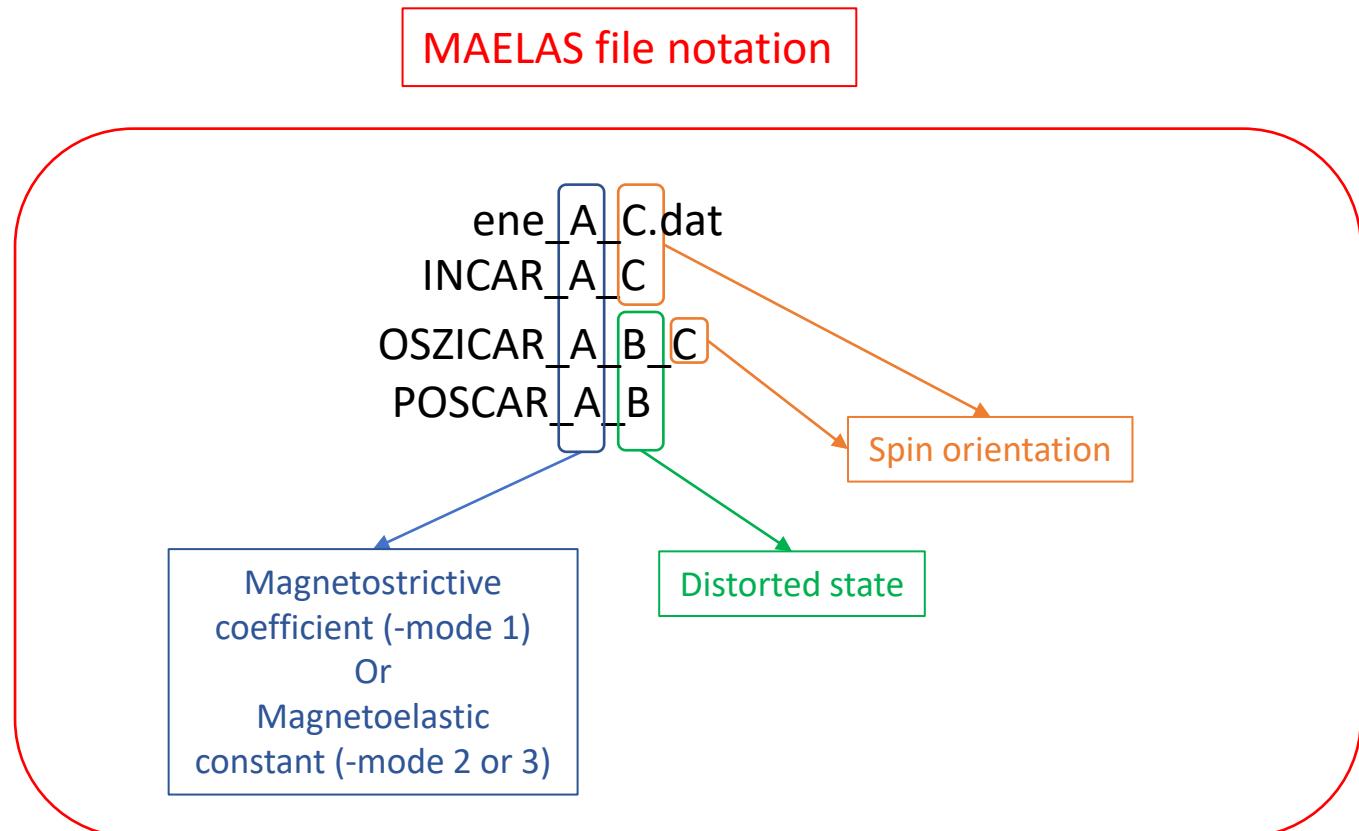
## Crystal systems supported by MAELAS v3.0

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 ( $c_{ij}$ )	Magnetoelastic constants ( $b$ )	Magnetostriction coefficients ( $\lambda$ )	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



# Methodology (-mode 1)

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

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

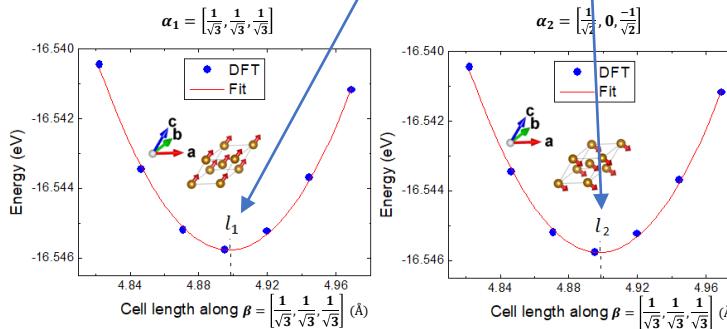
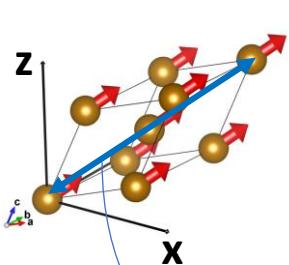
**Spin-polarized calculation with SOC**

$$E = E_{elas} + E_{me} + E_K^0$$

Fitting to a quadratic function

$$E(\alpha_j, l) = A_j l^2 + B_j l + C_j, \quad j = 1, 2$$

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



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

Table 2: Selected cell length ( $\beta$ ) and magnetization directions ( $\alpha_1, \alpha_2$ ) in MAELAS to calculate the anisotropic magnetostrictive coefficients according to Eq.48. The first column shows the crystal system and the corresponding lattice convention set in MAELAS based on the IEEE format [44]. The second column presents the equation of the relative length change that we used in Eq.48 for each crystal system. In the last column we show the values of the parameter  $\rho$  that is defined in Eq.48. The symbols  $a, b, c$  correspond to the lattice parameters of the relaxed (not distorted) unit cell.

Crystal system	$\frac{\Delta l}{l_0}$	Magnetostrictive coefficient	$\beta$	$\alpha_1$	$\alpha_2$	$\rho$
Cubic (I)	Eq.17	$\lambda_{001}$	$(0, 0, 1)$	$(0, 0, 1)$	$(1, 0, 0)$	$\frac{3}{2}$
$a \parallel \hat{x}, b \parallel \hat{y}, c \parallel \hat{z}$		$\lambda_{111}$	$(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$	$(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$	$(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}})$	$\frac{3}{2}$
Hexagonal (I)	Eq.25	$\lambda^{\alpha1,2}$	$(1, 0, 0)$	$(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$\frac{1}{3}$
$a \parallel \hat{x}, c \parallel \hat{z}$		$\lambda^{\alpha2,2}$	$(0, 0, 1)$	$(0, 0, 1)$	$(1, 0, 0)$	$1$
$b = \left(-\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0\right)$		$\lambda^{\gamma,2}$	$(1, 0, 0)$	$(1, 0, 0)$	$(0, 1, 0)$	$1$
$a = b \neq c$		$\lambda^{\epsilon,2}$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(\frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$\frac{2ac}{a^2+c^2}$
Trigonal (I)	Eq.35	$\lambda^{\alpha1,2}$	$(1, 0, 0)$	$(0, 0, 1)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$1$
$a \parallel \hat{x}, c \parallel \hat{z}$		$\lambda^{\alpha2,2}$	$(0, 0, 1)$	$(0, 0, 1)$	$(1, 0, 0)$	$1$
$b = \left(-\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0\right)$		$\lambda^{\gamma,1}$	$(1, 0, 0)$	$(1, 0, 0)$	$(0, 1, 0)$	$1$
$a = b \neq c$		$\lambda^{\gamma,2}$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}})$	$\frac{ac}{a^2+c^2}$
$\lambda_{12}$	$v2.0$	$(1, 0, 0)$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$	$(0, \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}})$	$v1.0$
$\lambda_{21}$		$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, 0)$	$\frac{1}{2}$
Tetragonal (I)	Eq.40	$\lambda^{\alpha1,2}$	$(1, 0, 0)$	$(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$\frac{1}{3}$
$a \parallel \hat{x}, b \parallel \hat{y}, c \parallel \hat{z}$		$\lambda^{\alpha2,2}$	$(0, 0, 1)$	$(0, 0, 1)$	$(1, 0, 0)$	$1$
$a = b \neq c$		$\lambda^{\gamma,2}$	$(1, 0, 0)$	$(1, 0, 0)$	$(0, 1, 0)$	$1$
		$\lambda^{\epsilon,2}$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(\frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$\frac{2ac}{a^2+c^2}$
		$\lambda^{\delta,2}$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$(\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$1$
Orthorhombic	Eq.44	$\lambda_1$	$(1, 0, 0)$	$(1, 0, 0)$	$(0, 0, 1)$	$1$
$a \parallel \hat{x}, b \parallel \hat{y}, c \parallel \hat{z}$		$\lambda_2$	$(1, 0, 0)$	$(0, 1, 0)$	$(0, 0, 1)$	$1$
$c < a < b$		$\lambda_3$	$(0, 1, 0)$	$(1, 0, 0)$	$(0, 0, 1)$	$1$
		$\lambda_4$	$(0, 1, 0)$	$(0, 1, 0)$	$(0, 0, 1)$	$1$
		$\lambda_5$	$(0, 0, 1)$	$(1, 0, 0)$	$(0, 0, 1)$	$1$
		$\lambda_6$	$(0, 0, 1)$	$(0, 1, 0)$	$(0, 0, 1)$	$1$
		$\lambda_7$	$\frac{(a,b,0)}{\sqrt{a^2+b^2}}$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$(0, 0, 1)$	$\frac{(a-b)(a[\lambda_1+\lambda_2]-b[\lambda_3+\lambda_4])+4ab\lambda_7}{2(a^2+b^2)\lambda_7}$
		$\lambda_8$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(0, 0, 1)$	$\frac{(a-c)(a[\lambda_1-\lambda_5]+4ac\lambda_8)}{2(a^2+c^2)\lambda_8}$
		$\lambda_9$	$\frac{(0,b,c)}{\sqrt{b^2+c^2}}$	$(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$	$(0, 0, 1)$	$\frac{(b-c)(b[\lambda_4-\lambda_6]+4bc\lambda_9)}{2(b^2+c^2)\lambda_9}$

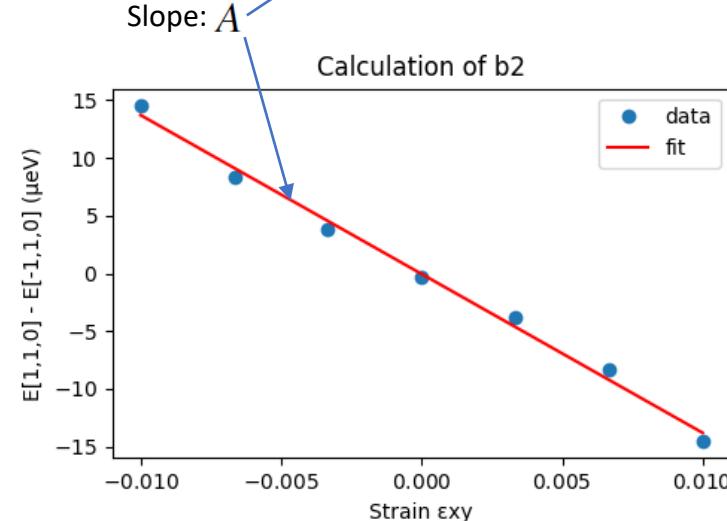
## Spin-polarized calculation with SOC

$$E = E_{elas} + E_{me} + E_K^0$$

$$\frac{1}{V_0} [E(\boldsymbol{\epsilon}^i(s), \boldsymbol{\alpha}_1^i) - E(\boldsymbol{\epsilon}^i(s), \boldsymbol{\alpha}_2^i)] = \Gamma_i b_i s + \Phi_i(K_1, K_2),$$

Fitting to a linear function

$$f(s) = As + B$$



## Methodology (-mode 2)

Table 1: Selected magnetization directions ( $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2$ ) in the new method implemented in MAELAS version 2.0 to calculate the anisotropic magnetoelastic constants. The first column shows the crystal system and the corresponding lattice convention set in MAELAS based on the IEEE format [3]. In the fifth and sixth columns we show the values of the parameters  $\Gamma$  and  $\Phi$  that are defined in Eq.2. Last column presents the equation of the deformation gradient  $F_{ij}$  that we used in Eq.2 for the calculation of each magnetoelastic constant. The symbols  $a, b, c$  correspond to the lattice parameters of the relaxed (not distorted) unit cell.

Crystal system	Magnetoelastic constant	$\boldsymbol{\alpha}_1$	$\boldsymbol{\alpha}_2$	$\Gamma$	$\Phi$	$F$
Cubic (I)	$b_1$	$(1, 0, 0)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$\frac{1}{2}$	$-\frac{K_1}{4}$	Eq.A.4
$\boldsymbol{a} \parallel \hat{x}, \boldsymbol{b} \parallel \hat{y}, \boldsymbol{c} \parallel \hat{z}$	$b_2$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$(\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	2	0	Eq.A.5
Hexagonal (I)	$b_{21}$	$(0, 0, 1)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	1	$-K_1 - K_2$	Eq.A.6
$\boldsymbol{a} \parallel \hat{x}, \boldsymbol{c} \parallel \hat{z}$	$b_{22}$	$(0, 0, 1)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	1	$-K_1 - K_2$	Eq.A.7
$\boldsymbol{b} = \left(-\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0\right)$	$b_3$	$(1, 0, 0)$	$(0, 1, 0)$	1	0	Eq.A.8
$a = b \neq c$	$b_4$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(\frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	2	0	Eq.A.9
Trigonal (I)	$b_{21}$	$(0, 0, 1)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	1	$-K_1 - K_2$	Eq.A.6
$\boldsymbol{a} \parallel \hat{x}, \boldsymbol{c} \parallel \hat{z}$	$b_{22}$	$(0, 0, 1)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	1	$-K_1 - K_2$	Eq.A.7
$\boldsymbol{b} = \left(-\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0\right)$	$b_3$	$(1, 0, 0)$	$(0, 1, 0)$	1	0	Eq.A.8
$a = b \neq c$	$b_4$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(\frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	2	0	Eq.A.9
	$b_{14}$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$(\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	2	0	Eq.A.10
	$b_{34}$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(\frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	2	0	Eq.A.11
Tetragonal (I)	$b_{21}$	$(0, 0, 1)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	1	$-K_1 - K_2$	Eq.A.6
$\boldsymbol{a} \parallel \hat{x}, \boldsymbol{b} \parallel \hat{y}, \boldsymbol{c} \parallel \hat{z}$	$b_{22}$	$(0, 0, 1)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	1	$-K_1 - K_2$	Eq.A.7
$a = b \neq c$	$b_3$	$(1, 0, 0)$	$(0, 1, 0)$	1	0	Eq.A.8
	$b_4$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(\frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	2	0	Eq.A.9
	$b'_3$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$(\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	2	0	Eq.A.12
Orthorhombic	$b_1$	$(1, 0, 0)$	$(0, 0, 1)$	1	$K_1$	Eq.A.13
$c < a < b$	$b_2$	$(0, 1, 0)$	$(0, 0, 1)$	1	$K_2$	Eq.A.13
	$b_3$	$(1, 0, 0)$	$(0, 0, 1)$	1	$K_1$	Eq.A.14
	$b_4$	$(0, 1, 0)$	$(0, 0, 1)$	1	$K_2$	Eq.A.14
	$b_5$	$(1, 0, 0)$	$(0, 0, 1)$	1	$K_1$	Eq.A.15
	$b_6$	$(0, 1, 0)$	$(0, 0, 1)$	1	$K_2$	Eq.A.15
	$b_7$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$(0, 0, 1)$	1	$\frac{K_1}{2} + \frac{K_2}{2}$	Eq.A.16
	$b_8$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(0, 0, 1)$	1	$\frac{K_1}{2}$	Eq.A.17
	$b_9$	$(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$	$(0, 0, 1)$	1	$\frac{K_2}{2}$	Eq.A.18

### Spin-polarized calculation without SOC

### Methodology (-mode 3)

$$E = E_{elas} + E_{me}^{iso}$$

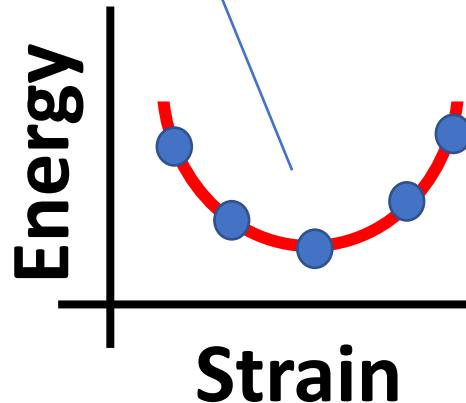
$$\frac{1}{V_0}E(\boldsymbol{\epsilon}^i(s)) = \Phi_i(C_{ij})s^2 + \Gamma_i b_i^{iso}s + \frac{1}{V_0}E_0$$

$$b_i^{iso}$$

Crystal system	$b_i^{iso}$	Convention	$(\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}, \epsilon_{yz}, \epsilon_{zx}, \epsilon_{xy})$	$\Gamma$
Cubic (I)	$b^{\alpha,2}$	Lacheisserie[1]	$(s, s, s, 0, 0, 0)$	1
Hexagonal (I)	$b_{11}$	Clark[17]	$(s, s, 0, 0, 0, 0)$	2
	$b_{12}$		$(0, 0, s, 0, 0, 0)$	1
Trigonal (I)	$b_{11}$	Cullen[18]	$(s, s, 0, 0, 0, 0)$	2
	$b_{12}$		$(0, 0, s, 0, 0, 0)$	1
Tetragonal (I)	$b_{11}$	Cullen[18]	$(s, s, 0, 0, 0, 0)$	2
	$b_{12}$		$(0, 0, s, 0, 0, 0)$	1
Orthorhombic	$b_1^{\alpha,0}$	Lacheisserie[1]	$(s, s, s, 0, 0, 0)$	1
	$b_2^{\alpha,0}$		$(-s/2, -s/2, s, 0, 0, 0)$	$\frac{1}{\sqrt{2}}$
	$b_3^{\alpha,0}$		$(s, -s, 0, 0, 0, 0)$	$\sqrt{\frac{2}{3}}$

Fitting to a cubic function

$$f(s) = As^3 + Bs^2 + Cs + D$$



#### Convention:

Lacheisserie: E. D. T. de Lacheisserie, Magnetostriiction: Theory and Application of Magnetoelasticity (CRC Press, Boca Raton, FL, 1993)

Clark: A. Clark, Handbook of Ferromagnetic Materials, Vol. 1 (Elsevier, Amsterdam, 1980), pp. 531–589.

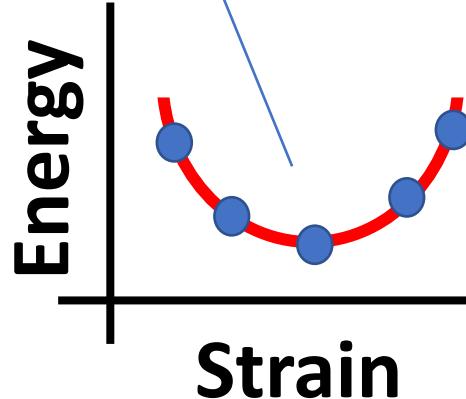
Cullen: J. R. Cullen, A. E. Clark, and K. B. Hathaway, in Materials, Science and Technology (VCH Publishing, 1994), pp. 529 – 565.

$$E = E_{elas} + E_{me} + E_K^0$$

$$\frac{1}{V_0} E(\boldsymbol{\epsilon}^i(s), \boldsymbol{\alpha} = (0, 0, 1)) = \Phi_i(C_{ij})s^2 + [\Gamma_i b_i^{iso} + \Lambda_i(b^{ani})]s + \frac{1}{V_0} E_0,$$

Fitting to a cubic function

$$f(s) = As^3 + Bs^2 + Cs + D$$



$$b_i^{iso} = \frac{C - \Lambda_i(b^{ani})}{\Gamma_i}$$

$$b_i^{iso}$$

Crystal system	$b_i^{iso}$	Convention	$(\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{yz}, \varepsilon_{zx}, \varepsilon_{xy})$	$\Gamma$	$\boldsymbol{\alpha}$	$\Lambda$
Cubic (I)	$b^{\alpha,2}$	Lacheisserie[1]	$(s, s, 0, 0, 0)$	1	$(0, 0, 1)$	0
Hexagonal (I)	$b_{11}$	Clark[17]	$(s, s, 0, 0, 0)$	2	$(0, 0, 1)$	$\frac{4}{3}b_{21}$
	$b_{12}$		$(0, 0, s, 0, 0, 0)$	1	$(0, 0, 1)$	$\frac{2}{3}b_{22}$
Trigonal (I)	$b_{11}$	Cullen[18]	$(s, s, 0, 0, 0, 0)$	2	$(0, 0, 1)$	$\frac{4}{3}b_{21}$
	$b_{12}$		$(0, 0, s, 0, 0, 0)$	1	$(0, 0, 1)$	$\frac{2}{3}b_{22}$
Tetragonal (I)	$b_{11}$	Cullen[18]	$(s, s, 0, 0, 0, 0)$	2	$(0, 0, 1)$	$\frac{4}{3}b_{21}$
	$b_{12}$		$(0, 0, s, 0, 0, 0)$	1	$(0, 0, 1)$	$\frac{2}{3}b_{22}$
Orthorhombic	$b_1^{\alpha,0}$	Lacheisserie[1]	$(s, s, s, 0, 0, 0)$	1	$(0, 0, 1)$	$\sqrt{2}b_1^{\alpha,2}$
	$b_2^{\alpha,0}$		$(-s/2, -s/2, s, 0, 0, 0)$	$\frac{1}{\sqrt{2}}$	$(0, 0, 1)$	$b_2^{\alpha,2}$
	$b_3^{\alpha,0}$		$(s, -s, 0, 0, 0, 0)$	$\sqrt{\frac{2}{3}}$	$(0, 0, 1)$	$\sqrt{\frac{2}{3}}b_3^{\alpha,2}$

(it requires file MAGANI generated in -mode 2 which contains the data for  $b^{ani}$ )

#### Convention:

Lacheisserie: E. D. T. de Lacheisserie, Magnetostriiction: Theory and Application of Magnetoelasticity (CRC Press, Boca Raton, FL, 1993)

Clark: A. Clark, Handbook of Ferromagnetic Materials, Vol. 1 (Elsevier, Amsterdam, 1980), pp. 531–589.

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

# CALCULATED QUANTITIES BY MAELAS

Crystal system	Clark <sup>†</sup> - Cullen <sup>‡</sup>			Callen <sup>♣</sup>	Birss <sup>♦</sup>	Mason <sup>◊</sup> -Nieves <sup>□</sup>			Lacheisserie <sup>△</sup>					
Space Group	$b$	-mode	$\lambda$	-mode	$\lambda$	-mode	$b$	-mode	$\lambda$	-mode	$b$	-mode	$\lambda$	-mode
Cubic (I) SG 230-207	$b_0$	*	$\lambda^\alpha$	3							$b^{\alpha,2}$	3	$\lambda^{\alpha,2}$	3
	$b_1$	1,2	$\lambda_{001}$	1,2							$b^{\gamma,2}$	1,2	$\lambda^{\gamma,2}$	1,2
	$b_2$	1,2	$\lambda_{111}$	1,2							$b^{\varepsilon,2}$	1,2	$\lambda^{\varepsilon,2}$	1,2
Hexagonal (I) SG 177-194	$b_{11}$	3	$\lambda^{\alpha1,0}$	3	$\lambda_{11}^\alpha$	*	$Q_0$	*	$\lambda^{\alpha1,0}$	*	$b_1^{\alpha,0}$	3	$\lambda_1^{\alpha,0}$	3
	$b_{12}$	3	$\lambda^{\alpha2,0}$	3	$\lambda_{21}^\alpha$	3	$Q_1$	*	$\lambda^{\alpha2,0}$	*	$b_2^{\alpha,0}$	3	$\lambda_2^{\alpha,0}$	3
	$b_{21}$	1,2	$\lambda^{\alpha1,2}$	1,2	$\lambda_{12}^\alpha$	1,2	$Q_2$	1,2	$\lambda_A$	1,2	$b_1^{\alpha,2}$	1,2	$\lambda_1^{\alpha,2}$	1,2
	$b_{22}$	1,2	$\lambda^{\alpha2,2}$	1,2	$\lambda_{22}^\alpha$	1,2	$Q_4$	1,2	$\lambda_B$	1,2	$b_2^{\alpha,2}$	1,2	$\lambda_2^{\alpha,2}$	1,2
	$b_3$	1,2	$\lambda^{\gamma,2}$	1,2	$\lambda^\gamma$	1,2	$Q_6$	1,2	$\lambda_C$	1,2	$b^{\varepsilon,2}$	1,2	$\lambda^{\varepsilon,2}$	1,2
	$b_4$	1,2	$\lambda^{\varepsilon,2}$	1,2	$\lambda^\varepsilon$	1,2	$Q_8$	1,2	$\lambda_D$	1,2	$b^{\zeta,2}$	1,2	$\lambda^{\zeta,2}$	1,2
Trigonal (I) SG 149-167	$b_{11}$	3	$\lambda^{\alpha1,0}$	3										
	$b_{12}$	3	$\lambda^{\alpha2,0}$	3										
	$b_{21}$	1,2	$\lambda^{\alpha1,2}$	1,2										
	$b_{22}$	1,2	$\lambda^{\alpha2,2}$	1,2										
	$b_3$	1,2	$\lambda^{\gamma 1}$	1,2										
	$b_4$	1,2	$\lambda^{\gamma 2}$	1,2										
	$b_{14}$	1,2	$\lambda_{12}$	1,2										
	$b_{34}$	1,2	$\lambda_{21}$	1,2										
Tetragonal (I) SG 89-142	$b_{11}$	3	$\lambda^{\alpha1,0}$	3										
	$b_{12}$	3	$\lambda^{\alpha2,0}$	3										
	$b_{21}$	1,2	$\lambda^{\alpha1,2}$	1,2										
	$b_{22}$	1,2	$\lambda^{\alpha2,2}$	1,2										
	$b_3$	1,2	$\lambda^{\gamma,2}$	1,2										
	$b_4$	1,2	$\lambda^{\varepsilon,2}$	1,2										
	$b'_3$	1,2	$\lambda^{\delta,2}$	1,2										
Orthorhombic SG 16-74							$b_{01}$	*	$\lambda^{\alpha1,0}$	*	$b_1^{\alpha,0}$	3	$\lambda_1^{\alpha,0}$	3
							$b_{02}$	*	$\lambda^{\alpha2,0}$	*	$b_2^{\alpha,0}$	3	$\lambda_2^{\alpha,0}$	3
							$b_{03}$	*	$\lambda^{\alpha3,0}$	*	$b_3^{\alpha,0}$	3	$\lambda_3^{\alpha,0}$	3
							$b_1$	1,2	$\lambda_1$	1,2	$b_1^{\alpha,2}$	1,2	$\lambda_1^{\alpha,2}$	1,2
							$b_2$	1,2	$\lambda_2$	1,2	$b_2^{\alpha,2}$	1,2	$\lambda_2^{\alpha,2}$	1,2
							$b_3$	1,2	$\lambda_3$	1,2	$b_3^{\alpha,2}$	1,2	$\lambda_3^{\alpha,2}$	1,2
							$b_4$	1,2	$\lambda_4$	1,2	$b_1^{\alpha,2'}$	1,2	$\lambda_1^{\alpha,2'}$	1,2
							$b_5$	1,2	$\lambda_5$	1,2	$b_2^{\alpha,2'}$	1,2	$\lambda_2^{\alpha,2'}$	1,2
							$b_6$	1,2	$\lambda_6$	1,2	$b_3^{\alpha,2'}$	1,2	$\lambda_3^{\alpha,2'}$	1,2
							$b_7$	1,2	$\lambda_7$	1,2	$b^{\beta,2}$	1,2	$\lambda^{\beta,2}$	1,2
							$b_8$	1,2	$\lambda_8$	1,2	$b^{\gamma,2}$	1,2	$\lambda^{\gamma,2}$	1,2
							$b_9$	1,2	$\lambda_9$	1,2	$b^{\delta,2}$	1,2	$\lambda^{\delta,2}$	1,2

<sup>†</sup>A. Clark, Handbook of Ferromagnetic Materials, vol. 1, Elsevier, 1980, pp. 531–589.

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

<sup>♣</sup>E. Callen, H.B. Callen, Phys. Rev. 139 (1965) A455–A471.

<sup>♦</sup>R. Birss, Adv. Phys. 8 (31) (1959) 252–291.

<sup>◊</sup>W.P. Mason, Phys. Rev. 96 (1954) 302–310.

<sup>□</sup>P. Nieves, S. Arapan, S.H. Zhang, A.P. Kadzielawa, R.F. Zhang and D. Legut, Comput. Phys. Commun. 264, 107964 (2021).

<sup>△</sup>E. D. Tremolet de Lacheisserie, Magnetostriction: Theory and Application of Magnetoelasticity (CRC Press, Boca Raton, FL, 1993).

\*The definition of these quantities does not fully decouple isotropic and anisotropic interactions, so that they cannot be calculated with a single mode implemented in MAELAS automatically. These quantities can be manually calculated by inserting the isotropic and anisotropic quantities obtained with MAELAS in the equations given in the following Table:

Crystal system	Convention	*	=	Convention
Cubic (I)	Clark-Cullen	$b_0$	$\frac{1}{3}(b^{\alpha,2} + b^{\gamma,2})$	Lacheisserie
Hexagonal (I)	Callen	$\lambda_{11}^\alpha$	$2\lambda^{\alpha1,0} + \lambda^{\alpha2,0} + 2\lambda^{\alpha1,2} + \lambda^{\alpha2,2}$	Clark-Cullen
	Birss	$Q_0$	$\lambda^{\alpha1,0} + \frac{2}{3}\lambda^{\alpha1,2}$	Clark-Cullen
	Birss	$Q_1$	$\lambda^{\alpha2,0} + \frac{2}{3}\lambda^{\alpha2,2} - \lambda^{\alpha1,0} - \frac{2}{3}\lambda^{\alpha1,2}$	Clark-Cullen
	Mason-Nieves	$\lambda^{\alpha1,0}$	$\lambda^{\alpha1,0} + \frac{2}{3}\lambda^{\alpha1,2}$	Clark-Cullen
	Mason-Nieves	$\lambda^{\alpha2,0}$	$\lambda^{\alpha2,0} + \frac{2}{3}\lambda^{\alpha2,2}$	Clark-Cullen
Tetragonal (I)	Mason-Nieves	$\lambda^{\alpha1,0}$	$\lambda^{\alpha1,0} + \frac{2}{3}\lambda^{\alpha1,2}$	Clark-Cullen
	Mason-Nieves	$\lambda^{\alpha2,0}$	$\lambda^{\alpha2,0} + \frac{2}{3}\lambda^{\alpha2,2}$	Clark-Cullen
Orthorhombic	Mason-Nieves	$b_{01}$	$\frac{1}{3}(b_1^{\alpha,0} + \sqrt{2}b_1^{\alpha,2} - \frac{1}{\sqrt{2}}b_2^{\alpha,0} - b_2^{\alpha,2}) + \frac{1}{\sqrt{6}}(b_3^{\alpha,0} + b_3^{\alpha,2})$	Lacheisserie
	Mason-Nieves	$b_{02}$	$\frac{1}{3}(b_1^{\alpha,0} + \sqrt{2}b_1^{\alpha,2} - \frac{1}{\sqrt{2}}b_2^{\alpha,0} - b_2^{\alpha,2}) - \frac{1}{\sqrt{6}}(b_3^{\alpha,0} + b_3^{\alpha,2})$	Lacheisserie
	Mason-Nieves	$b_{03}$	$\frac{1}{3}(b_1^{\alpha,0} + \sqrt{2}b_1^{\alpha,2} + \sqrt{2}b_2^{\alpha,0} + 2b_2^{\alpha,2})$	Lacheisserie
	Mason-Nieves	$\lambda^{\alpha1,0}$	$\frac{1}{3}(\lambda_1^{\alpha,0} + \lambda_1^{\alpha,2} - \lambda_2^{\alpha,0} - \lambda_2^{\alpha,2}) + \lambda_3^{\alpha,0} + \lambda_3^{\alpha,2}$	Lacheisserie
	Mason-Nieves	$\lambda^{\alpha2,0}$	$\frac{1}{3}(\lambda_1^{\alpha,0} + \lambda_1^{\alpha,2} - \lambda_2^{\alpha,0} - \lambda_2^{\alpha,2}) - \lambda_3^{\alpha,0} - \lambda_3^{\alpha,2}$	Lacheisserie
	Mason-Nieves	$\lambda^{\alpha3,0}$	$\frac{1}{3}(\lambda_1^{\alpha,0} + \lambda_1^{\alpha,2} + 2\lambda_2^{\alpha,0} + 2\lambda_2^{\alpha,2})$	Lacheisserie

# Workflow

## CUBIC (I)

SG 207-230

## Cubic (I)

# Workflow

### Elastic energy

$$\begin{aligned}\frac{E_{el}^{cub} - E_0}{V_0} &= \frac{C_{11}}{2}(\tilde{\epsilon}_1^2 + \tilde{\epsilon}_2^2 + \tilde{\epsilon}_3^2) + C_{12}(\tilde{\epsilon}_1\tilde{\epsilon}_2 + \tilde{\epsilon}_1\tilde{\epsilon}_3 + \tilde{\epsilon}_2\tilde{\epsilon}_3) \\ &\quad + \frac{C_{44}}{2}(\tilde{\epsilon}_4^2 + \tilde{\epsilon}_5^2 + \tilde{\epsilon}_6^2) \\ &= \frac{c_{xxxx}}{2}(\epsilon_{xx}^2 + \epsilon_{yy}^2 + \epsilon_{zz}^2) + c_{xxyy}(\epsilon_{xx}\epsilon_{yy} + \epsilon_{xx}\epsilon_{zz} + \epsilon_{yy}\epsilon_{zz}) \\ &\quad + 2c_{yzyz}(\epsilon_{xy}^2 + \epsilon_{yz}^2 + \epsilon_{xz}^2),\end{aligned}$$

### Magnetoelastic energy

$$\begin{aligned}\frac{E_{me}^{cub(I)}}{V_0} &= b_0(\tilde{\epsilon}_1 + \tilde{\epsilon}_2 + \tilde{\epsilon}_3) + b_1(\alpha_x^2\tilde{\epsilon}_1 + \alpha_y^2\tilde{\epsilon}_2 + \alpha_z^2\tilde{\epsilon}_3) \\ &\quad + b_2(\alpha_x\alpha_y\tilde{\epsilon}_6 + \alpha_x\alpha_z\tilde{\epsilon}_5 + \alpha_y\alpha_z\tilde{\epsilon}_4) \\ &= b_0(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) + b_1(\alpha_x^2\epsilon_{xx} + \alpha_y^2\epsilon_{yy} + \alpha_z^2\epsilon_{zz}) \\ &\quad + 2b_2(\alpha_x\alpha_y\epsilon_{xy} + \alpha_x\alpha_z\epsilon_{xz} + \alpha_y\alpha_z\epsilon_{yz}),\end{aligned}$$



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

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

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

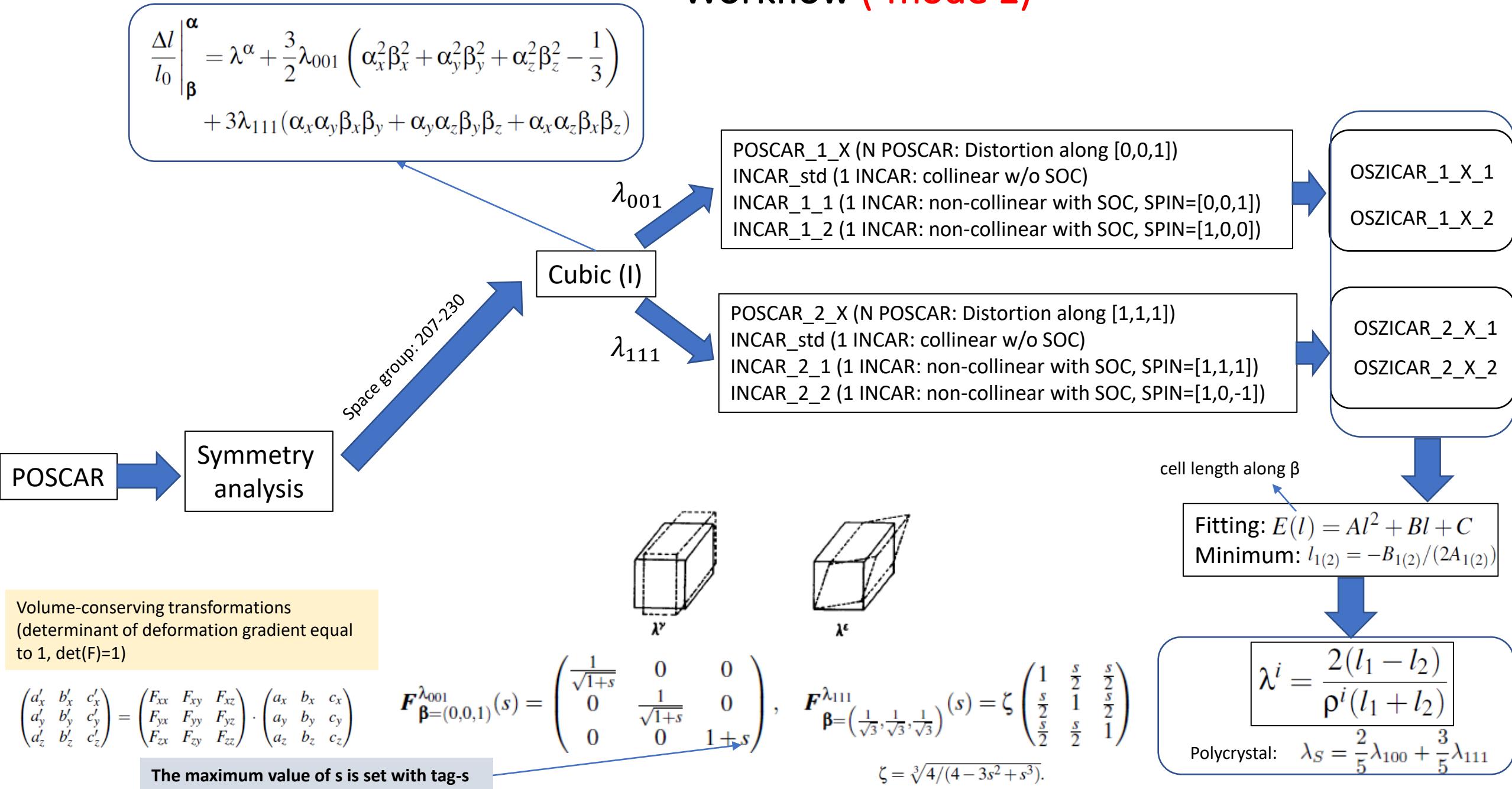
$$\begin{aligned}\frac{\Delta l}{l_0} \Bigg|_{\beta}^{\alpha} &= \lambda^{\alpha} + \frac{3}{2}\lambda_{001} \left( \alpha_x^2 \beta_x^2 + \alpha_y^2 \beta_y^2 + \alpha_z^2 \beta_z^2 - \frac{1}{3} \right) \\ &\quad + 3\lambda_{111} (\alpha_x \alpha_y \beta_x \beta_y + \alpha_y \alpha_z \beta_y \beta_z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

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

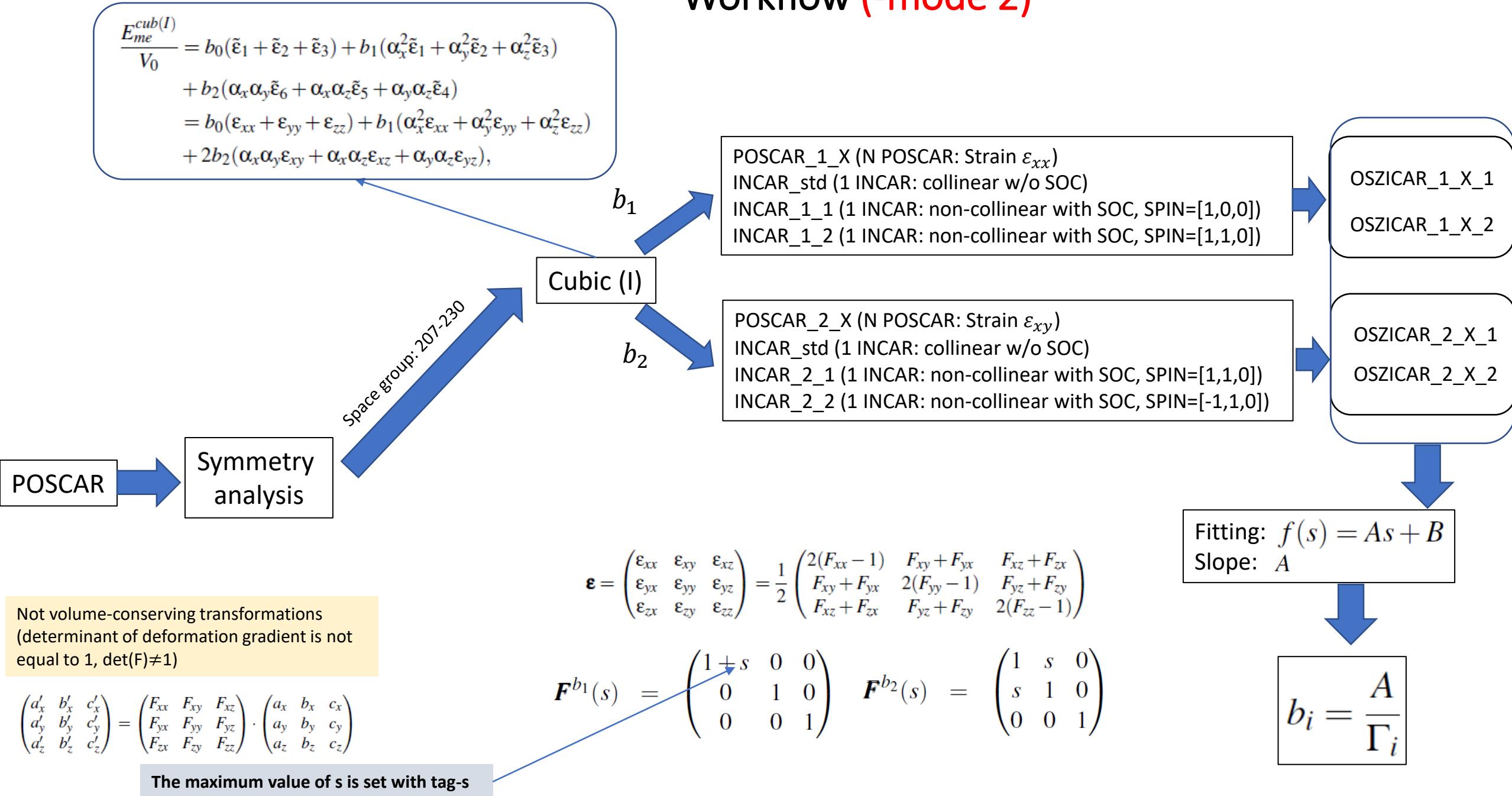
$$\lambda_{001} = \frac{-2b_1}{3(c_{11} - c_{12})},$$

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

# Workflow (-mode 1)



# Workflow (-mode 2)



### Spin-polarized calculation without SOC

$$E_{me} = E_{me}^{iso} + E_{me}^{ani}$$

$$E_{me}^{iso} = \frac{1}{3} b^{\alpha,2} (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$E_{me}^{ani} = b^{\gamma,2} \left( \left[ \alpha_x^2 - \frac{1}{3} \right] \varepsilon_{xx} + \left[ \alpha_y^2 - \frac{1}{3} \right] \varepsilon_{yy} + \left[ \alpha_z^2 - \frac{1}{3} \right] \varepsilon_{zz} \right) \\ + 2b^{\varepsilon,2} (\alpha_y \alpha_z \varepsilon_{yz} + \alpha_z \alpha_x \varepsilon_{zx} + \alpha_x \alpha_y \varepsilon_{xy})$$

$$b^{\alpha,2} = 3b_0 + b_1 \\ b^{\gamma,2} = b_1 \\ b^{\varepsilon,2} = b_2$$

Cubic (I)

Space group: 207-230

POSCAR

Symmetry analysis

Not volume-conserving transformations  
(determinant of deformation gradient is not equal to 1,  $\det(F) \neq 1$ )

$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

The maximum value of s is set with tag -s

## Workflow (-mode 3)

This convention fully decouples isotropic and anisotropic interactions

E. D. T. de Lacheisserie, Magnetostriction: Theory and Application of Magnetoelasticity (CRC Press, Boca Raton, FL, 1993)

$b^{\alpha,2}$

POSCAR\_1\_X (N POSCAR)  
INCAR\_std (1 INCAR: collinear w/o SOC)

OSZICAR\_1\_X\_1

Fitting:  $f(s) = As^3 + Bs^2 + Cs + D$

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

$$\boldsymbol{\varepsilon} = \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & s \end{pmatrix}$$

$$b^{\alpha,2} = C$$

$$b_k^{iso} = \frac{C}{\Gamma_k}$$

Spontaneous volume magnetostriction (isotropic contribution):  $\omega_S^{iso} \approx \lambda^{\alpha,2} = \frac{-b^{\alpha,2}}{c_{11}+2c_{12}}$

### Spin-polarized calculation with SOC

$$E_{me} = E_{me}^{iso} + E_{me}^{ani}$$

$$E_{me}^{iso} = \frac{1}{3} b^{\alpha,2} (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$\begin{aligned} E_{me}^{ani} &= b^{\gamma,2} \left( \left[ \alpha_x^2 - \frac{1}{3} \right] \varepsilon_{xx} + \left[ \alpha_y^2 - \frac{1}{3} \right] \varepsilon_{yy} + \left[ \alpha_z^2 - \frac{1}{3} \right] \varepsilon_{zz} \right) \\ &\quad + 2b^{\varepsilon,2} (\alpha_y \alpha_z \varepsilon_{yz} + \alpha_z \alpha_x \varepsilon_{zx} + \alpha_x \alpha_y \varepsilon_{xy}) \end{aligned}$$

$$\begin{aligned} b^{\alpha,2} &= 3b_0 + b_1 \\ b^{\gamma,2} &= b_1 \\ b^{\varepsilon,2} &= b_2 \end{aligned}$$

Space group: 207-230

Cubic (I)

POSCAR

Symmetry analysis

Not volume-conserving transformations  
(determinant of deformation gradient is not equal to 1,  $\det(F) \neq 1$ )

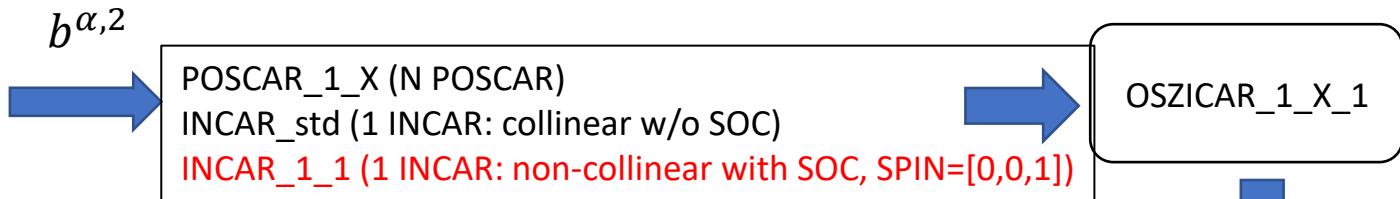
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

The maximum value of s is set with tag -s

# Workflow (-mode 3 including anisotropic magnetic interactions)

This convention fully decouples isotropic and anisotropic interactions

E. D. T. de Lacheisserie, Magnetostriction: Theory and Application of Magnetoelasticity (CRC Press, Boca Raton, FL, 1993)



$$\text{Fitting: } f(s) = As^3 + Bs^2 + Cs + D$$

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

(it requires file MAGANI generated in -mode 2)

$$\boldsymbol{\varepsilon} = \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & s \end{pmatrix}$$

$$\text{Spontaneous volume magnetostriction (isotropic contribution): } \omega_S^{iso} \simeq \lambda^{\alpha,2} = \frac{-b^{\alpha,2}}{c_{11}+2c_{12}}$$

$$b_i^{iso} = \frac{C - \Lambda_i(b^{ani})}{\Gamma_i}$$

# Workflow

HEXAGONAL (I)

SG 177-194

## Hexagonal (I)

# Workflow

### Elastic energy

$$\begin{aligned} \frac{E_{el}^{hex} - E_0}{V_0} &= \frac{1}{2}C_{11}(\tilde{\epsilon}_1^2 + \tilde{\epsilon}_2^2) + C_{12}\tilde{\epsilon}_1\tilde{\epsilon}_2 + C_{13}(\tilde{\epsilon}_1 + \tilde{\epsilon}_2)\tilde{\epsilon}_3 + \frac{1}{2}C_{33}\tilde{\epsilon}_3^2 \\ &\quad + \frac{1}{2}C_{44}(\tilde{\epsilon}_4^2 + \tilde{\epsilon}_5^2) + \frac{1}{4}(C_{11} - C_{12})\tilde{\epsilon}_6^2 \\ &= \frac{1}{2}c_{xxxx}(\epsilon_{xx}^2 + \epsilon_{yy}^2) + c_{xxyy}\epsilon_{xx}\epsilon_{yy} + c_{xxzz}(\epsilon_{xx} + \epsilon_{yy})\epsilon_{zz} + \frac{1}{2}c_{zzzz}\epsilon_{zz}^2 \\ &\quad + 2c_{yzyz}(\epsilon_{yz}^2 + \epsilon_{xz}^2) + (c_{xxxx} - c_{xxyy})\epsilon_{xy}^2 \end{aligned}$$

### Magnetoelastic energy

$$\begin{aligned} \frac{E_{me}^{hex(I)}}{V_0} &= b_{11}(\epsilon_{xx} + \epsilon_{yy}) + b_{12}\epsilon_{zz} + b_{21}\left(\alpha_z^2 - \frac{1}{3}\right)(\epsilon_{xx} + \epsilon_{yy}) + b_{22}\left(\alpha_z^2 - \frac{1}{3}\right)\epsilon_{zz} \\ &\quad + b_3\left[\frac{1}{2}(\alpha_x^2 - \alpha_y^2)(\epsilon_{xx} - \epsilon_{yy}) + 2\alpha_x\alpha_y\epsilon_{xy}\right] + 2b_4(\alpha_x\alpha_z\epsilon_{xz} + \alpha_y\alpha_z\epsilon_{yz}). \end{aligned}$$

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

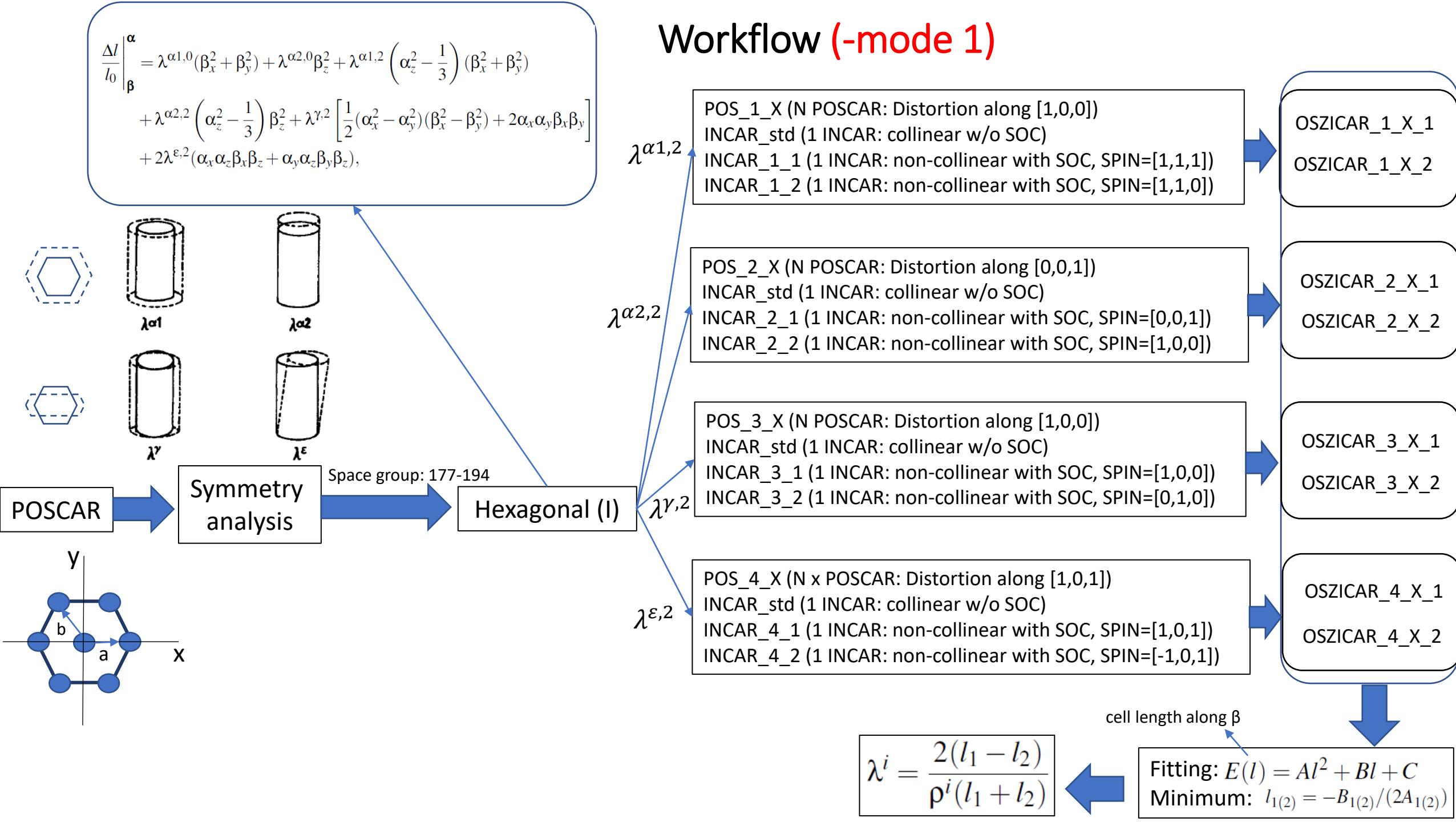
$\downarrow$

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

$\downarrow$

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

$$\begin{aligned} \frac{\Delta l}{l_0} \Big|_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} &= \lambda^{\alpha 1,0}(\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0}\beta_z^2 + \lambda^{\alpha 1,2}\left(\alpha_z^2 - \frac{1}{3}\right)(\beta_x^2 + \beta_y^2) \\ &\quad + \lambda^{\alpha 2,2}\left(\alpha_z^2 - \frac{1}{3}\right)\beta_z^2 + \lambda^{\gamma,2}\left[\frac{1}{2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + 2\alpha_x\alpha_y\beta_x\beta_y\right] \\ &\quad + 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z), \\ \lambda^{\alpha 1,0} &= \frac{b_{11}c_{33} + b_{12}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 2,0} &= \frac{2b_{11}c_{13} - b_{12}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 1,2} &= \frac{-b_{21}c_{33} + b_{22}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 2,2} &= \frac{2b_{21}c_{13} - b_{22}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\gamma,2} &= \frac{-b_3}{c_{11} - c_{12}}, \\ \lambda^{\varepsilon,2} &= \frac{-b_4}{2c_{44}}. \end{aligned}$$



Hexagonal (I)

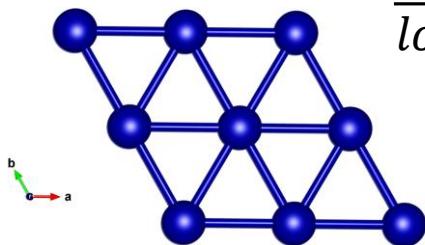
# Distorted states (-mode 1)

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

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

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

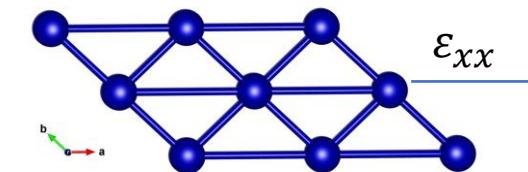
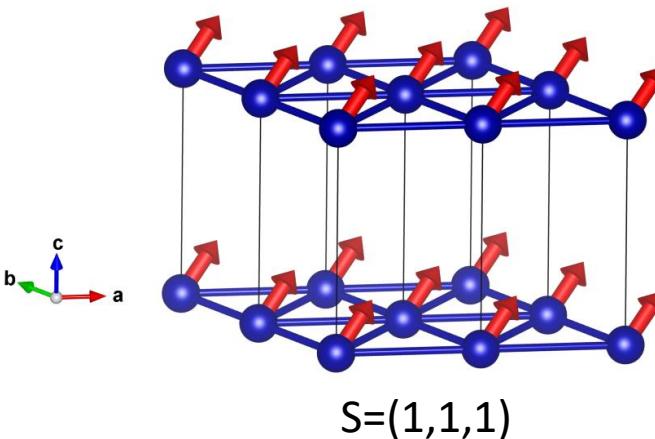
$$\mathbf{F} \Big|_{\beta=(1,0,0)}^{\lambda^{\alpha 1,2}}(s) = \begin{pmatrix} 1+s & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+s}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+s}} \end{pmatrix}$$



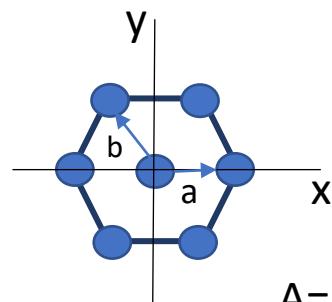
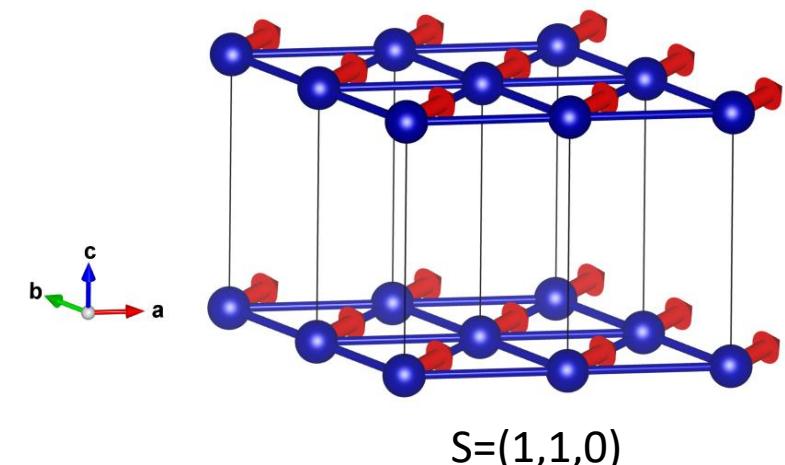
$$\lambda^{\alpha 1,2}$$

$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$



volume-conserving  
 $\text{Det}(\mathbf{F})=1$

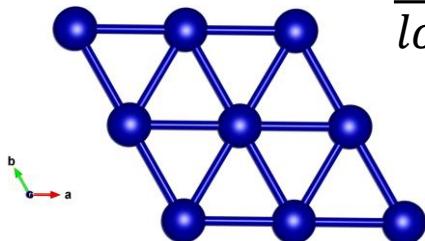


$$\mathbf{A} = \begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

Hexagonal (I)

# Distorted states (-mode 1)

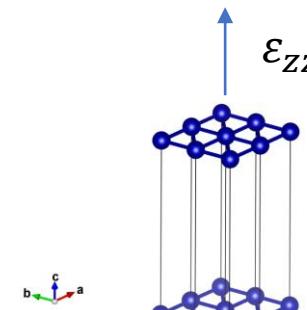
$$\frac{\Delta l^\alpha}{l o_\beta}$$



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

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

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

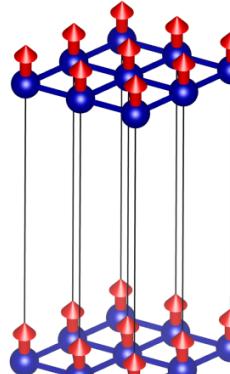
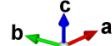


volume-conserving  
 $\text{Det}(F)=1$

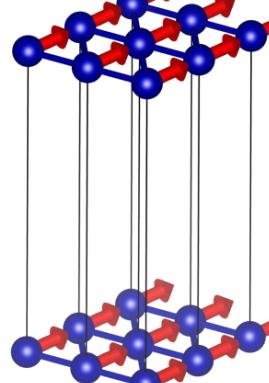
$$\lambda^{\alpha 2,2}$$

$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

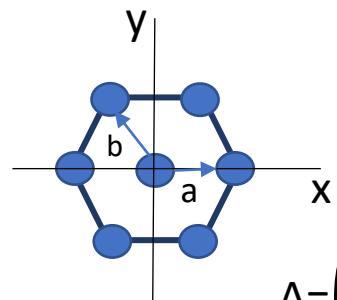
$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$



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



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



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

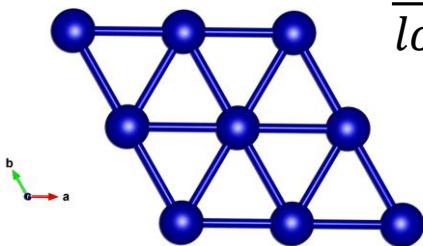
Hexagonal (I)

# Distorted states (-mode 1)

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

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

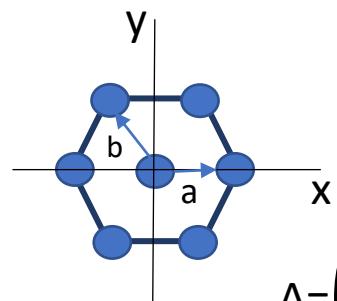
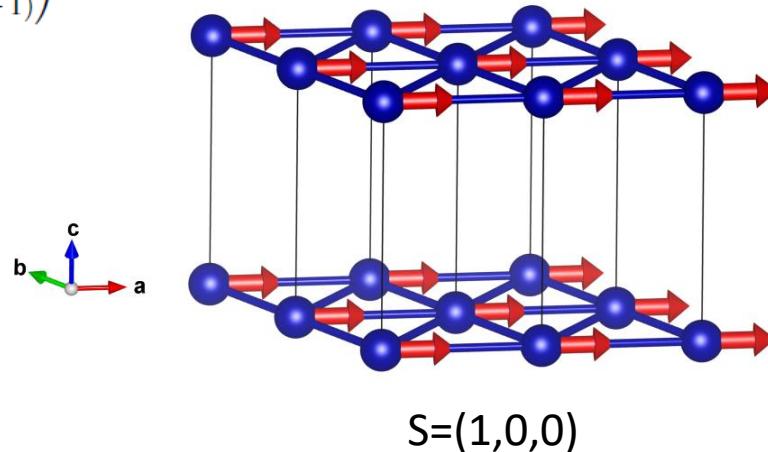
$$\mathbf{F}^{\lambda \gamma^2}_{\beta=(1,0,0)}(s) = \begin{pmatrix} 1+s & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+s}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+s}} \end{pmatrix}$$



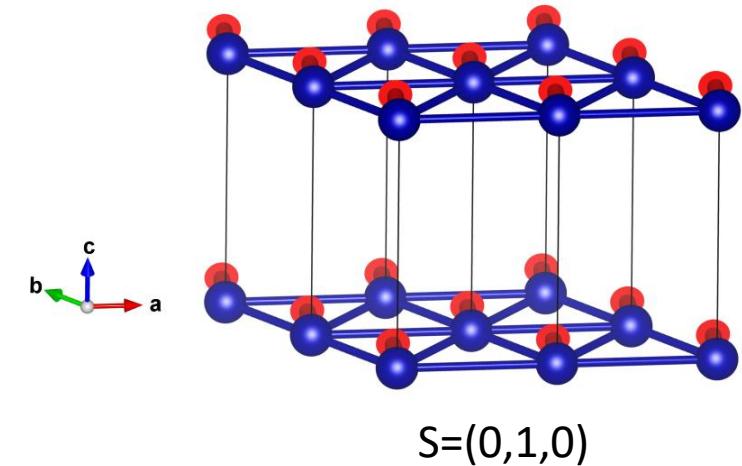
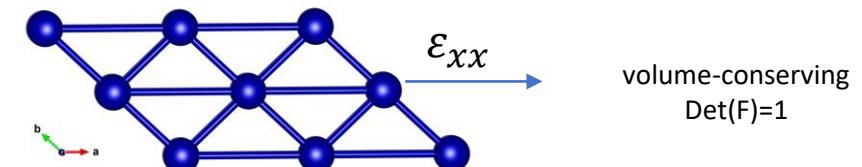
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

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

$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$



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

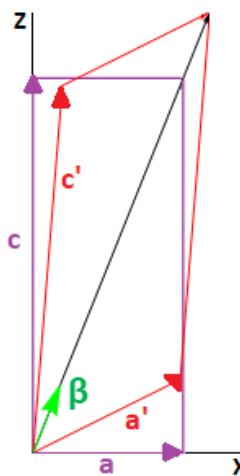


Hexagonal (I)

# Distorted states (-mode 1)

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

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

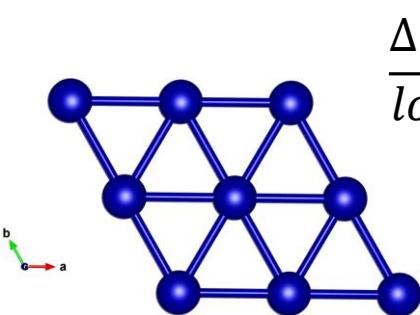


$$A = \begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

$$\epsilon = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

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



$$\frac{\Delta l^\alpha}{l_0 \beta}$$

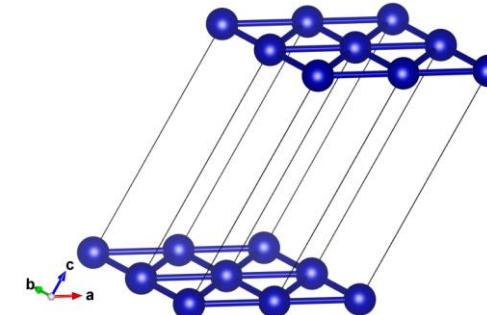
$$|\alpha| = 1, |\beta| = 1$$

$$\text{shear along xz: } \beta = \left( \frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right)$$

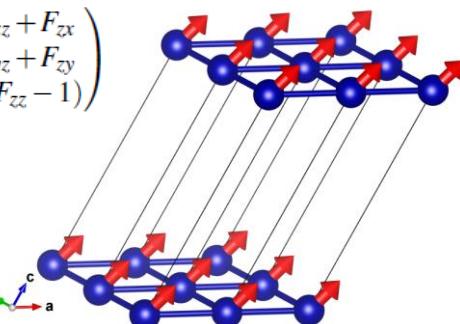
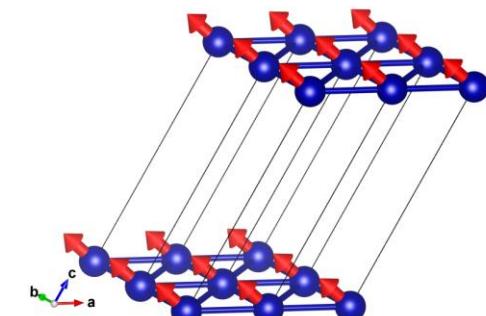
$$F \Big|_{\beta = \frac{(a,0,c)}{\sqrt{a^2+c^2}}}^{\lambda^{\epsilon,2}} (s) = \omega \begin{pmatrix} 1 & 0 & \frac{sc}{2a} \\ 0 & 1 & 0 \\ \frac{sa}{2c} & 0 & 1 \end{pmatrix}$$

$$\varepsilon_{xz}$$

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



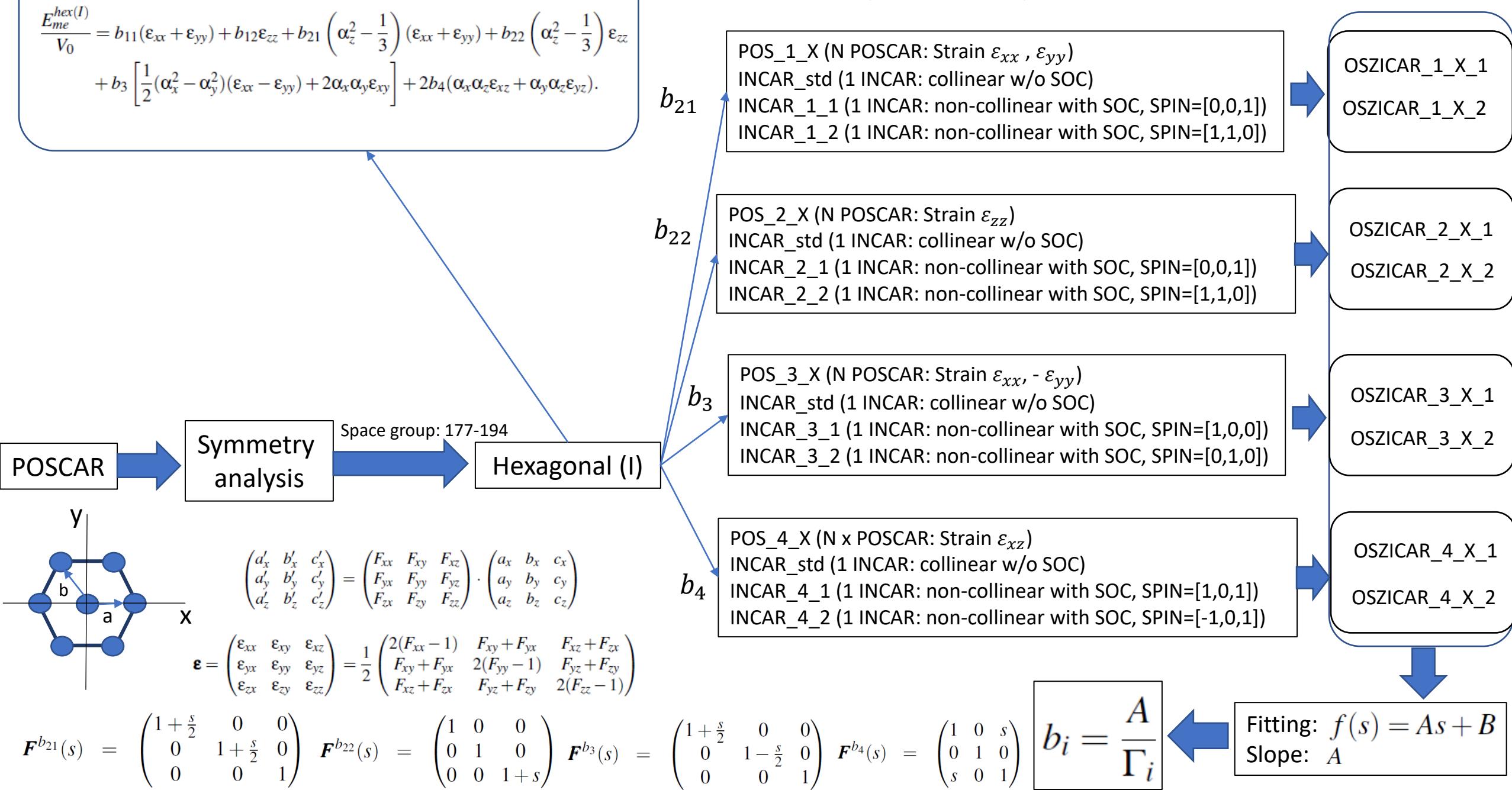
volume-conserving  
 $\text{Det}(F)=1$



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

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

# Workflow (-mode 2)



# Relation between different notations

Hexagonal system

Clark

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Gauge direction			Magnetization direction						$\lambda(x,y)_0 - \lambda(x,y)_f$	Magnetostriiction coefficients	Eq. (3)	Mason <sup>a</sup>	Birss <sup>b</sup>
$\beta_x$	$\beta_y$	$\beta_z$	$\alpha_x$	$\alpha_y$	$\alpha_z$	$\alpha_x$	$\alpha_y$	$\alpha_z$					
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	$\lambda(a,a) - \lambda(c,a)$	$\lambda_A$	$-Q_2$		
$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\lambda(d,d) - \lambda(e,d)$	$-\frac{1}{2}\lambda_A - \frac{1}{2}\lambda_C + 2\lambda_D$	$\frac{1}{2}Q_6$		
$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$					
2	2	2	2	2	2	2	2	2					

<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

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19 JULY 1965

Callen

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

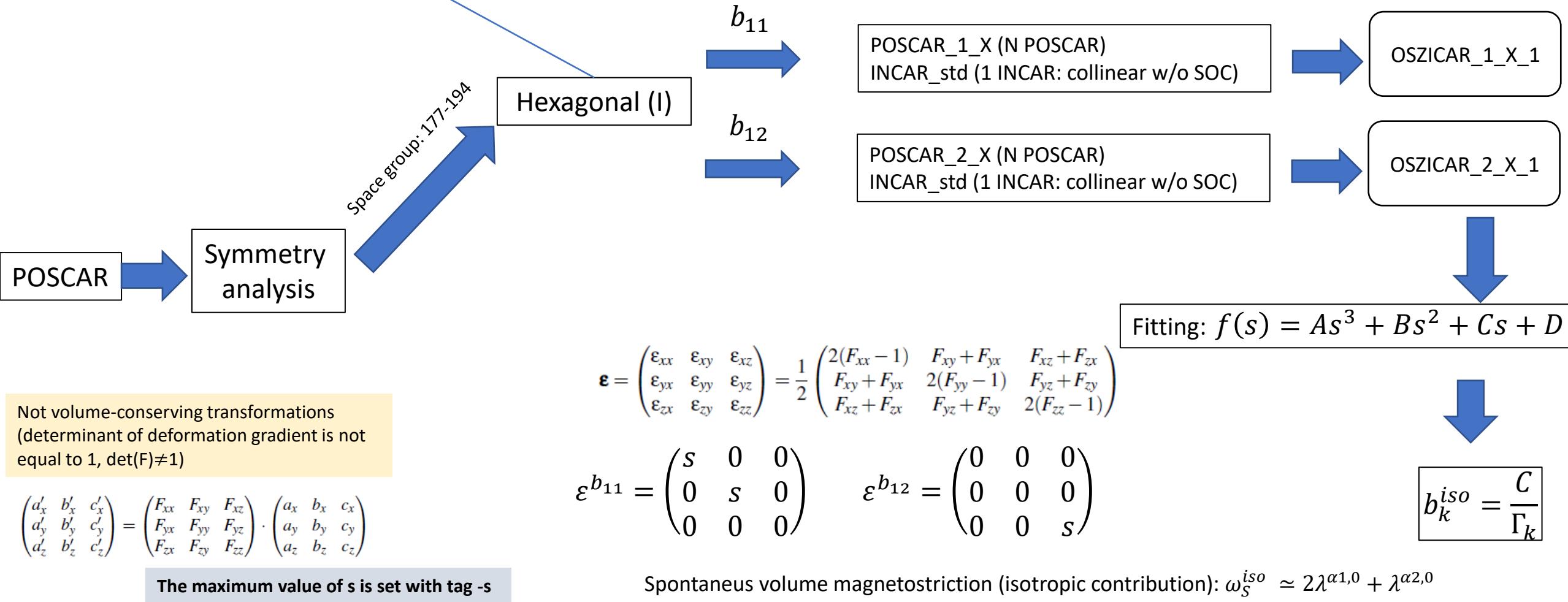
$$\lambda^{\epsilon} = \lambda^{\epsilon,2}$$

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

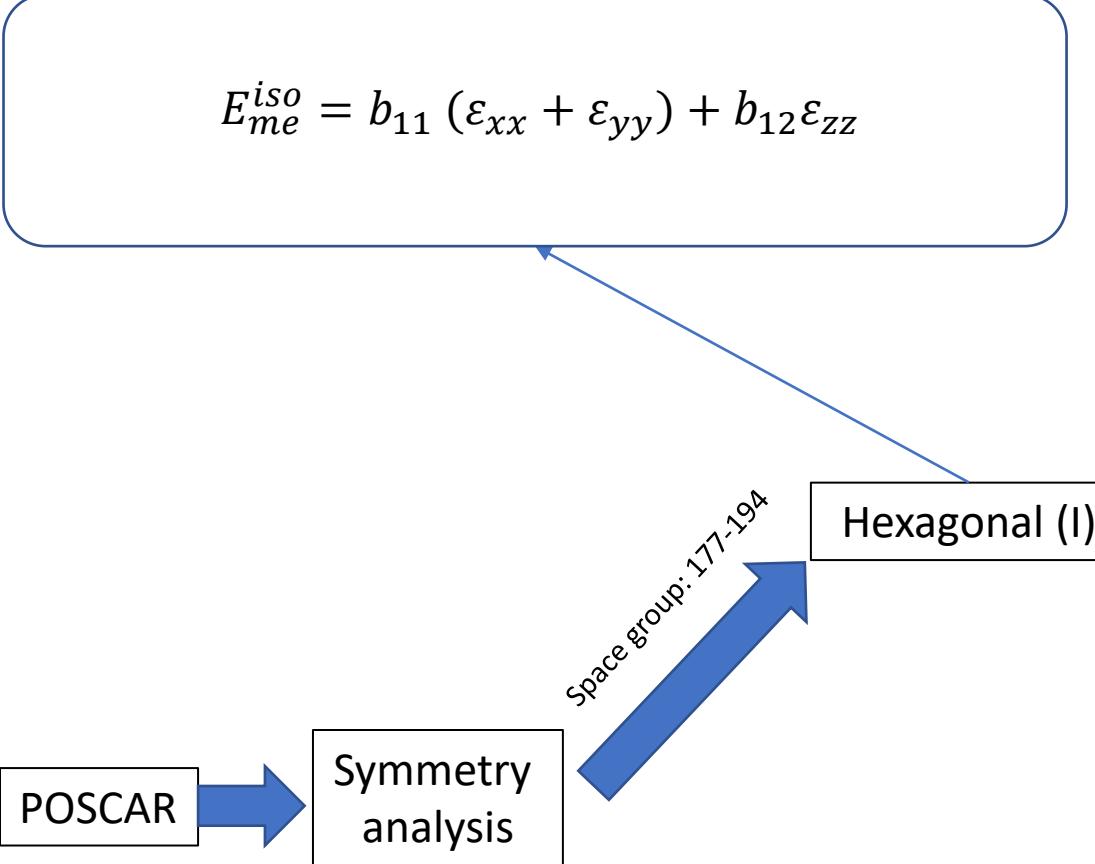
The calculated magnetostriictive coefficients are written in Clark, Mason, Birss and Callen notation in MAELAS code

Spin-polarized calculation **without SOC**

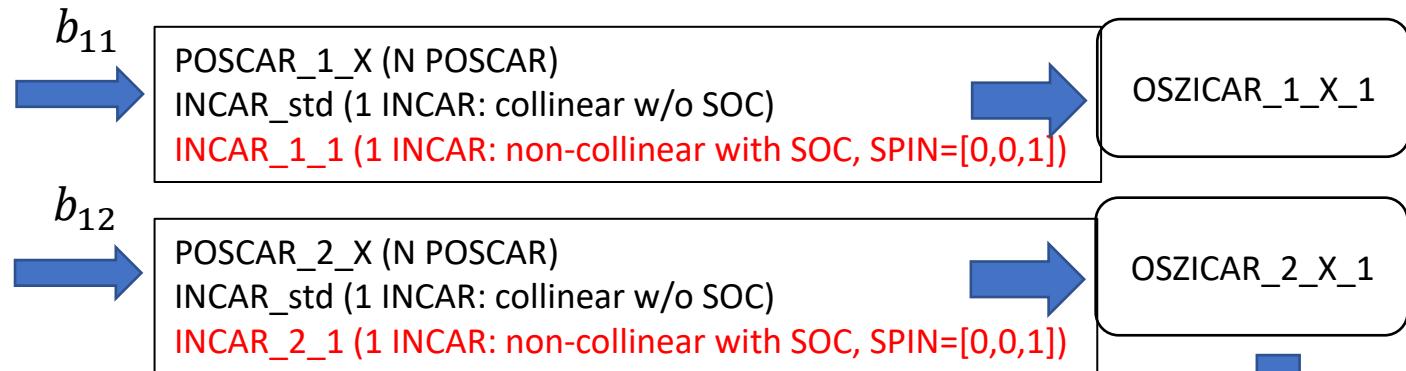
$$E_{me}^{iso} = b_{11} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12} \varepsilon_{zz}$$



$$E_{me}^{iso} = b_{11} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12} \varepsilon_{zz}$$



# Workflow (-mode 3 including anisotropic magnetic interactions)



$$\text{Fitting: } f(s) = As^3 + Bs^2 + Cs + D$$

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

$$\varepsilon^{b_{11}} = \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \varepsilon^{b_{12}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & s \end{pmatrix}$$

(it requires file MAGANI generated in -mode 2)

$$b_i^{iso} = \frac{\mathcal{C} - \Lambda_i(b^{ani})}{\Gamma_i}$$

Not volume-conserving transformations  
(determinant of deformation gradient is not equal to 1,  $\det(F) \neq 1$ )

$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

The maximum value of s is set with tag -s

Spontaneous volume magnetostriction (isotropic contribution):  $\omega_S^{iso} \simeq 2\lambda^{\alpha 1,0} + \lambda^{\alpha 2,0}$

Workflow

# TRIGONAL (I)

SG 149-167

## Trigonal (I)

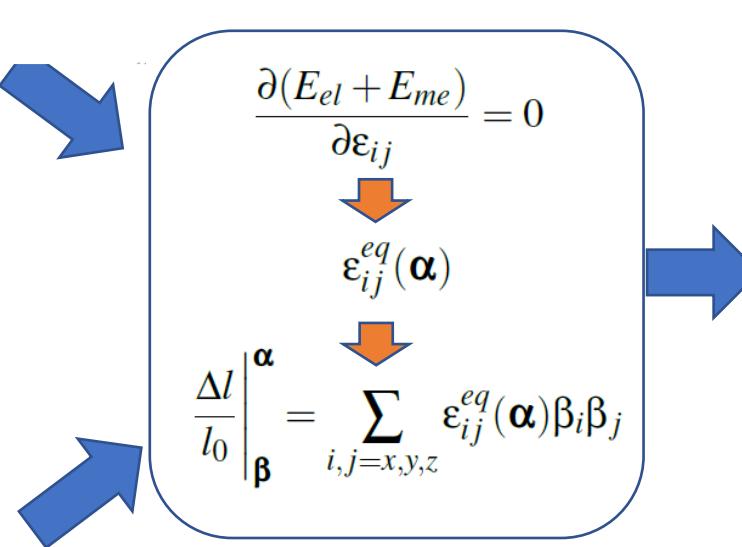
# Workflow

### Elastic energy

$$\begin{aligned} \frac{E_{el}^{trig(I)} - E_0}{V_0} &= \frac{1}{2}C_{11}(\tilde{\epsilon}_1^2 + \tilde{\epsilon}_2^2) + C_{12}\tilde{\epsilon}_1\tilde{\epsilon}_2 + C_{13}(\tilde{\epsilon}_1 + \tilde{\epsilon}_2)\tilde{\epsilon}_3 + \frac{1}{2}C_{33}\tilde{\epsilon}_3^2 \\ &\quad + \frac{1}{2}C_{44}(\tilde{\epsilon}_5^2 + \tilde{\epsilon}_4^2) + \frac{1}{4}(C_{11} - C_{12})\tilde{\epsilon}_6^2 + C_{14}(\tilde{\epsilon}_6\tilde{\epsilon}_5 + \tilde{\epsilon}_1\tilde{\epsilon}_4 - \tilde{\epsilon}_2\tilde{\epsilon}_4). \\ &= \frac{1}{2}c_{xxxx}(\epsilon_{xx}^2 + \epsilon_{yy}^2) + c_{xxyy}\epsilon_{xx}\epsilon_{yy} + c_{xxzz}(\epsilon_{xx} + \epsilon_{yy})\epsilon_{zz} + \frac{1}{2}c_{zzzz}\epsilon_{zz}^2 \\ &\quad + 2c_{yzyz}(\epsilon_{xz}^2 + \epsilon_{yz}^2) + (c_{xxxx} - c_{xxyy})\epsilon_{xy}^2 \\ &\quad + c_{xxyz}(4\epsilon_{xy}\epsilon_{xz} + 2\epsilon_{xx}\epsilon_{yz} - 2\epsilon_{yy}\epsilon_{yz}). \end{aligned}$$

### Magnetoelastic energy

$$\begin{aligned} \frac{E_{me}^{trig(I)}}{V_0} &= b_{11}(\epsilon_{xx} + \epsilon_{yy}) + b_{12}\epsilon_{zz} + b_{21}\left(\alpha_z^2 - \frac{1}{3}\right)(\epsilon_{xx} + \epsilon_{yy}) + b_{22}\left(\alpha_z^2 - \frac{1}{3}\right)\epsilon_{zz} \\ &\quad + b_3\left[\frac{1}{2}(\alpha_x^2 - \alpha_y^2)(\epsilon_{xx} - \epsilon_{yy}) + 2\alpha_x\alpha_y\epsilon_{xy}\right] + 2b_4(\alpha_x\alpha_z\epsilon_{xz} + \alpha_y\alpha_z\epsilon_{yz}) \\ &\quad + b_{14}\left[(\alpha_x^2 - \alpha_y^2)\epsilon_{yz} + 2\alpha_x\alpha_y\epsilon_{xz}\right] + b_{34}\left[\frac{1}{2}\alpha_y\alpha_z(\epsilon_{xx} - \epsilon_{yy}) + 2\alpha_x\alpha_z\epsilon_{xy}\right]. \end{aligned}$$



We corrected these errors in v2.0

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

### Old (v1.0)

$$\begin{aligned} \lambda^{\alpha 1,0} &= \frac{b_{11}c_{33} + b_{12}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 2,0} &= \frac{2b_{11}c_{13} - b_{12}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 1,2} &= \frac{-b_{21}c_{33} + b_{22}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 2,2} &= \frac{2b_{21}c_{13} - b_{22}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \end{aligned}$$

$$\begin{aligned} \lambda^{\gamma,1} &= \frac{c_{14}b_{14} - c_{44}b_3}{1/2c_{44}(c_{11} - c_{12}) - c_{14}^2}, \\ \lambda^{\gamma,2} &= \frac{1/2b_4(c_{11} - c_{12}) - b_{34}c_{14}}{1/2c_{44}(c_{11} - c_{12}) - c_{14}^2}, \\ \lambda_{12} &= \frac{c_{14}b_4 - c_{44}b_{34}}{1/2c_{44}(c_{11} - c_{12}) - c_{14}^2}, \\ \lambda_{21} &= \frac{1/2b_{14}(c_{11} - c_{12}) - b_3c_{14}}{1/2c_{44}(c_{11} - c_{12}) - c_{14}^2} \end{aligned}$$

### New (v2.0)

$$\begin{aligned} \lambda^{\alpha 1,0} &= \frac{b_{11}C_{33} + b_{12}C_{13}}{C_{33}(C_{11} + C_{12}) - 2C_{13}^2}, \\ \lambda^{\alpha 2,0} &= \frac{2b_{11}C_{13} - b_{12}(C_{11} + C_{12})}{C_{33}(C_{11} + C_{12}) - 2C_{13}^2}, \\ \lambda^{\alpha 1,2} &= \frac{-b_{21}C_{33} + b_{22}C_{13}}{C_{33}(C_{11} + C_{12}) - 2C_{13}^2}, \\ \lambda^{\alpha 2,2} &= \frac{2b_{21}C_{13} - b_{22}(C_{11} + C_{12})}{C_{33}(C_{11} + C_{12}) - 2C_{13}^2}, \\ \lambda^{\gamma,1} &= \frac{1/2C_{44}b_{14} - 1/2C_{44}b_3}{1/2C_{44}(C_{11} - C_{12}) - C_{14}^2}, \\ \lambda^{\gamma,2} &= \frac{-1/2b_4(C_{11} - C_{12}) + b_{34}C_{14}}{1/2C_{44}(C_{11} - C_{12}) - C_{14}^2}, \\ \lambda_{12} &= \frac{C_{14}b_4 - C_{44}b_{34}}{1/2C_{44}(C_{11} - C_{12}) - C_{14}^2}, \\ \lambda_{21} &= \frac{-1/2b_{14}(C_{11} - C_{12}) + b_3C_{14}}{1/2C_{44}(C_{11} - C_{12}) - C_{14}^2}. \end{aligned}$$

## Trigonal (I)

## Workflow (-mode 1)

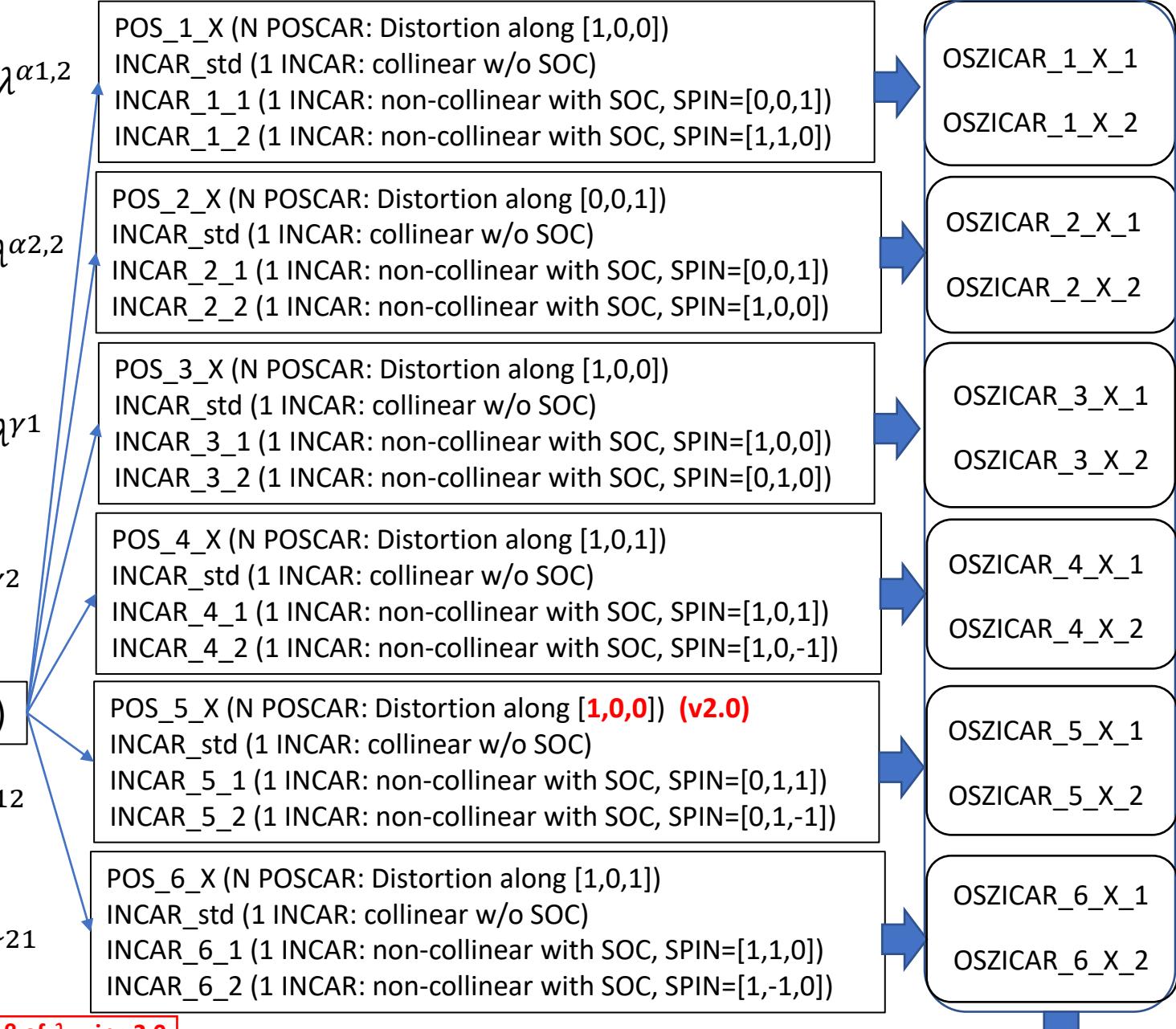
$$\frac{\Delta l}{l_0} \Bigg|_{\beta}^{\alpha} = \lambda^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0} \beta_z^2 + \lambda^{\alpha 1,2} \left( \alpha_z^2 - \frac{1}{3} \right) (\beta_x^2 + \beta_y^2) \\ + \lambda^{\alpha 2,2} \left( \alpha_z^2 - \frac{1}{3} \right) \beta_z^2 \\ + \lambda^{\gamma,1}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



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

$$F \Big|_{\beta=(0,0,1)}^{\lambda^{\alpha 2,2}} (s) = \begin{pmatrix} \frac{1}{\sqrt{1+s}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+s}} & 0 \\ 0 & 0 & 1+s \end{pmatrix} \quad F \Big|_{\beta=\frac{(a,0,c)}{\sqrt{a^2+c^2}}}^{\lambda^{\gamma,2}} (s) = F \Big|_{\beta=\frac{(a,0,c)}{\sqrt{a^2+c^2}}}^{\lambda_{21}} (s) = \Omega \begin{pmatrix} 1 & 0 & \frac{sc}{2a} \\ 0 & 1 & 0 \\ \frac{sa}{2c} & 0 & 1 \end{pmatrix}$$

$$\Omega = [4/(4-s^2)]^{1/3}$$



We have replaced the deformation gradient (F) and measuring length direction  $\beta$  of  $\lambda_{12}$  in v2.0

$$F \Big|_{\beta=\frac{(a,0,c)}{\sqrt{a^2+c^2}}}^{\lambda_{12}(\text{version1.0})} (s) = \Omega \begin{pmatrix} 1 & 0 & \frac{sc}{2a} \\ 0 & 1 & 0 \\ \frac{sa}{2c} & 0 & 1 \end{pmatrix} \rightarrow F \Big|_{\beta=(1,0,0)}^{\lambda_{12}(\text{version2.0})} (s) = \begin{pmatrix} 1+s & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+s}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+s}} \end{pmatrix}$$

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

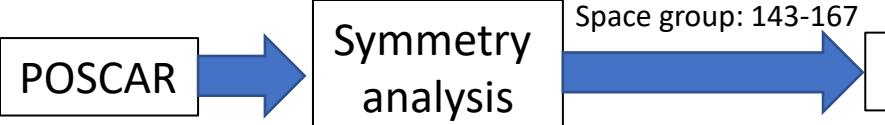
$$\text{Fitting: } E(l) = Al^2 + Bl + C \\ \text{Minimum: } l_{1(2)} = -B_{1(2)}/(2A_{1(2)})$$

## Trigonal (I)

## Workflow (-mode 2)

$$\frac{E_{me}^{trig(I)}}{V_0} = b_{11}(\epsilon_{xx} + \epsilon_{yy}) + b_{12}\epsilon_{zz} + b_{21} \left( \alpha_z^2 - \frac{1}{3} \right) (\epsilon_{xx} + \epsilon_{yy}) + b_{22} \left( \alpha_z^2 - \frac{1}{3} \right) \epsilon_{zz} \\ + b_3 \left[ \frac{1}{2}(\alpha_x^2 - \alpha_y^2)(\epsilon_{xx} - \epsilon_{yy}) + 2\alpha_x\alpha_y\epsilon_{xy} \right] + 2b_4(\alpha_x\alpha_z\epsilon_{xz} + \alpha_y\alpha_z\epsilon_{yz}) \\ + b_{14}[(\alpha_x^2 - \alpha_y^2)\epsilon_{yz} + 2\alpha_x\alpha_y\epsilon_{xz}] + b_{34} \left[ \frac{1}{2}\alpha_y\alpha_z(\epsilon_{xx} - \epsilon_{yy}) + 2\alpha_x\alpha_z\epsilon_{xy} \right].$$

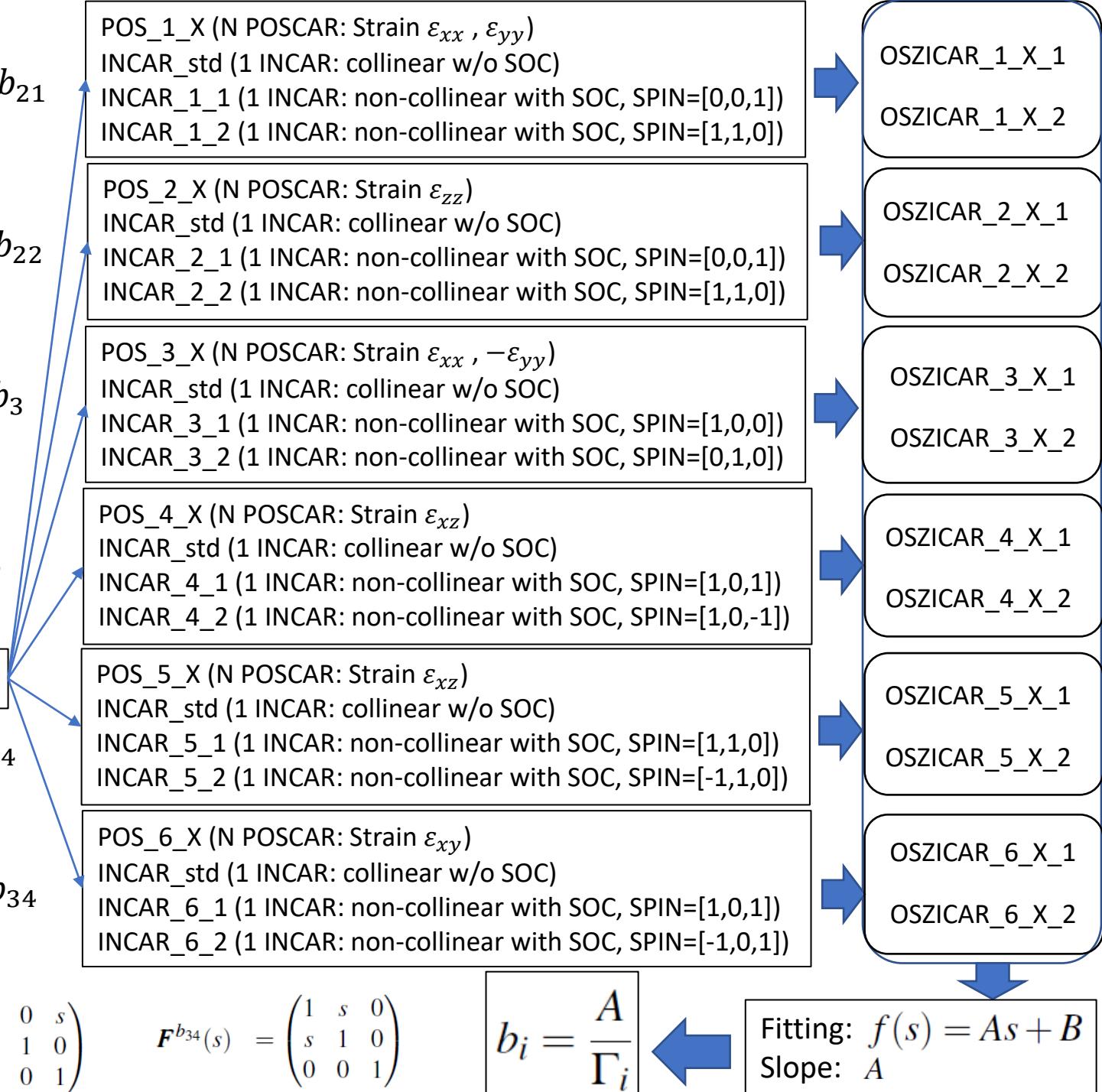
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$



$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

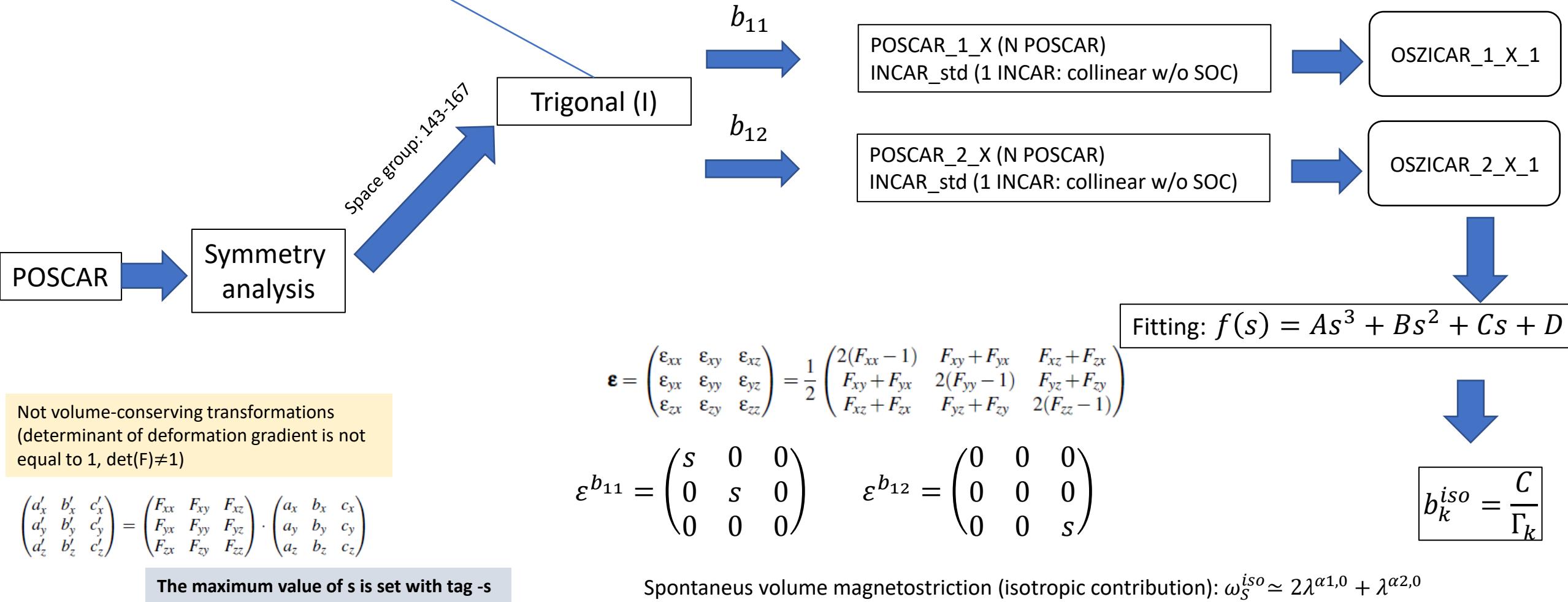
$$\mathbf{F}^{b_{21}}(s) = \begin{pmatrix} 1 + \frac{s}{2} & 0 & 0 \\ 0 & 1 + \frac{s}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_{22}}(s) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+s \end{pmatrix}$$

$$\mathbf{F}^{b_3}(s) = \begin{pmatrix} 1 + \frac{s}{2} & 0 & 0 \\ 0 & 1 - \frac{s}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_4}(s) = \begin{pmatrix} 1 & 0 & s \\ 0 & 1 & 0 \\ s & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_{14}}(s) = \begin{pmatrix} 1 & 0 & s \\ 0 & 1 & 0 \\ s & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_{34}}(s) = \begin{pmatrix} 1 & s & 0 \\ s & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

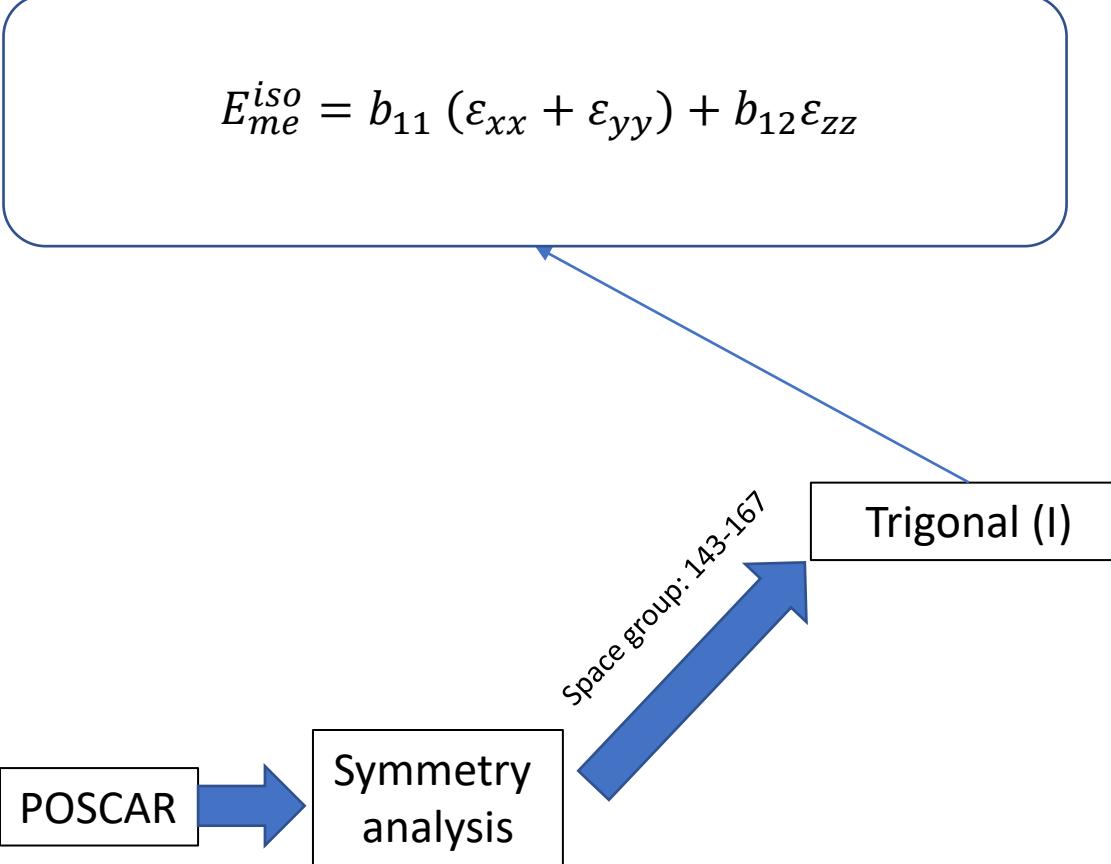


Spin-polarized calculation **without SOC**

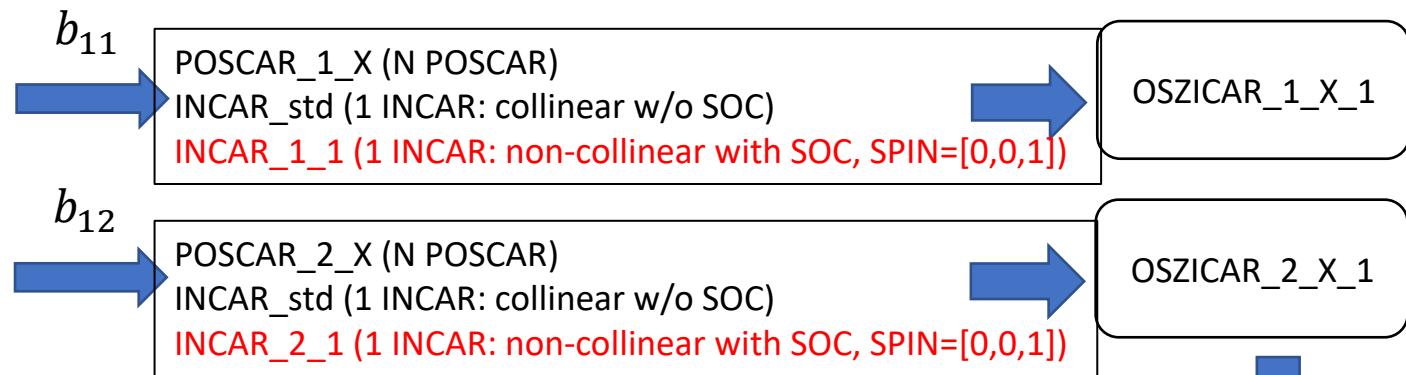
$$E_{me}^{iso} = b_{11} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12} \varepsilon_{zz}$$



$$E_{me}^{iso} = b_{11} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12} \varepsilon_{zz}$$



# Workflow (-mode 3 including anisotropic magnetic interactions)



$$\text{Fitting: } f(s) = As^3 + Bs^2 + Cs + D$$

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

(it requires file MAGANI generated in -mode 2)

$$\boldsymbol{\varepsilon}^{b_{11}} = \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \boldsymbol{\varepsilon}^{b_{12}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & s \end{pmatrix}$$

$$b_i^{iso} = \frac{\mathcal{C} - \Lambda_i(b^{ani})}{\Gamma_i}$$

Not volume-conserving transformations  
(determinant of deformation gradient is not equal to 1,  $\det(\mathbf{F}) \neq 1$ )

$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

The maximum value of s is set with tag -s

Spontaneous volume magnetostriction (isotropic contribution):  $\omega_S^{iso} \simeq 2\lambda^{\alpha 1,0} + \lambda^{\alpha 2,0}$

Workflow

# TETRAGONAL (I)

SG 89-142

# Workflow

Tetragonal (I)

Elastic energy

$$\begin{aligned} \frac{E_{el}^{tet(I)} - E_0}{V_0} &= \frac{1}{2} C_{11}(\tilde{\epsilon}_1^2 + \tilde{\epsilon}_2^2) + C_{12}\tilde{\epsilon}_1\tilde{\epsilon}_2 + C_{13}(\tilde{\epsilon}_1 + \tilde{\epsilon}_2)\tilde{\epsilon}_3 + \frac{1}{2}C_{33}\tilde{\epsilon}_3^2 \\ &\quad + \frac{1}{2}C_{44}(\tilde{\epsilon}_4^2 + \tilde{\epsilon}_5^2) + \frac{1}{2}C_{66}\tilde{\epsilon}_6^2 \\ &= \frac{1}{2}c_{xxxx}(\epsilon_{xx}^2 + \epsilon_{yy}^2) + c_{xyyy}\epsilon_{xx}\epsilon_{yy} + c_{xzxz}(\epsilon_{xx} + \epsilon_{yy})\epsilon_{zz} + \frac{1}{2}c_{zzzz}\epsilon_{zz}^2 \\ &\quad + 2c_{yzyz}(\epsilon_{yz}^2 + \epsilon_{xz}^2) + 2c_{xyxy}\epsilon_{xy}^2 \end{aligned}$$

Magnetoelastic energy

$$\begin{aligned} \frac{E_{me}^{tet(I)}}{V_0} &= b_{11}(\epsilon_{xx} + \epsilon_{yy}) + b_{12}\epsilon_{zz} + b_{21}\left(\alpha_z^2 - \frac{1}{3}\right)(\epsilon_{xx} + \epsilon_{yy}) + b_{22}\left(\alpha_z^2 - \frac{1}{3}\right)\epsilon_{zz} \\ &\quad + \frac{1}{2}b_3(\alpha_x^2 - \alpha_y^2)(\epsilon_{xx} - \epsilon_{yy}) + 2b'_3\alpha_x\alpha_y\epsilon_{xy} + 2b_4(\alpha_x\alpha_z\epsilon_{xz} + \alpha_y\alpha_z\epsilon_{yz}). \end{aligned}$$

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

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

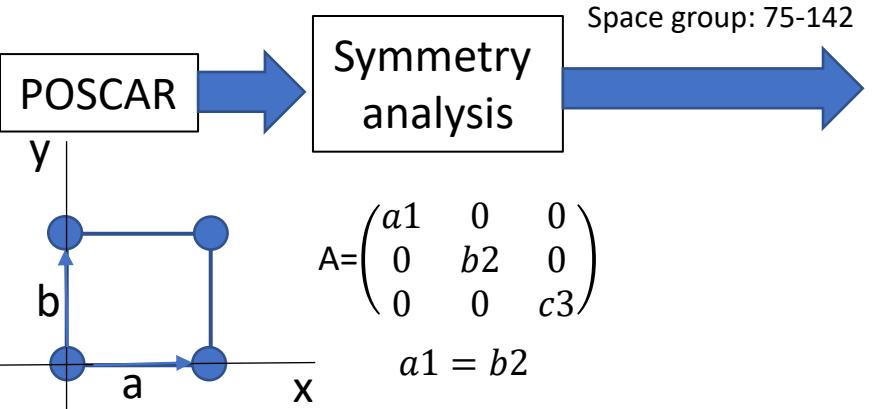
$$\frac{\Delta l}{l_0} \Bigg|_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} = \sum_{i,j=x,y,z} \epsilon_{ij}^{eq}(\boldsymbol{\alpha}) \beta_i \beta_j$$

$$\begin{aligned} \frac{\Delta l}{l_0} \Bigg|_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} &= \lambda^{\alpha 1,0}(\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0}\beta_z^2 + \lambda^{\alpha 1,2}\left(\alpha_z^2 - \frac{1}{3}\right)(\beta_x^2 + \beta_y^2) \\ &\quad + \lambda^{\alpha 2,2}\left(\alpha_z^2 - \frac{1}{3}\right)\beta_z^2 + \frac{1}{2}\lambda^{\gamma,2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + 2\lambda^{\delta,2}\alpha_x\alpha_y\beta_x\beta_y \\ &\quad + 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z), \\ \lambda^{\alpha 1,0} &= \frac{b_{11}c_{33} + b_{12}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 2,0} &= \frac{2b_{11}c_{13} - b_{12}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 1,2} &= \frac{-b_{21}c_{33} + b_{22}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\alpha 2,2} &= \frac{2b_{21}c_{13} - b_{22}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2}, \\ \lambda^{\gamma,2} &= \frac{-b_3}{c_{11} - c_{12}}, \\ \lambda^{\delta,2} &= \frac{-b'_3}{2c_{66}}, \\ \lambda^{\varepsilon,2} &= \frac{-b_4}{2c_{44}}. \end{aligned}$$

# Workflow (-mode 1)

same files as the hexagonal (I) case (-mode 1)

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



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

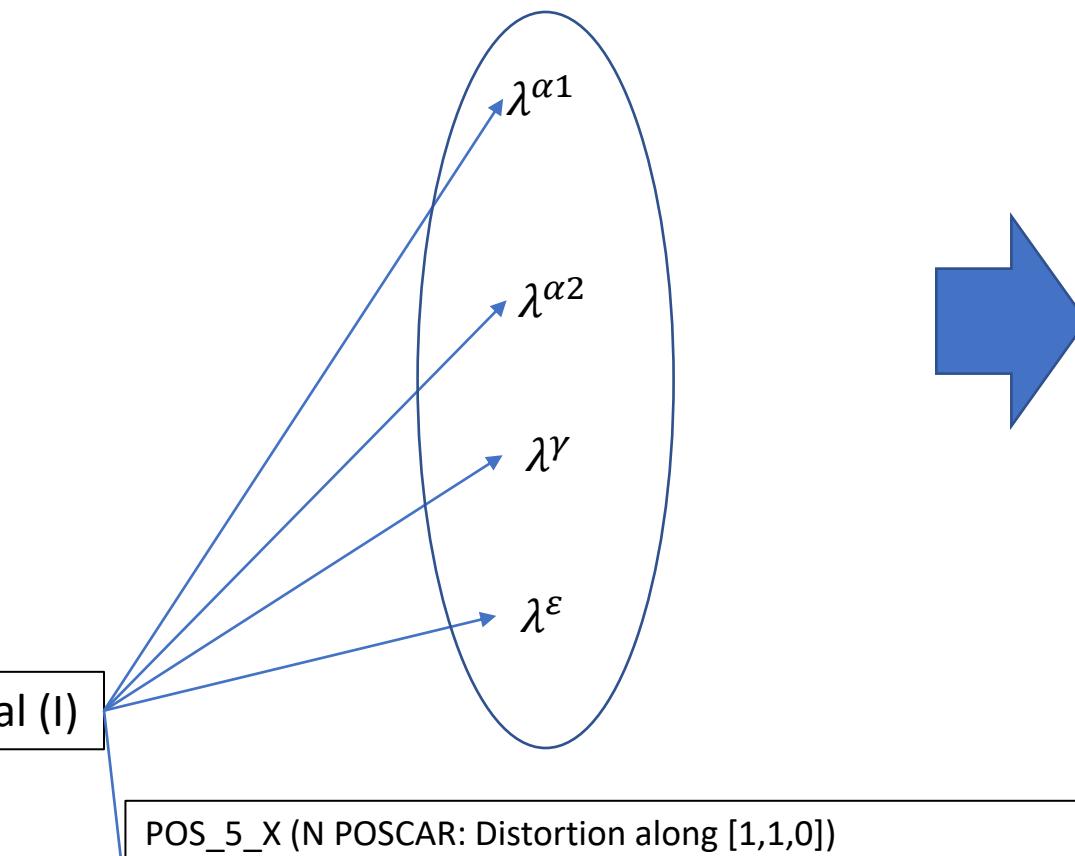
$$\begin{pmatrix} d'_x & b'_x & c'_x \\ d'_y & b'_y & c'_y \\ d'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

$$F \Big|_{\beta = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)}^{s=2} = \mathcal{Q} \begin{pmatrix} 1 & \frac{s}{2} & 0 \\ \frac{s}{2} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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

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



# Relation between different notations

## Tetragonal (I)

Cullen

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



Mason

$$\frac{\Delta l}{l_0} \Bigg|_{\beta}^{\alpha} = \lambda_{Mason}^{\alpha 1,0}(\beta_x^2 + \beta_y^2) + \lambda_{Mason}^{\alpha 2,0}\beta_z^2 + \frac{1}{2} \lambda_1 [(\alpha_x \beta_x - \alpha_y \beta_y)^2 - (\alpha_x \beta_y + \alpha_y \beta_x)^2 \\ + (1 - \beta_z^2)(1 - \alpha_z^2) - 2\alpha_z \beta_z (\alpha_x \beta_x + \alpha_y \beta_y)] + 4\lambda_2 \alpha_z \beta_z (\alpha_x \beta_x + \alpha_y \beta_y) \\ + 4\lambda_3 \alpha_x \alpha_y \beta_x \beta_y + \lambda_4 [\beta_z^2(1 - \alpha_z^2) - \alpha_z \beta_z (\alpha_x \beta_x + \alpha_y \beta_y)] \\ + \frac{1}{2} \lambda_5 [(\alpha_x \beta_y - \alpha_y \beta_x)^2 - (\alpha_x \beta_x + \alpha_y \beta_y)^2 + (1 - \beta_z^2)(1 - \alpha_z^2)].$$

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

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

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

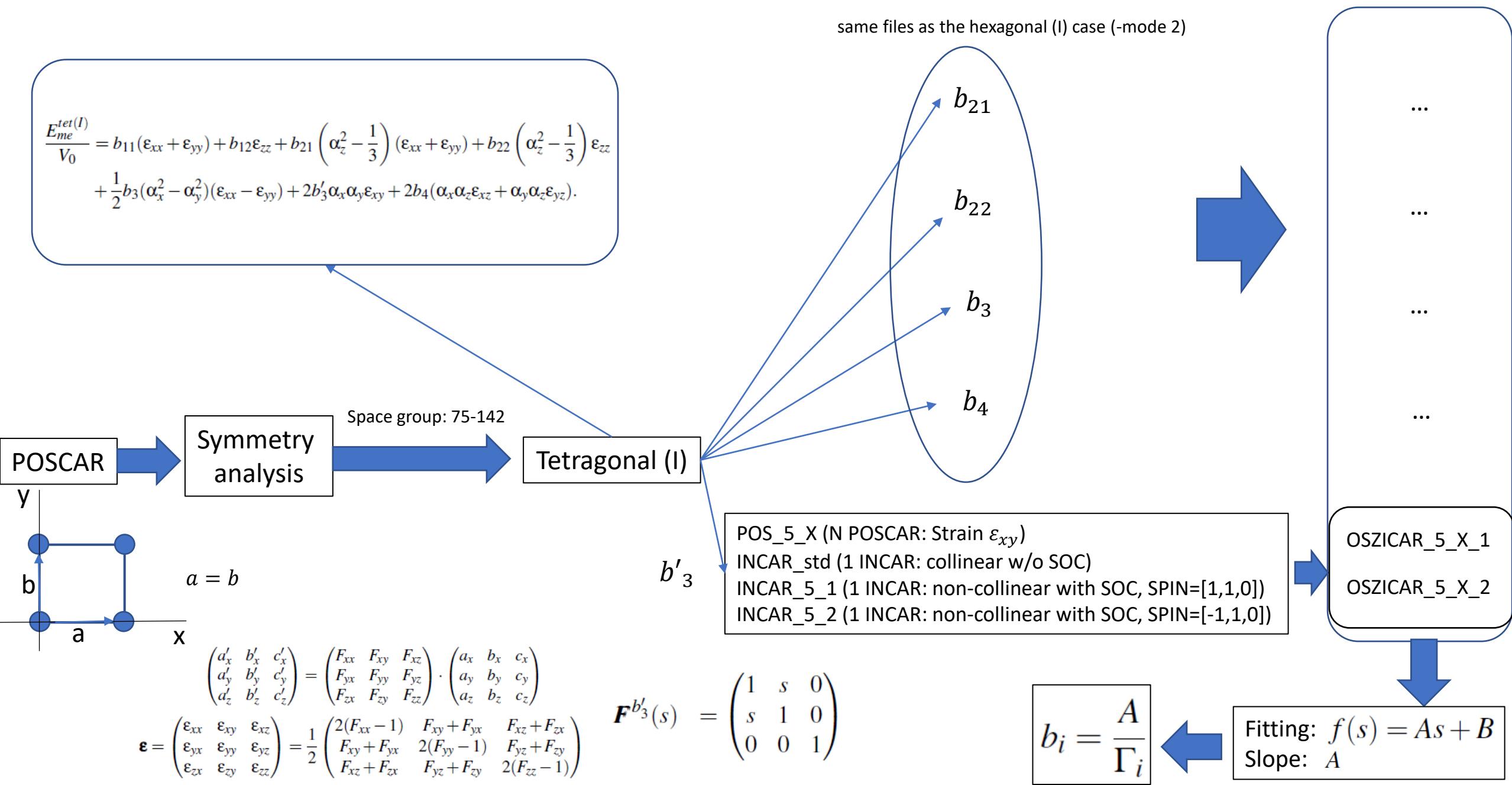
$$\lambda_2 = \frac{1}{2} \lambda^{\varepsilon,2} - \frac{1}{4} \lambda^{\alpha 2,2} - \frac{1}{4} \lambda^{\alpha 1,2} + \frac{1}{8} \lambda^{\gamma,2}$$

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

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

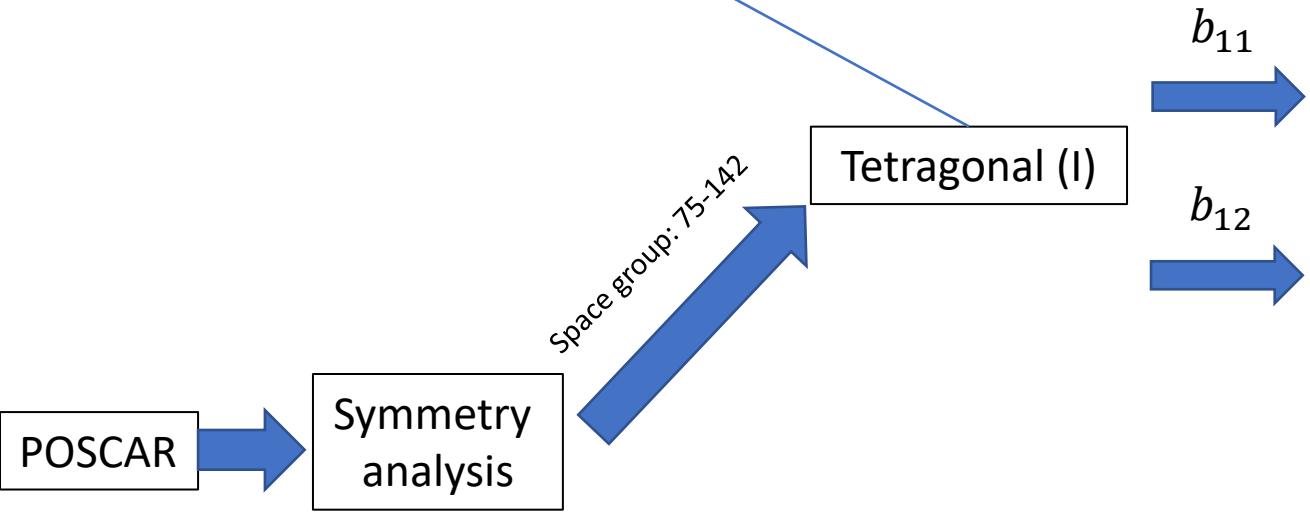
$$\lambda_5 = -\lambda^{\alpha 1,2} - \frac{1}{2} \lambda^{\gamma,2}.$$

# Workflow (-mode 2)



Spin-polarized calculation **without SOC**

$$E_{me}^{iso} = b_{11} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12} \varepsilon_{zz}$$



## Workflow (-mode 3)

Not volume-conserving transformations  
(determinant of deformation gradient is not equal to 1,  $\det(F) \neq 1$ )

$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

The maximum value of s is set with tag -s

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

$$\varepsilon^{b_{11}} = \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \varepsilon^{b_{12}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & s \end{pmatrix}$$

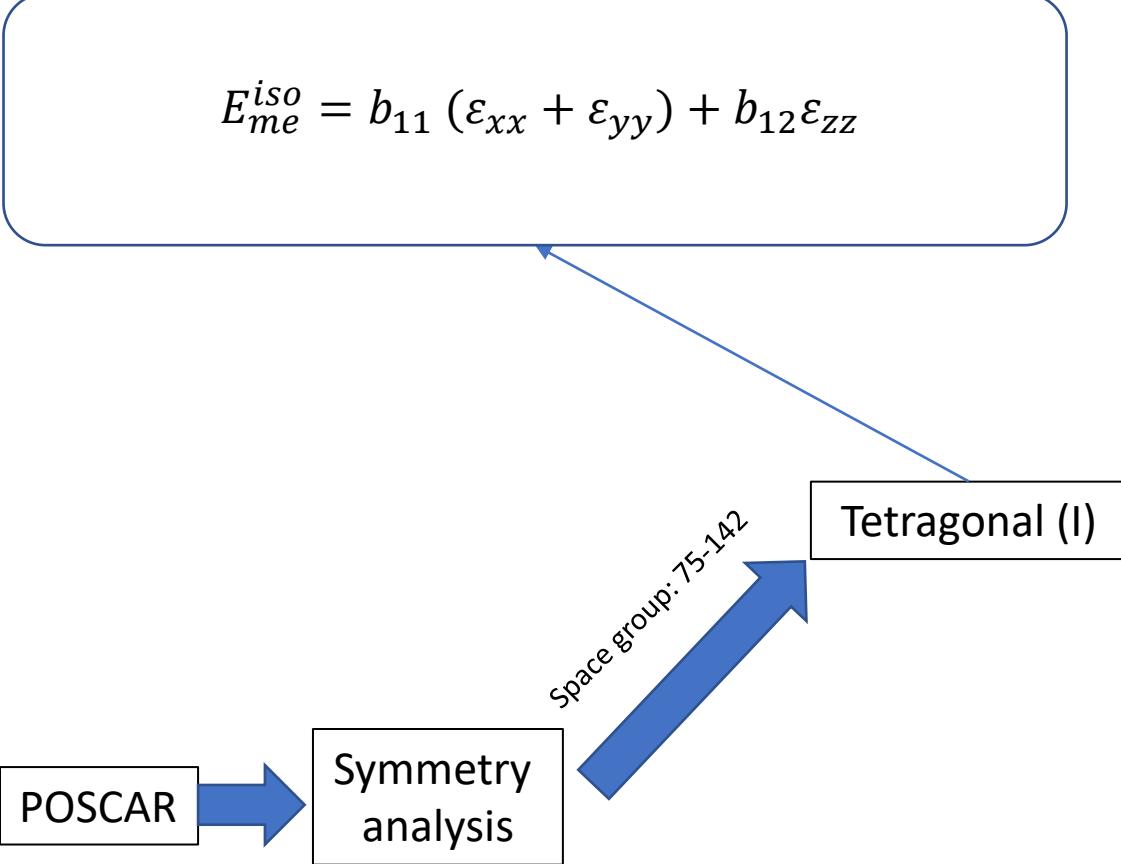
$$\text{Fitting: } f(s) = As^3 + Bs^2 + Cs + D$$

$$b_k^{iso} = \frac{C}{\Gamma_k}$$

Spontaneous volume magnetostriction (isotropic contribution):  $\omega_S^{iso} \simeq 2\lambda^{\alpha 1,0} + \lambda^{\alpha 2,0}$

Spin-polarized calculation **with SOC**

$$E_{me}^{iso} = b_{11} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{12} \varepsilon_{zz}$$

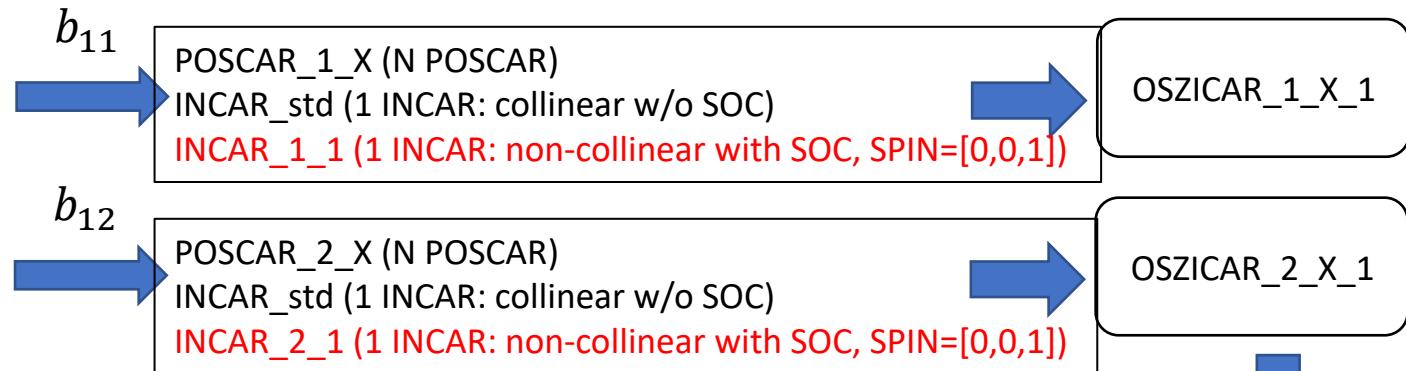


Not volume-conserving transformations  
(determinant of deformation gradient is not equal to 1,  $\det(F) \neq 1$ )

$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

The maximum value of s is set with tag -s

# Workflow (-mode 3 including anisotropic magnetic interactions)



$$\text{Fitting: } f(s) = As^3 + Bs^2 + Cs + D$$

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

$$\varepsilon^{b_{11}} = \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \varepsilon^{b_{12}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & s \end{pmatrix}$$

(it requires file MAGANI generated in -mode 2)

$$b_i^{iso} = \frac{\mathcal{C} - \Lambda_i(b^{ani})}{\Gamma_i}$$

Spontaneous volume magnetostriction (isotropic contribution):  $\omega_S^{iso} \simeq 2\lambda^{\alpha 1,0} + \lambda^{\alpha 2,0}$

Workflow

# ORTHORHOMBIC

SG 16-74

## Orthorhombic

# Workflow

### Elastic energy

$$\begin{aligned}\frac{E_{el}^{ortho} - E_0}{V_0} &= \frac{1}{2}C_{11}\tilde{\epsilon}_1^2 + \frac{1}{2}C_{22}\tilde{\epsilon}_2^2 + C_{12}\tilde{\epsilon}_1\tilde{\epsilon}_2 + C_{13}\tilde{\epsilon}_1\tilde{\epsilon}_3 + C_{23}\tilde{\epsilon}_2\tilde{\epsilon}_3 + \frac{1}{2}C_{33}\tilde{\epsilon}_3^2 \\ &\quad + \frac{1}{2}C_{44}\tilde{\epsilon}_4^2 + \frac{1}{2}C_{55}\tilde{\epsilon}_5^2 + \frac{1}{2}C_{66}\tilde{\epsilon}_6^2 \\ &= \frac{1}{2}c_{xxxx}\epsilon_{xx}^2 + \frac{1}{2}c_{yyyy}\epsilon_{yy}^2 + c_{xxyy}\epsilon_{xx}\epsilon_{yy} + c_{xxzz}\epsilon_{xx}\epsilon_{zz} + c_{yyzz}\epsilon_{yy}\epsilon_{zz} \\ &\quad + \frac{1}{2}c_{zzzz}\epsilon_{zz}^2 + 2c_{zyz}\epsilon_{yz}^2 + 2c_{xzx}\epsilon_{xz}^2 + 2c_{xyx}\epsilon_{xy}^2.\end{aligned}$$



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



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



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



### Magnetoelastic energy

$$\begin{aligned}\frac{E_{me}^{ortho}}{V_0} &= b_{01}\epsilon_{xx} + b_{02}\epsilon_{yy} + b_{03}\epsilon_{zz} + b_1\alpha_x^2\epsilon_{xx} + b_2\alpha_y^2\epsilon_{xx} + b_3\alpha_x^2\epsilon_{yy} + b_4\alpha_y^2\epsilon_{yy} \\ &\quad + b_5\alpha_x^2\epsilon_{zz} + b_6\alpha_y^2\epsilon_{zz} + 2b_7\alpha_x\alpha_y\epsilon_{xy} + 2b_8\alpha_x\alpha_z\epsilon_{xz} + 2b_9\alpha_y\alpha_z\epsilon_{yz},\end{aligned}$$



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

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

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

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

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

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

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

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

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

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

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

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

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

Orthorhombic

# Workflow (-mode 1)

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

Mason convention



MAELAS uses the same lattice convention as AELAS code:

$$c < a < b$$

$$\mathbf{F} \Big|_{\beta=(1,0,0)}^{\lambda_2}(s) = \mathbf{F} \Big|_{\beta=(1,0,0)}^{\lambda_1}(s) = \begin{pmatrix} 1+s & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+s}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+s}} \end{pmatrix}$$

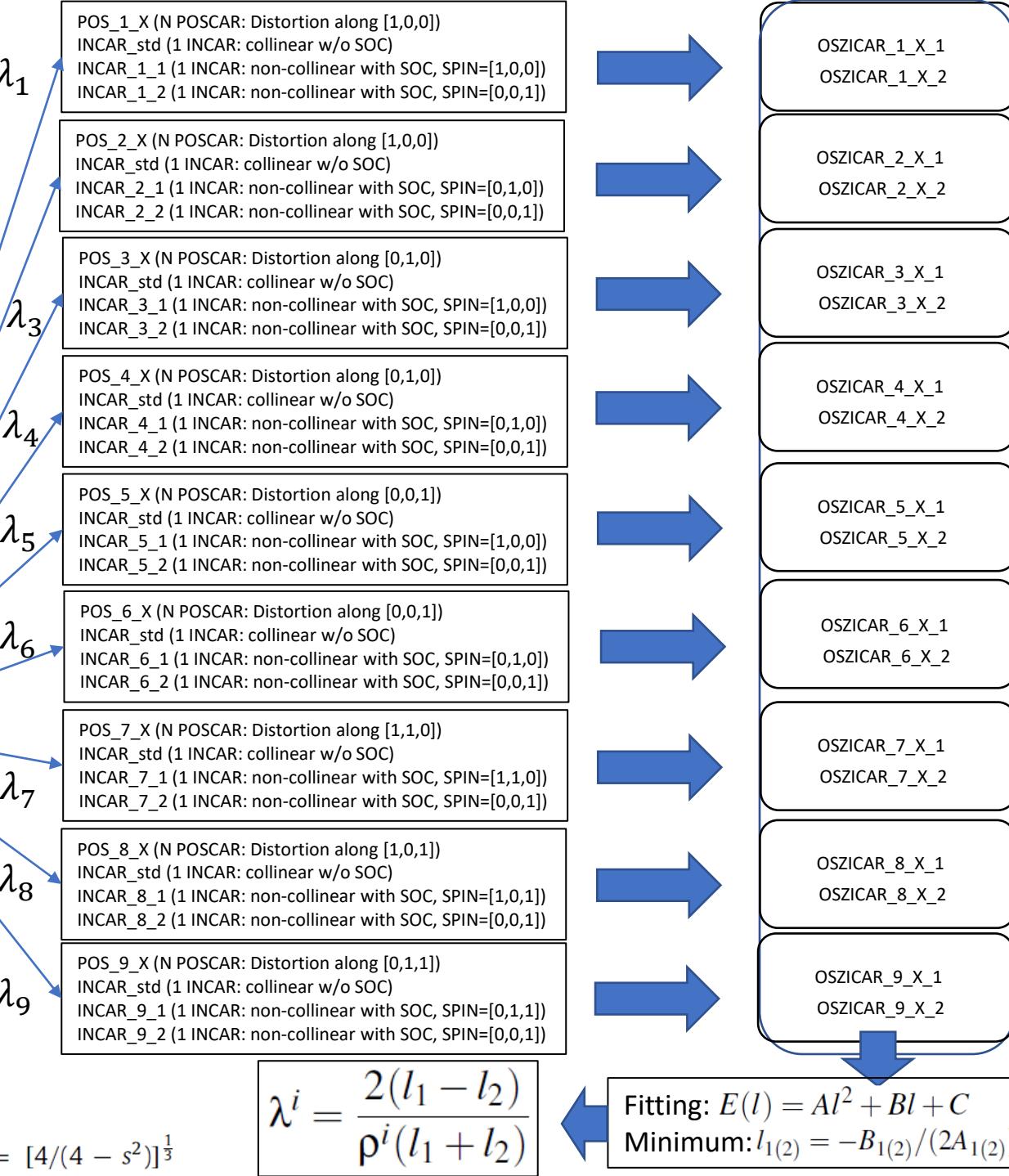
$$\mathbf{F} \Big|_{\beta=(0,1,0)}^{\lambda_4}(s) = \mathbf{F} \Big|_{\beta=(0,1,0)}^{\lambda_3}(s) = \begin{pmatrix} \frac{1}{\sqrt{1+s}} & 0 & 0 \\ 0 & 1+s & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+s}} \end{pmatrix}$$

$$\mathbf{F} \Big|_{\beta=(0,0,1)}^{\lambda_6}(s) = \mathbf{F} \Big|_{\beta=(0,0,1)}^{\lambda_5}(s) = \begin{pmatrix} \frac{1}{\sqrt{1+s}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+s}} & 0 \\ 0 & 0 & 1+s \end{pmatrix}$$

$$\mathbf{F} \Big|_{\beta=\frac{(a,b,0)}{\sqrt{a^2+b^2}}}^{\lambda_7}(s) = \Omega \begin{pmatrix} 1 & \frac{sb}{2a} & 0 \\ \frac{sa}{2b} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\mathbf{F} \Big|_{\beta=\frac{(a,0,c)}{\sqrt{a^2+c^2}}}^{\lambda_8}(s) = \Omega \begin{pmatrix} 1 & 0 & \frac{sc}{2a} \\ 0 & 1 & 0 \\ \frac{sa}{2c} & 0 & 1 \end{pmatrix}$$

$$\mathbf{F} \Big|_{\beta=\frac{(0,b,c)}{\sqrt{b^2+c^2}}}^{\lambda_9}(s) = \Omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{sc}{2b} \\ 0 & \frac{sb}{2c} & 1 \end{pmatrix}$$



Orthorhombic

# Workflow (-mode 2)

$$\frac{E_{me}^{ortho}}{V_0} = b_{01}\epsilon_{xx} + b_{02}\epsilon_{yy} + b_{03}\epsilon_{zz} + b_1\alpha_x^2\epsilon_{xx} + b_2\alpha_y^2\epsilon_{xx} + b_3\alpha_x^2\epsilon_{yy} + b_4\alpha_y^2\epsilon_{yy} + b_5\alpha_x^2\epsilon_{zz} + b_6\alpha_y^2\epsilon_{zz} + 2b_7\alpha_x\alpha_y\epsilon_{xy} + 2b_8\alpha_x\alpha_z\epsilon_{xz} + 2b_9\alpha_y\alpha_z\epsilon_{yz},$$

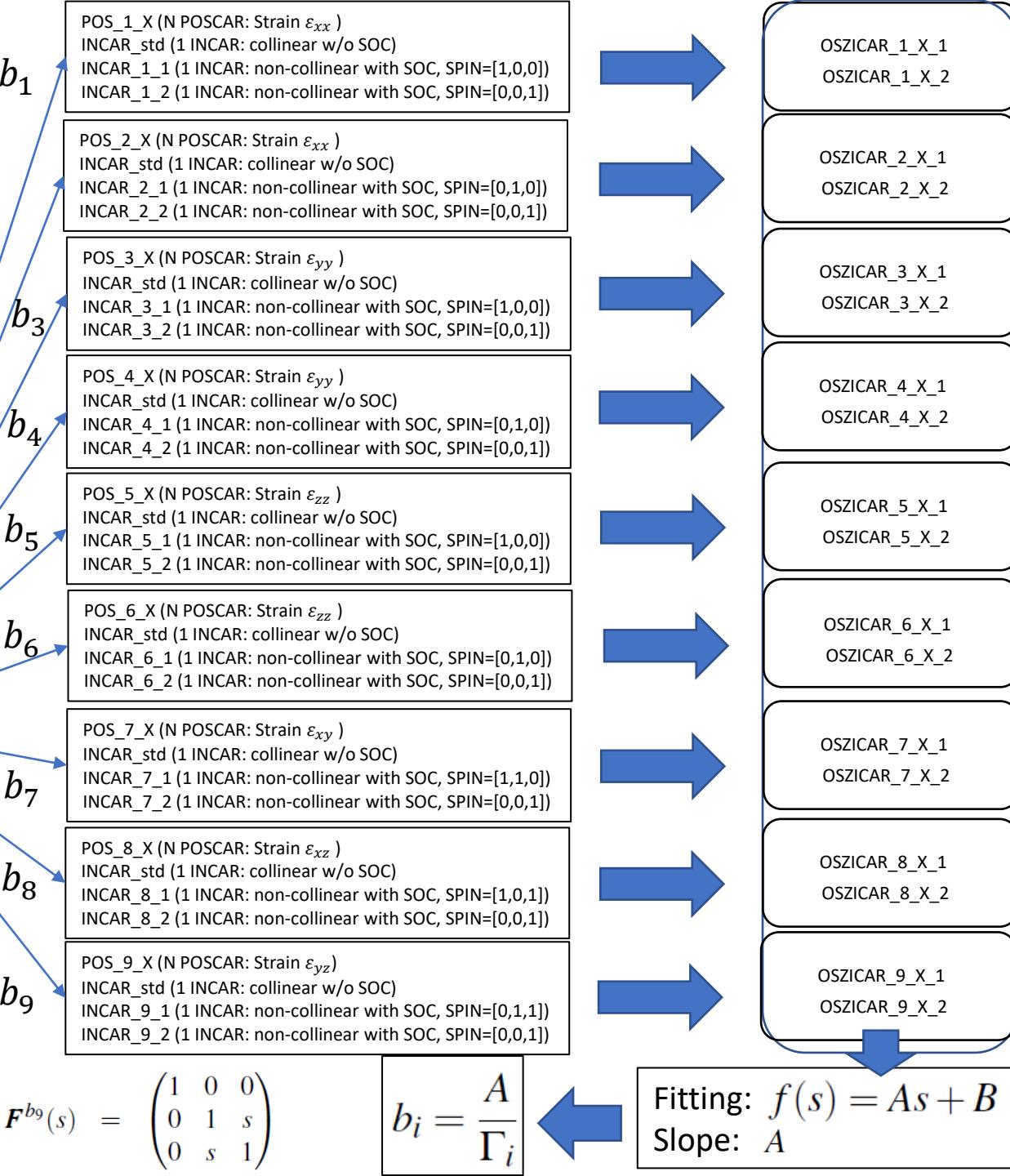


MAELAS uses the same lattice convention as AELAS code:

$$c < a < b$$

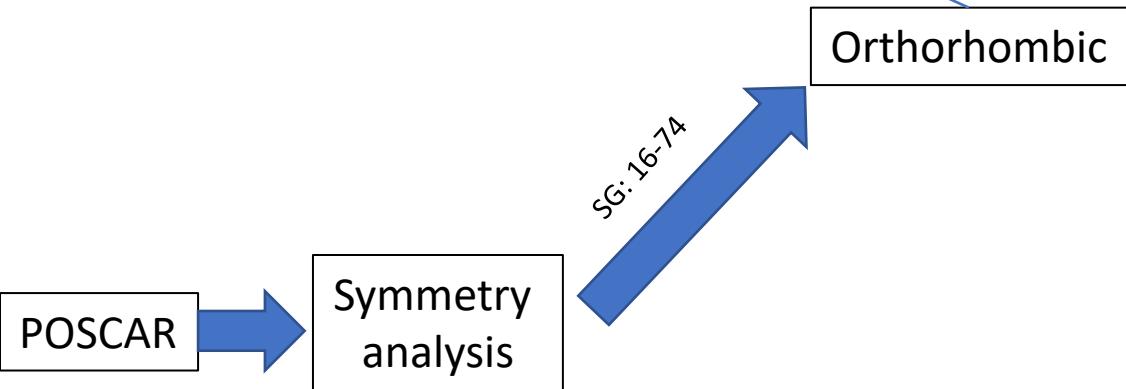
$$\mathbf{F}^{b_1}(s) = \mathbf{F}^{b_2}(s) = \begin{pmatrix} 1+s & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_5}(s) = \mathbf{F}^{b_6}(s) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+s \end{pmatrix}$$

$$\mathbf{F}^{b_3}(s) = \mathbf{F}^{b_4}(s) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+s & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_7}(s) = \begin{pmatrix} 1 & s & 0 \\ s & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_8}(s) = \begin{pmatrix} 1 & 0 & s \\ 0 & 1 & 0 \\ s & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_9}(s) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & s \\ 0 & s & 1 \end{pmatrix}$$



### Spin-polarized calculation **without SOC**

$$E_{me}^{iso} = \frac{1}{3} b_1^{\alpha,0} (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \frac{\sqrt{2}}{3} b_2^{\alpha,0} \left( \varepsilon_{zz} - \frac{\varepsilon_{xx} + \varepsilon_{yy}}{2} \right) + \frac{1}{\sqrt{6}} b_3^{\alpha,0} (\varepsilon_{xx} - \varepsilon_{yy})$$



Not volume-conserving transformations  
(determinant of deformation gradient is not equal to 1,  $\det(F) \neq 1$ )

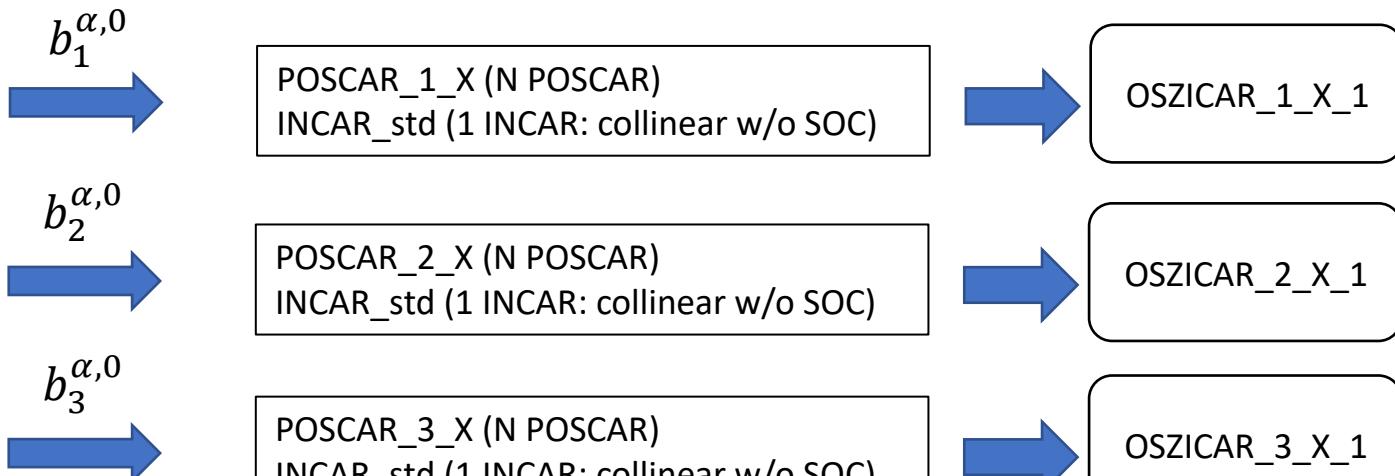
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

The maximum value of  $s$  is set with tag `-s`

## Workflow (-mode 3)

This convention fully decouples isotropic and anisotropic interactions

E. D. T. de Lacheisserie, Magnetostriiction: Theory and Application of Magnetoelasticity (CRC Press, Boca Raton, FL, 1993)



$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

$$\text{Fitting: } f(s) = As^3 + Bs^2 + Cs + D$$

$$\varepsilon^{b_1^{\alpha,0}} = \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & s \end{pmatrix} \quad \varepsilon^{b_2^{\alpha,0}} = \begin{pmatrix} -s/2 & 0 & 0 \\ 0 & -s/2 & 0 \\ 0 & 0 & s \end{pmatrix} \quad \varepsilon^{b_3^{\alpha,0}} = \begin{pmatrix} s & 0 & 0 \\ 0 & -s & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

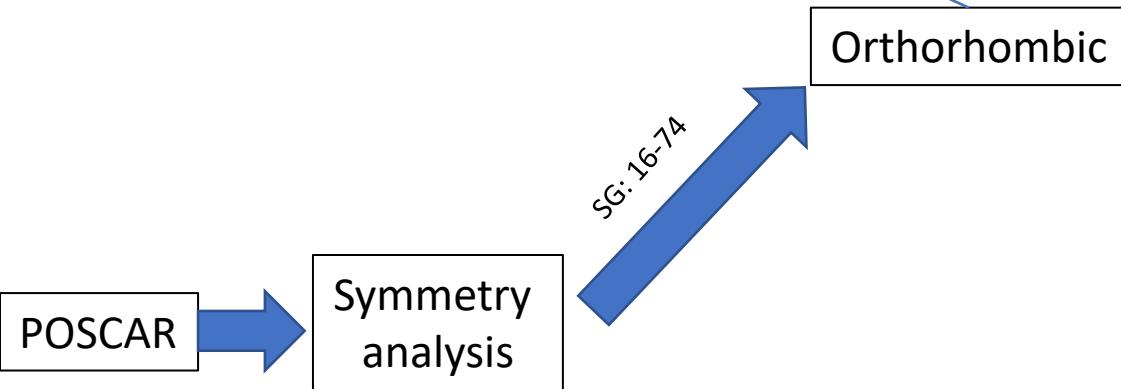
Spontaneous volume magnetostriiction (isotropic contribution):

$$\omega_S^{iso} \simeq \lambda_a + \lambda_b + \lambda_c = \lambda_1^{\alpha,0} \quad \text{Lacheisserie convention}$$

$$b_k^{iso} = \frac{C}{\Gamma_k}$$

### Spin-polarized calculation **with SOC**

$$E_{me}^{iso} = \frac{1}{3} b_1^{\alpha,0} (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \frac{\sqrt{2}}{3} b_2^{\alpha,0} \left( \varepsilon_{zz} - \frac{\varepsilon_{xx} + \varepsilon_{yy}}{2} \right) + \frac{1}{\sqrt{6}} b_3^{\alpha,0} (\varepsilon_{xx} - \varepsilon_{yy})$$



Not volume-conserving transformations  
(determinant of deformation gradient is not equal to 1,  $\det(F) \neq 1$ )

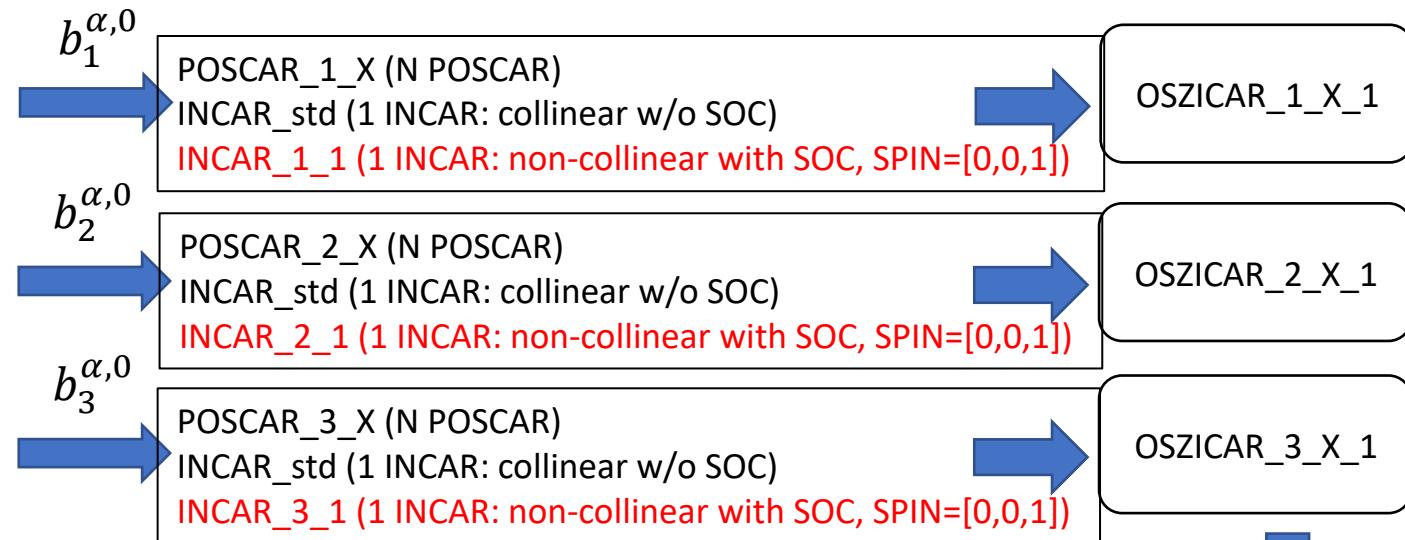
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

The maximum value of s is set with tag -s

## Workflow (-mode 3 including anisotropic magnetic interactions)

This convention fully decouples isotropic and anisotropic interactions

E. D. T. de Lacheisserie, Magnetostriiction: Theory and Application of Magnetoelasticity (CRC Press, Boca Raton, FL, 1993)



$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1) & F_{yz}+F_{zy} \\ F_{xz}+F_{zx} & F_{yz}+F_{zy} & 2(F_{zz}-1) \end{pmatrix}$$

$$\text{Fitting: } f(s) = As^3 + Bs^2 + Cs + D$$

(it requires file MAGANI generated in -mode 2)

$$\varepsilon^{b_1^{\alpha,0}} = \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & s \end{pmatrix} \quad \varepsilon^{b_2^{\alpha,0}} = \begin{pmatrix} -s/2 & 0 & 0 \\ 0 & -s/2 & 0 \\ 0 & 0 & s \end{pmatrix} \quad \varepsilon^{b_3^{\alpha,0}} = \begin{pmatrix} s & 0 & 0 \\ 0 & -s & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Spontaneous volume magnetostriiction (isotropic contribution):

$$\omega_S^{iso} \simeq \lambda_a + \lambda_b + \lambda_c = \lambda_1^{\alpha,0} \quad \text{Lacheisserie convention}$$

$$b_i^{iso} = \frac{C - \Lambda_i(b^{ani})}{\Gamma_i}$$

# BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

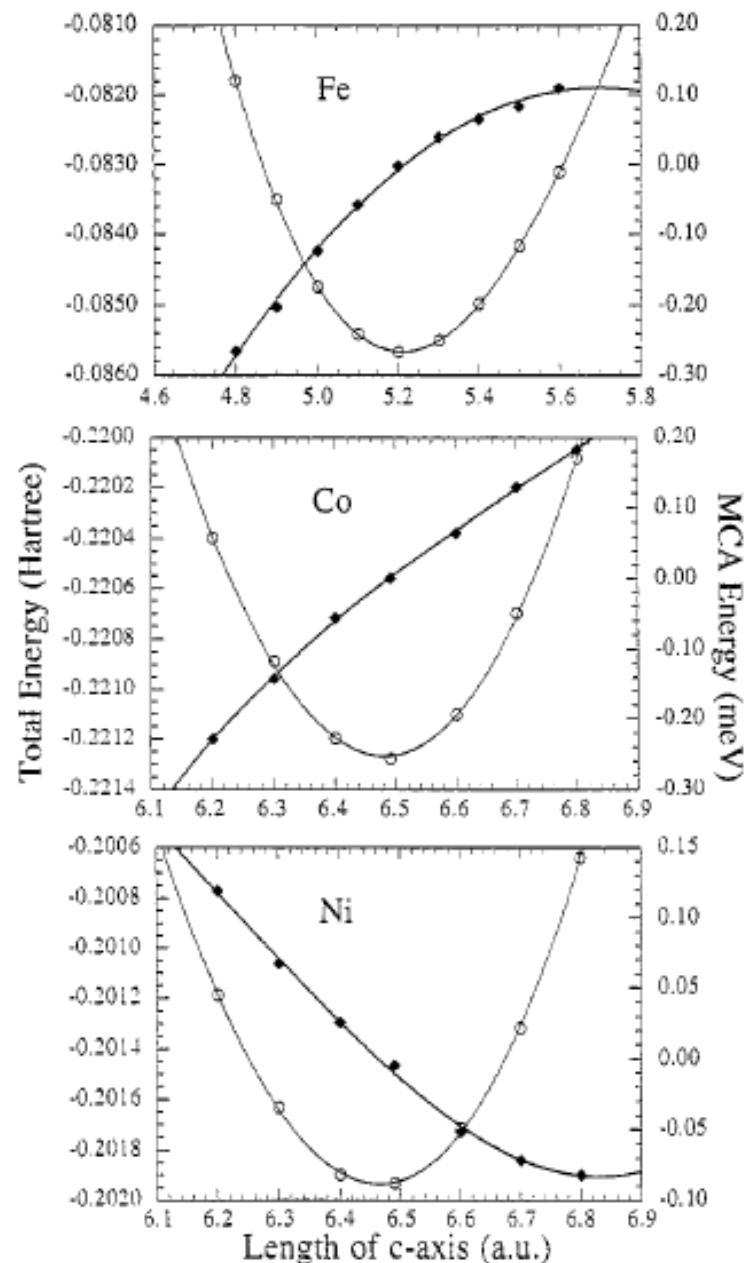
## Cubic systems: Itinerant magnets

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

	$a$ (a.u.)	$\sigma$	$M_s(\mu_B)$	$M_L(\mu_B)$	$\lambda_{001}(10^{-6})$
<b>bcc Fe</b>					
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
<b>fcc Co</b>					
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
<b>fcc Ni</b>					
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.

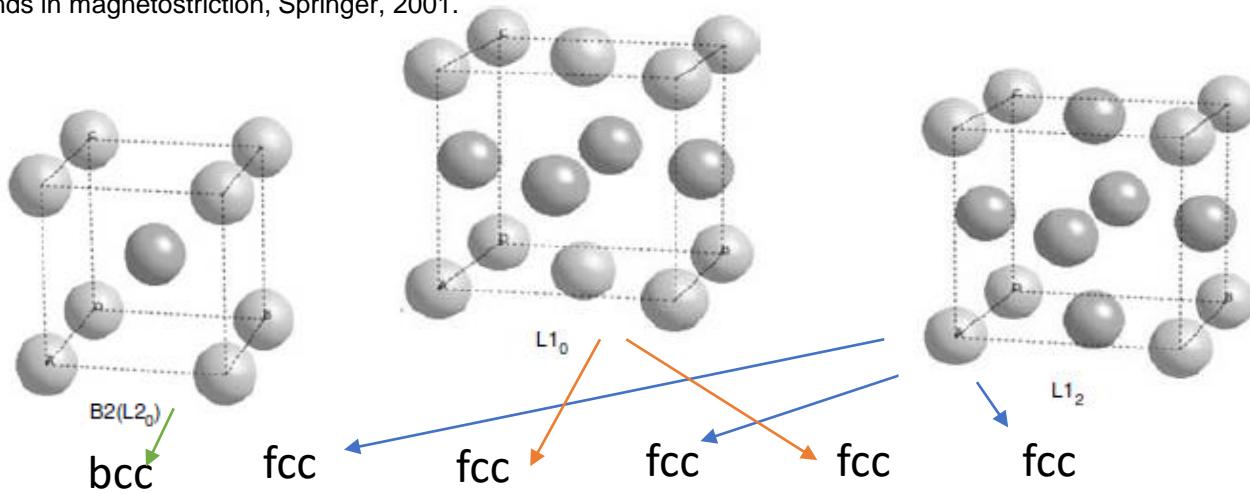
	$T = 4.2\text{ K}$		Room Temperature		
	$\lambda_{100}(\lambda^{z,2})$	$\lambda_{111}(\lambda^{z,2})$	$\lambda_{100}(\lambda^{z,2})$	$\lambda_{111}(\lambda^{z,2})$	Polycrystal $\lambda_s$
<i>3d Metals</i>					
BCC-Fe	26	-30	21	-21	-7
HCP-Co <sup>a</sup>	(-150)	(45)	(-140)	(50)	(-62)
FCC-Ni	-60	-35	-46	-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



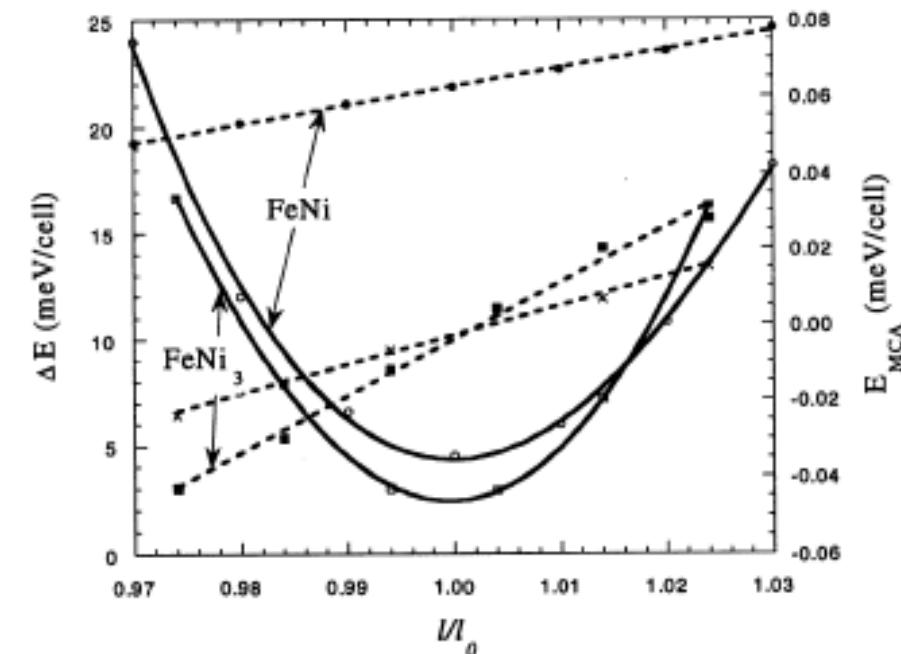
# BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

## Cubic systems: Itinerant 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 (5.39)	6.70	6.76 (6.76)	6.70 (6.71)	6.62 (6.67)	6.66 (6.65)
c (a.u.)	5.38 (5.39)	6.70	6.76 (6.76)	6.70 (6.71)	6.78 (6.67)	6.66 (6.65)
E <sub>MCA</sub> (μeV)	0	0	63	0	143	0
σ	-0.35	-0.36	-0.33	-0.35	-0.34	-0.36
λ <sub>001</sub> (10 <sup>-6</sup> )	83 (125)	-68 (12)	10 (13)	27 (13)	42 (42-100)	33



# BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

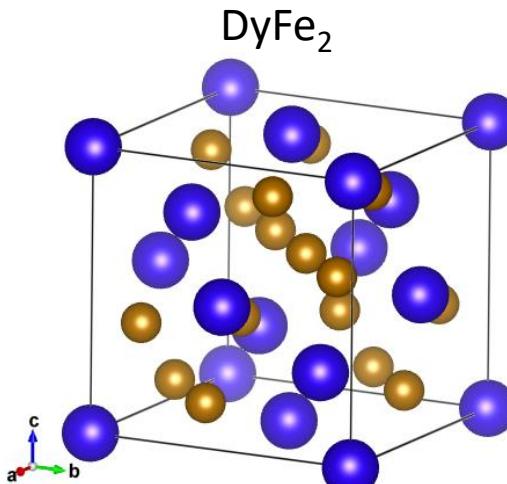
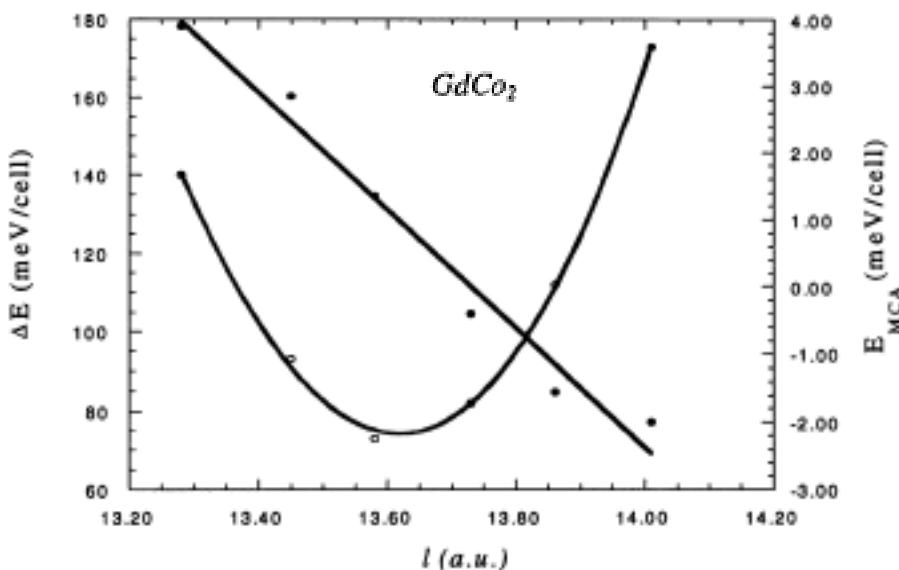
G. Engdahl, Handbook of giant magnetostrictive materials, Academic Press, 1999

## Cubic systems: Rare-Earth magnets

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

### C15 cubic Laves phase

	Theory	Experiment
$\lambda_{001}$ ( $\text{GdCo}_2$ )	-407	-1200
$\lambda_{111}$ ( $\text{GdCo}_2$ )	19	< 10
$\lambda_{001}$ ( $\text{SmCo}_2$ )	-290	---
$\lambda_{001}$ ( $\text{ErCo}_2$ )	-516	-1000
$\lambda_{001}$ ( $\text{GdFe}_2$ )	44	39



**Table 16-10.** Low-temperature magnetostriction constants for  $\text{RCO}_2$  crystals [from Levitin and Markosyan (1990) unless otherwise noted].

R in $\text{RCO}_2$	$10^6 \lambda_{111}$	$10^6 \lambda_{100}$	$T_c$ (K) <sup>a</sup>
Gd	$< 10^{-5}$	-1200	409
Tb	4500	-1200 <sup>b</sup>	256
Dy	5000 <sup>b, c</sup>	-2000 <sup>d</sup> -1300 <sup>e</sup>	159
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	$\lambda_{111} (10^{-6})$	$\lambda_{100} (10^{-6})$	$T_c$ (K)
$\text{NdAl}_2$	—	-700	61
$\text{TbAl}_2$	-3000	—	114
$\text{DyAl}_2$	—	-1700	68
$\text{TbMn}_2$	-3000	—	40
$\text{TbFe}_2$	4000, 4500	—	711
$\text{DyFe}_2$	—	-70	635
$\text{HoFe}_2$	—	-750	612
$\text{TmFe}_2$	-3500, -2600	—	610
$\text{TbCo}_2$	4400	—	256
$\text{DyCo}_2$	—	-2000	159
$\text{HoCo}_2$	—	-2200	85
$\text{ErCo}_2$	-2500	—	36
$\text{TbNi}_2$	1500	—	45
$\text{DyNi}_2$	—	-1300	30
$\text{HoNi}_2$	—	-1000	22

**Table 1.7.** Magnitudes of Single-Crystal Magnetostriction in Rare Earth- $\text{Fe}_2$  Compounds

Compound	$\frac{1}{2}\lambda_{111} (10^{-6})$ (calculated at 0 K)	$\frac{1}{2}\lambda_{111} (10^{-6})$ (measured at room temperature)	$T_c$
$\text{SmFe}_2$	-4800	-3150	676
$\text{TbFe}_2$	6600	3690	697, 711
$\text{DyFe}_2$	6300	1890	635
$\text{HoFe}_2$	2400	288	606
$\text{ErFe}_2$	-2250	-450	590, 597
$\text{TmFe}_2$	-5550	-315	560

# BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

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

Element	$\lambda_1^{\alpha,2}$	$\lambda_2^{\alpha,2}$	$\lambda^{\gamma,2}$	$\lambda^{\epsilon,2}$	$\lambda_1^{\alpha,0} - \frac{1}{3}\lambda_1^{\alpha,2}$	$\lambda_2^{\alpha,0} - \frac{1}{3}\lambda_2^{\alpha,2}$	$\lambda^{\gamma,4}$
<b>Hexagonal Rare-Earth</b>	<b>Gadolinium<sup>a)</sup></b>	<b>0.14</b>	<b>-0.13</b>	<b>0.11</b>	<b>0.02</b>	-	-
	<b>Terbium<sup>b)</sup></b>	<b>-2.6<sup>c)</sup></b>	<b>9.0<sup>c)</sup></b>	<b>8.7</b>	<b>15.0<sup>c)</sup></b>	<b>-0.8</b>	<b>4.3</b>
	<b>Dysprosium<sup>b)</sup></b>	-	-	<b>9.4</b>	<b>5.5</b>	<b>-2.0</b>	<b>7.3</b>
	<b>Holmium<sup>b)</sup></b>	-	-	<b>2.5<sup>c)</sup></b>	-	<b>-3.9</b>	<b>7.1</b>
	<b>Erbium<sup>b)</sup></b>	-	-	<b>-5.1<sup>c)</sup></b>	-	<b>+0.3</b>	<b>6.2</b>

<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.

Table 14.4. Magnetostriiction constants of spinel-type ferrites (mainly after Tsuya<sup>49</sup>).

Composition	$\lambda_{100}$	$\lambda_{111}$	Temp.	Ref.
MnFe <sub>2</sub> O <sub>4</sub>	$-31 \times 10^{-6}$	$6.5 \times 10^{-6}$		38
Fe <sub>3</sub> O <sub>4</sub>	-20	78	20°C	39
Co <sub>0.8</sub> Fe <sub>2.2</sub> O <sub>4</sub>	-590	120	20°C	40
NiFe <sub>2</sub> O <sub>4</sub>	-42	-14		41
CuFe <sub>2</sub> O <sub>4</sub>	-57.5	4.7		42
MgFe <sub>2</sub> O <sub>4</sub>	-10.5	1.7		41
Li <sub>0.5</sub> Fe <sub>2.5</sub> O <sub>4</sub>	-26	-3.8		38
Mn <sub>0.6</sub> Fe <sub>2.4</sub> O <sub>4</sub>	-5	45	20°C	43
Mn <sub>0.28</sub> Zn <sub>0.16</sub> Fe <sub>2.37</sub> O <sub>4</sub>	-0.5	36		44
Mn <sub>1.04</sub> Zn <sub>0.22</sub> Fe <sub>1.82</sub> O <sub>4</sub>	-22	3		44
Mg <sub>0.63</sub> Fe <sub>1.26</sub> Mn <sub>1.11</sub> O <sub>4</sub>	49.5	-2.6		45
Co <sub>0.32</sub> Zn <sub>0.22</sub> Fe <sub>2.2</sub> O <sub>4</sub>	-210	110		40
Co <sub>0.1</sub> Ni <sub>0.9</sub> Fe <sub>2</sub> O <sub>4</sub>	-109	-38.6		46
Li <sub>0.43</sub> Zn <sub>0.14</sub> Fe <sub>2.07</sub> O <sub>4</sub>	-27.1	3.2		41
Li <sub>0.5</sub> Al <sub>0.35</sub> Fe <sub>2.15</sub> O <sub>4</sub>	-19.1	0.2		47
Li <sub>0.56</sub> Ti <sub>0.10</sub> Fe <sub>2.35</sub> O <sub>4</sub>	-16.0	4.3		47
Li <sub>0.5</sub> Ga <sub>1.4</sub> Fe <sub>1.1</sub> O <sub>4</sub>	-12.3	2.9		47
Ti <sub>0.18</sub> Fe <sub>2.82</sub> O <sub>4</sub>	47	109	290 K	48
		142	80 K	48
Ti <sub>0.56</sub> Fe <sub>2.44</sub> O <sub>4</sub>	170	92	290 K	48
	990	(330)	80 K	48

# ANALYSIS OF THE ACCURACY OF THE METHODS IN MAELAS

$$b_i^{\text{Rel. Error}} (\%) = \frac{b_i^{\text{exact}} - b_i^{\text{MAELAS}}}{b_i^{\text{exact}}} \times 100,$$

$$\lambda_i^{\text{Rel. Error}} (\%) = \frac{\lambda_i^{\text{exact}} - \lambda_i^{\text{MAELAS}}}{\lambda_i^{\text{exact}}} \times 100.$$

$$E^{\text{exact}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = E_{el}^{\text{exact}}(\boldsymbol{\varepsilon}) + E_{me}^{\text{exact}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}).$$



We can estimate this error using the theoretical equation for the elastic and magnetoelastic energies (exact energy)

Methodology

Source of errors in MAELAS

Evaluation of energies (DFT)

The method -mode 2 is more accurate than -mode 1, especially for non-cubic crystals.

Table 2: Summary of the analysis of the accuracy of the methods implemented in MAELAS.

Crystal system	$C_{ij}$	$C_{ij}^{\text{exact}}$ (GPa)	$b$	$b^{\text{exact}}$ (MPa)	$\lambda$	$\lambda^{\text{exact}}$ ( $\times 10^{-6}$ )	-mode 1 $b^{\text{Rel. Error}}$ (%)	-mode 1 $\lambda^{\text{Rel. Error}}$ (%)	-mode 2 $b^{\text{Rel. Error}}$ (%)	-mode 2 $\lambda^{\text{Rel. Error}}$ (%)
Cubic (I) $a = 2.8293\text{\AA}$	$C_{11}$	243	$b_1$	-4.1	$\lambda_{001}$	26.0317	0.015	0.013	$7 \cdot 10^{-6}$	$8 \cdot 10^{-6}$
	$C_{12}$	138	$b_2$	10.9	$\lambda_{111}$	-29.7814	0.005	0.004	$6 \cdot 10^{-6}$	$3 \cdot 10^{-6}$
	$C_{44}$	122								
Hexagonal (I) $a = 2.4561\text{\AA}$ $c = 3.9821\text{\AA}$	$C_{11}$	307	$b_{21}$	-31.9	$\lambda^{\alpha 1,2}$	95.0656	-17.6	-17.6	$6 \cdot 10^{-6}$	$1 \cdot 10^{-5}$
	$C_{12}$	165	$b_{22}$	25.5	$\lambda^{\alpha 2,2}$	-125.9316	-17.4	-17.5	$8 \cdot 10^{-6}$	$2 \cdot 10^{-5}$
	$C_{13}$	103	$b_3$	-8.1	$\lambda^{\gamma,2}$	57.0423	17.0	17.0	$6 \cdot 10^{-6}$	$6 \cdot 10^{-6}$
	$C_{33}$	358	$b_4$	42.9	$\lambda^{\epsilon,2}$	-286.0	0.002	0.002	$5 \cdot 10^{-6}$	$7 \cdot 10^{-6}$
	$C_{44}$	75								
Trigonal (I) $a = 3.9249\text{\AA}$ $c = 4.8311\text{\AA}$	$C_{11}$	428	$b_{21}$	43.1	$\lambda^{\alpha 1,2}$	-104.9605	22.9	10.8	$1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
	$C_{12}$	164	$b_{22}$	-34.2	$\lambda^{\alpha 2,2}$	143.1326	-38.6	-16.4	$1 \cdot 10^{-5}$	$8 \cdot 10^{-5}$
	$C_{13}$	133	$b_3$	60.7	$\lambda^{\gamma,1}$	-202.6605	-11.9	-8.8	$1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
	$C_{14}$	-27	$b_4$	-34.3	$\lambda^{\gamma,2}$	204.2029	-15.8	-42.3	$1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
	$C_{33}$	434	$b_{14}$	-42.4	$\lambda_{12}$	-377.9282	-28.1	46.8	$1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
	$C_{44}$	118	$b_{34}$	55.4	$\lambda_{21}$	266.5791	37.9	-34.8	$1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
Tetragonal (I) $a = 2.6973\text{\AA}$ $c = 3.7593\text{\AA}$	$C_{11}$	324	$b_{21}$	-2.4	$\lambda^{\alpha 1,2}$	-20.4581	42.4	7.3	$8 \cdot 10^{-6}$	$-2 \cdot 10^{-5}$
	$C_{12}$	67	$b_{22}$	-15.2	$\lambda^{\alpha 2,2}$	78.1888	18.3	15.4	$6 \cdot 10^{-6}$	$-4 \cdot 10^{-5}$
	$C_{13}$	133	$b_3$	-7.9	$\lambda^{\gamma,2}$	30.7393	-14.2	-14.2	$6 \cdot 10^{-6}$	$-2 \cdot 10^{-5}$
	$C_{33}$	264	$b_4$	-5.6	$\lambda^{\epsilon,2}$	27.7228	0.002	0.002	$5 \cdot 10^{-6}$	$7 \cdot 10^{-6}$
	$C_{44}$	101	$b'_3$	-7.9	$\lambda^{\delta,2}$	106.7568	0.007	0.007	$5 \cdot 10^{-6}$	$6 \cdot 10^{-6}$
	$C_{66}$	37								
Orthorhombic $a = 4.0686\text{\AA}$ $b = 10.3157\text{\AA}$ $c = 3.8956\text{\AA}$	$C_{11}$	76	$b_1$	43.1	$\lambda_1$	-632.9614	37.4	24.7	$7 \cdot 10^{-6}$	$5 \cdot 10^{-6}$
	$C_{12}$	45	$b_2$	-34.2	$\lambda_2$	681.5787	6.9	7.9	$6 \cdot 10^{-6}$	$6 \cdot 10^{-6}$
	$C_{13}$	48	$b_3$	60.7	$\lambda_3$	-752.4503	19.6	0.03	$7 \cdot 10^{-6}$	$7 \cdot 10^{-6}$
	$C_{23}$	55	$b_4$	-34.3	$\lambda_4$	471.7839	-11.6	-18.5	$6 \cdot 10^{-6}$	$6 \cdot 10^{-6}$
	$C_{22}$	102	$b_5$	-42.4	$\lambda_5$	809.6944	-46.8	-10.8	$7 \cdot 10^{-6}$	$5 \cdot 10^{-6}$
	$C_{33}$	141	$b_6$	55.4	$\lambda_6$	-808.9638	-7.6	-5.6	$6 \cdot 10^{-6}$	$6 \cdot 10^{-6}$
	$C_{44}$	40	$b_7$	35.4	$\lambda_7$	-284.9353	47.3	54.3	$6 \cdot 10^{-6}$	$7 \cdot 10^{-6}$
	$C_{55}$	27	$b_8$	-22.6	$\lambda_8$	253.4425	43.2	11.6	$9 \cdot 10^{-6}$	$8 \cdot 10^{-6}$
	$C_{66}$	39	$b_9$	38.7	$\lambda_9$	-326.1699	-119.8	-85.6	$5 \cdot 10^{-6}$	$2 \cdot 10^{-5}$

# MAELAS TESTS

Table 3: Anisotropic magnetostrictive coefficients and magnetoelastic constants calculated with the two methods (-mode 1 and -mode 2) available in MAELAS v2.0. In parenthesis we show the magnetostrictive coefficients with Mason's definitions [1, 8]. These data correspond to the simulations with the same VASP settings, relaxed unit cell and elastic constants as in Ref. [1]. For  $\text{Fe}_2\text{Si}$  we repeated the calculations with -mode 1 as implemented in version 2.0 [v2.0], that is, including the corrections described in Section 2.2.

Material	Crystal system	DFT Exchange Correlation	Magnetostrictive coefficient	MAELAS -mode 1 ( $\times 10^{-6}$ )	MAELAS -mode 2 ( $\times 10^{-6}$ )	Expt. ( $\times 10^{-6}$ )	Magnetoelastic constant	MAELAS -mode 1 (MPa)	MAELAS -mode 2 (MPa)	Expt. (MPa)
FCC Ni	Cubic (I) SG 225	GGA	$\lambda_{001}$	-78.4 <sup>b</sup>	-72.7	-60 <sup>a</sup>	$b_1$	15.5 <sup>b</sup>	14.4	9.9 <sup>b</sup>
			$\lambda_{111}$	-46.1 <sup>b</sup>	-44.0	-35 <sup>a</sup>	$b_2$	19.4 <sup>b</sup>	18.5	13.9 <sup>b</sup>
BCC Fe	Cubic (I) SG 229	GGA	$\lambda_{001}$	25.7 <sup>b</sup>	29.1	26 <sup>a</sup>	$b_1$	-5.2 <sup>b</sup>	-5.9	-4.1 <sup>b</sup>
			$\lambda_{111}$	17.2 <sup>b</sup>	15.7	-30 <sup>a</sup>	$b_2$	-5.3 <sup>b</sup>	-4.9	10.9 <sup>b</sup>
HCP Co	Hexagonal (I) SG 194	LSDA+U $J = 0.8\text{eV}$ $U = 3\text{eV}$	$\lambda^{a1,2} (\lambda_A)$	111 (-109) <sup>b</sup>	75 (-74)	95 (-66) <sup>c</sup>	$b_{21}$	-21.3 <sup>b</sup>	-16.2	-31.9 <sup>b</sup>
			$\lambda^{a2,2} (\lambda_B)$	-251 (-114) <sup>b</sup>	-156 (-77)	-126 (-123) <sup>c</sup>	$b_{22}$	48.3 <sup>b</sup>	28.4	25.5 <sup>b</sup>
			$\lambda^{c1,2} (\lambda_C)$	4 (251) <sup>b</sup>	2 (156)	57 (126) <sup>c</sup>	$b_3$	-0.7 <sup>b</sup>	-0.4	-8.1 <sup>b</sup>
			$\lambda^{c2,2} (\lambda_D)$	-51 (10) <sup>b</sup>	-57 (-8)	-286 (-128) <sup>c</sup>	$b_4$	7.1 <sup>b</sup>	7.9	42.9 <sup>b</sup>
$\text{Fe}_2\text{Si}$	Trigonal (I) SG 164	GGA	$\lambda^{a1,2}$	-9 <sup>b</sup> [v1.0]	-5		$b_{21}$	3.1 <sup>b</sup> [v1.0]	0.7	
			$\lambda^{a2,2}$	15 <sup>b</sup> [v1.0]	17		$b_{22}$	-4.2 <sup>b</sup> [v1.0]	-6.2	
			$\lambda^{c1,2}$	8 <sup>b</sup> [v1.0]	6		$b_3$	-0.7 <sup>b</sup> [v1.0]	-1.9	
			$\lambda^{c2,2}$	29 <sup>b</sup> [v1.0]	29		$b_4$	3.3 <sup>b</sup> [v1.0]	-3.5	
			$\lambda_{12}$	-3 <sup>b</sup> [v1.0]	-5		$b_{14}$	-1.4 <sup>b</sup> [v1.0]	1.9	
		GGA	$\lambda_{21}$	-13 <sup>b</sup> [v1.0]	-14		$b_{34}$	-0.4 <sup>b</sup> [v1.0]	1.4	
			$\lambda^{a1,2}$	-9 [v2.0]			$b_{21}$	3.1 [v2.0]		
			$\lambda^{a2,2}$	15 [v2.0]			$b_{22}$	-4.2 [v2.0]		
			$\lambda^{c1,2}$	8 [v2.0]			$b_3$	-2.5 [v2.0]		
			$\lambda^{c2,2}$	29 [v2.0]			$b_4$	-3.7 [v2.0]		
L1 <sub>0</sub> FePd	Tetragonal (I) SG 123	GGA	$\lambda_{12}$	-11 [v2.0]			$b_{14}$	2.0 [v2.0]		
			$\lambda_{21}$	-13 [v2.0]			$b_{34}$	2.2 [v2.0]		
			$\lambda^{a1,2}$	-21 <sup>b</sup>	-41		$b_{21}$	-2.4 <sup>b</sup>	5.1	
			$\lambda^{a2,2}$	79 <sup>b</sup>	82		$b_{22}$	-15.2 <sup>b</sup>	-10.7	
			$\lambda^{c1,2}$	31 <sup>b</sup>	27		$b_3$	-7.9 <sup>b</sup>	-6.9	
YCo	Orthorhombic SG 63	LSDA+U $J = 0.8\text{eV}$ $U = 1.9\text{eV}$	$\lambda^{c2,2}$	28 <sup>b</sup>	26		$b_4$	-5.6 <sup>b</sup>	-5.3	
			$\lambda^{c3,2}$	106 <sup>b</sup>	106		$b'_3$	-7.9 <sup>b</sup>	-7.9	
			$\lambda_1$	-11 <sup>b</sup>	-36		$b_1$	-1.7 <sup>b</sup>	0.8	
			$\lambda_2$	32 <sup>b</sup>	57		$b_2$	1.2 <sup>b</sup>	-2.9	
			$\lambda_3$	70 <sup>b</sup>	75		$b_3$	-3.8 <sup>b</sup>	-2.2	
			$\lambda_4$	-74 <sup>b</sup>	-64		$b_4$	4.3 <sup>b</sup>	0.6	
			$\lambda_5$	-30 <sup>b</sup>	-35		$b_5$	-0.1 <sup>b</sup>	1.7	
			$\lambda_6$	7 <sup>b</sup>	24		$b_6$	2.3 <sup>b</sup>	-2.2	
			$\lambda_7$	36 <sup>b</sup>	38		$b_7$	-4.4 <sup>b</sup>	-4.2	
			$\lambda_8$	-20 <sup>b</sup>	-34		$b_8$	1.1 <sup>b</sup>	1.8	
			$\lambda_9$	35 <sup>b</sup>	-7		$b_9$	-8.7 <sup>b</sup>	-0.5	

<sup>a</sup>Ref.[9], <sup>b</sup>Ref.[1], <sup>c</sup>Ref.[10]

# MAELAS TESTS

Table 4: Isotropic magnetoelastic constants, isotropic magnetostrictive coefficients and isotropic contribution to spontaneous volume magnetostriction calculated with the new method (-mode 3) available in MAELAS v3.0. The symbol [SOC] means that this quantity has been calculated with SOC following the methodology described in Section 2.2, where the anisotropic magnetoelastic constants (required to compute  $\Lambda(b^{ani})$ ) are taken from the publication of version 2.0 [14] using -mode 2. The quantities without symbol [SOC] were calculated without SOC according to the methodology described in Section 2.1. Note that these calculations depend strongly on the lattice parameters which are shown in the first column.

Material	Crystal system	DFT Exchange Correlation	Isotropic magnetoelastic constant	MAELAS -mode 3 (MPa)	Isotropic magnetostrictive coefficient	MAELAS -mode 3 ( $\times 10^{-6}$ )	Spontaneous volume magnetostriction	MAELAS -mode 3 ( $\times 10^{-6}$ )	Expt. ( $\times 10^{-6}$ )
bcc Fe $a_0^{FM} = 2.83099\text{\AA}$	Cubic (I) SG 229	GGA	$b^{\alpha,2}$	-112.5	$\lambda^{\alpha,2}$	194.7	$\omega_s^{iso}$	194.7	400 <sup>a</sup> 3300 <sup>b</sup>
fcc Ni $a_0^{FM} = 3.52048\text{\AA}$	Cubic (I) SG 225	GGA	$b^{\alpha,2}$	-1.3	$\lambda^{\alpha,2}$	2.3	$\omega_s^{iso}$	2.3	375 <sup>c</sup> -510 <sup>d</sup>
hcp Co $a_0^{FM} = 2.48896\text{\AA}$ $c_0^{FM} = 4.02347\text{\AA}$	Hexagonal (I) SG 194	LSDA+U $J = 0.8\text{eV}$ $U = 3\text{eV}$	$b_{11}$ $b_{12}$ $b_{11}[\text{SOC}]$ $b_{12}[\text{SOC}]$	-316.5 -2755.9 -383.2 -2824.2	$\lambda^{\alpha1,0}$ $\lambda^{\alpha2,0}$ $\lambda^{\alpha1,0}[\text{SOC}]$ $\lambda^{\alpha2,0}[\text{SOC}]$	-3953.6 10857.6 -4209.2 10993.9	$\omega_s^{iso}$	2950.2	
Fe <sub>2</sub> Si $a_0^{FM} = 3.9249\text{\AA}$ $c_0^{FM} = 4.8311\text{\AA}$	Trigonal (I) SG 164	GGA	$b_{11}$ $b_{12}$ $b_{11}[\text{SOC}]$ $b_{12}[\text{SOC}]$	-94.1 -83.6 -135.4 -123.3	$\lambda^{\alpha1,0}$ $\lambda^{\alpha2,0}$ $\lambda^{\alpha1,0}[\text{SOC}]$ $\lambda^{\alpha2,0}[\text{SOC}]$	-234.7 110.2 -339.5 166.7	$\omega_s^{iso}$	-359.1	
L1 <sub>0</sub> FePd $a_0^{FM} = 2.6973\text{\AA}$ $c_0^{FM} = 3.7593\text{\AA}$	Tetragonal (I) SG 123	GGA	$b_{11}$ $b_{12}$ $b_{11}[\text{SOC}]$ $b_{12}[\text{SOC}]$	-2123.9 -1993.3 -2086.4 -2004.3	$\lambda^{\alpha1,0}$ $\lambda^{\alpha2,0}$ $\lambda^{\alpha1,0}[\text{SOC}]$ $\lambda^{\alpha2,0}[\text{SOC}]$	-12218.9 3158.2 -12094.7 3370.0	$\omega_s^{iso}$	-21279.7	
YCo $a_0^{FM} = 4.0686\text{\AA}$ $b_0^{FM} = 10.3157\text{\AA}$ $c_0^{FM} = 3.8957\text{\AA}$	Orthorhombic SG 63	LSDA+U $J = 0.8\text{eV}$ $U = 1.9\text{eV}$	$b_1^{\alpha,0}$ $b_2^{\alpha,0}$ $b_3^{\alpha,0}$ $b_1^{\alpha,0}[\text{SOC}]$ $b_2^{\alpha,0}[\text{SOC}]$ $b_3^{\alpha,0}[\text{SOC}]$	-522.3 14.7 85.1 -512.8 -38.1 81.3	$\lambda_1^{\alpha,0}$ $\lambda_2^{\alpha,0}$ $\lambda_3^{\alpha,0}$ $\lambda_1^{\alpha,0}[\text{SOC}]$ $\lambda_2^{\alpha,0}[\text{SOC}]$ $\lambda_3^{\alpha,0}[\text{SOC}]$	2258.8 -946.6 -1171.9 2148.6 -274.6 -1019.8	$\omega_s^{iso}$	2258.8	

# MAELAS TESTS: FCC Ni (-mode 1)

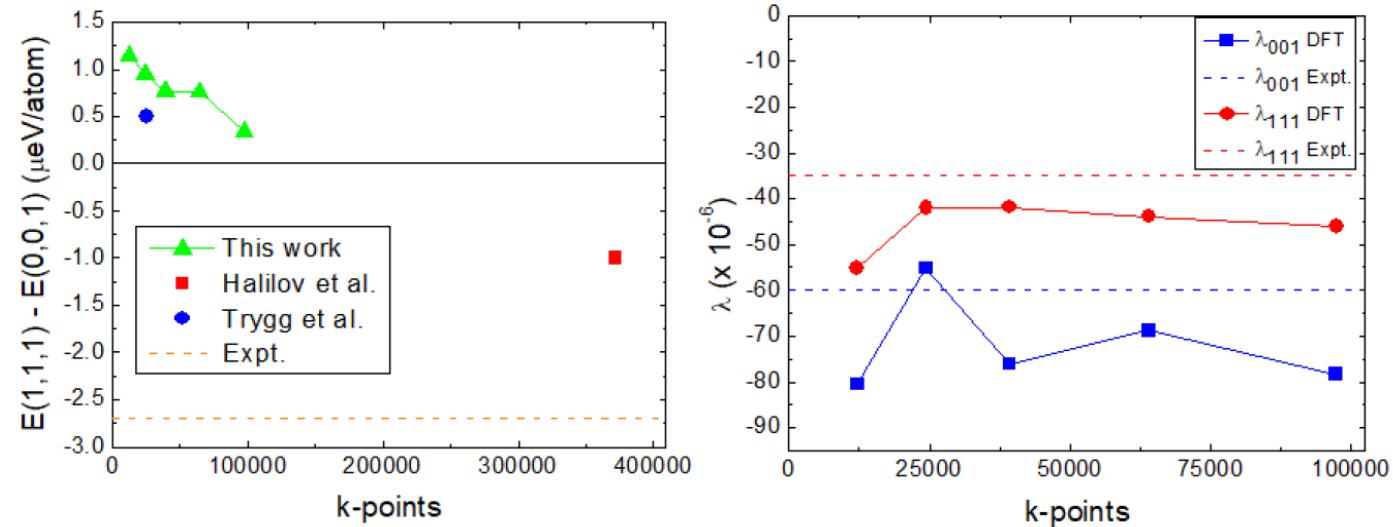


Figure 3: Calculation of (left) MAE of the unstrained unit cell and (right) magnetostrictive coefficients for FCC Ni as a function of k-points.

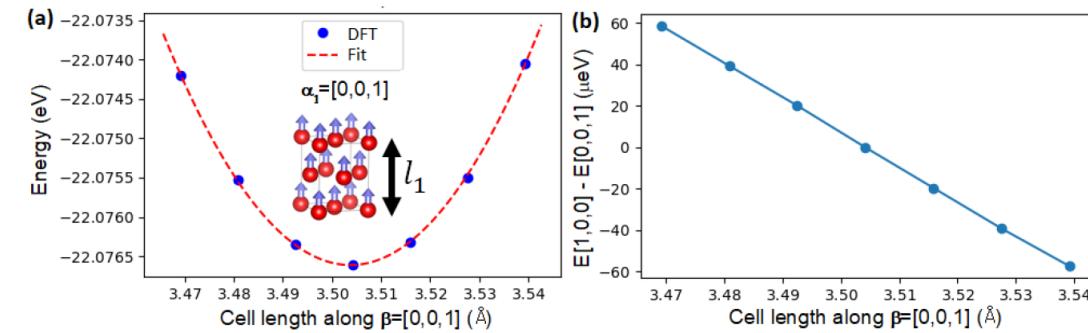


Figure 4: Calculation of  $\lambda_{001}$  for FCC Ni using MAELAS. (Left) Quadratic curve fit to the energy versus cell length along  $\beta = (0, 0, 1)$  with spin direction  $\alpha_1 = (0, 0, 1)$ . (Right) Energy difference between states with spin directions  $\alpha_2 = (1, 0, 0)$  and  $\alpha_1 = (0, 0, 1)$  against the cell length along  $\beta = (0, 0, 1)$ .

# MAELAS TESTS: FCC Ni (-mode 2)

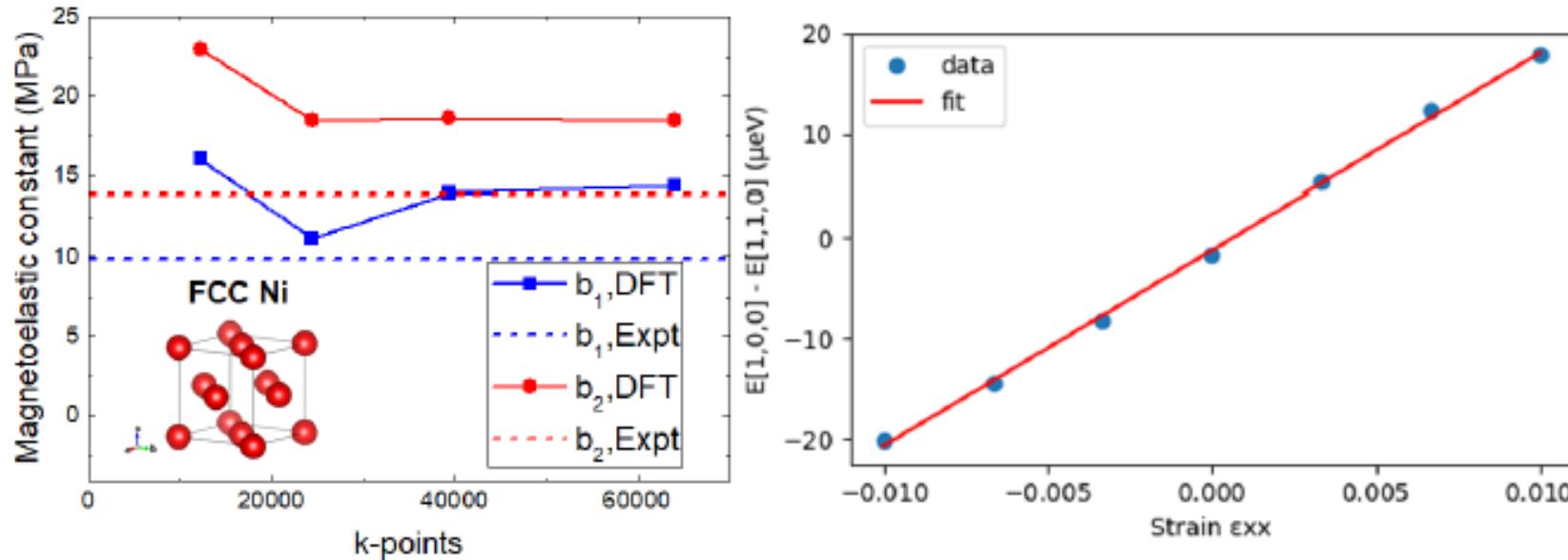


Figure 3: (Left) Calculated magnetoelastic constants for FCC Ni with the new method implemented in MAELAS v2.0 (-mode 2). (Right) Calculation of  $b_1$  for FCC Ni through a linear fitting of the energy difference between magnetization directions  $\alpha_1 = (1, 0, 0)$  and  $\alpha_2 = (1/\sqrt{2}, 1/\sqrt{2}, 0)$  versus strain ( $\epsilon_{xx}$ ) data.

# MAELAS TESTS: BCC Fe (-mode 1)

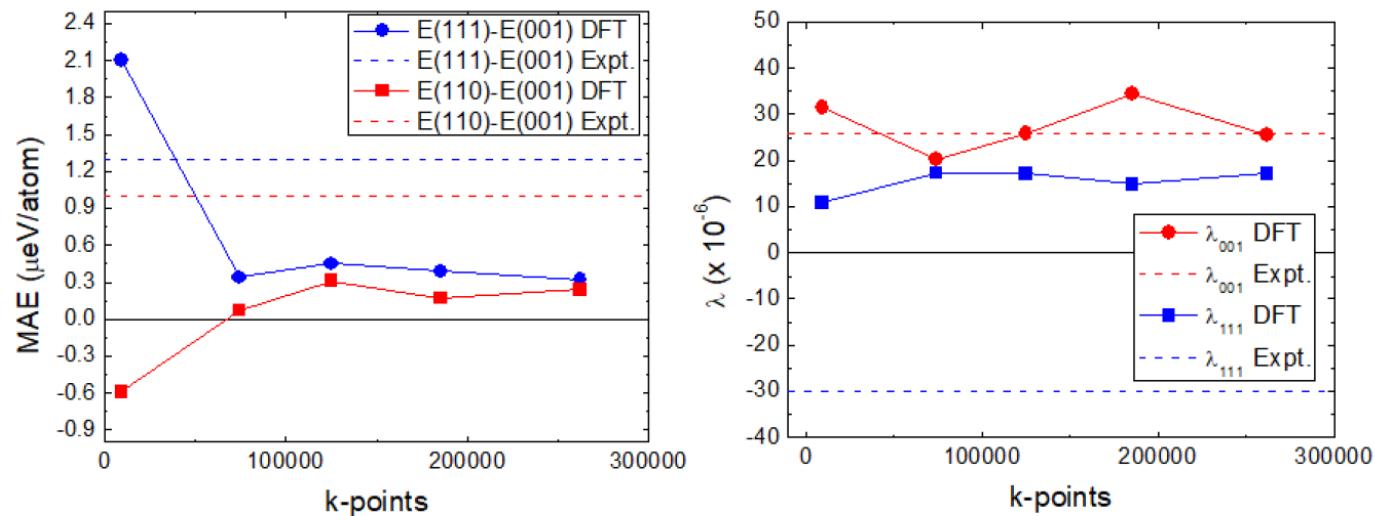


Figure 5: Calculation of (left) MAE of the unstrained unit cell and (right) magnetostrictive coefficients for BCC Fe as a function of k-points.

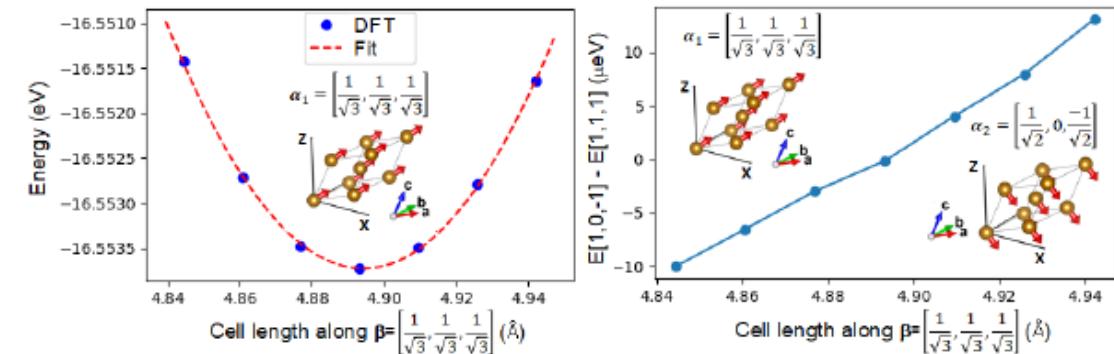


Figure 6: Calculation of  $\lambda_{111}$  for BCC Fe using MAELAS. (Left) Quadratic curve fit to the energy versus cell length along  $\beta = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$  with spin direction  $\alpha_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$ . (Right) Energy difference between states with spin directions  $\alpha_2 = \left(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}}\right)$  and  $\alpha_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$  against the cell length along  $\beta = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$ .

# MAELAS TESTS: BCC Fe (-mode 2)

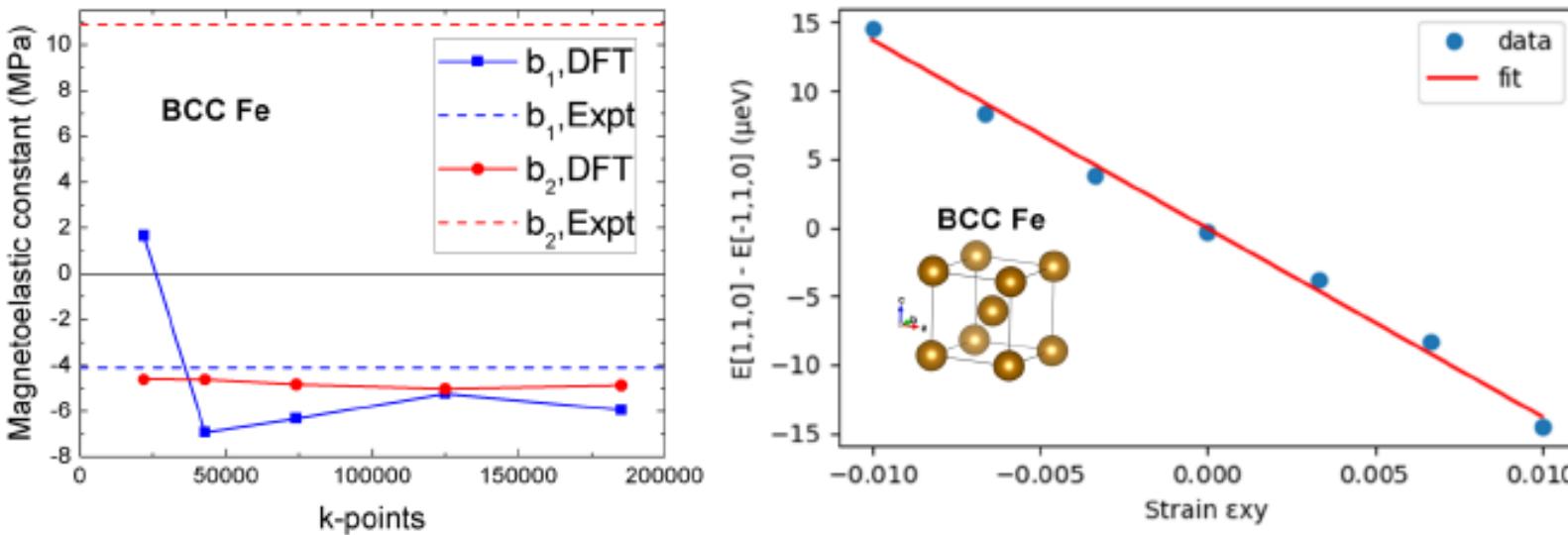


Figure 4: (Left) Calculated magnetoelastic constants for BCC Fe with the new method implemented in MAELAS v2.0 (-mode 2). (Right) Calculation of  $b_2$  for BCC Fe through a linear fitting of the energy difference between magnetization directions  $\alpha_1 = (1/\sqrt{2}, 1/\sqrt{2}, 0)$  and  $\alpha_2 = (-1/\sqrt{2}, 1/\sqrt{2}, 0)$  versus strain ( $\epsilon_{xy}$ ) data.

# MAELAS TESTS: HCP Co (-mode 1)

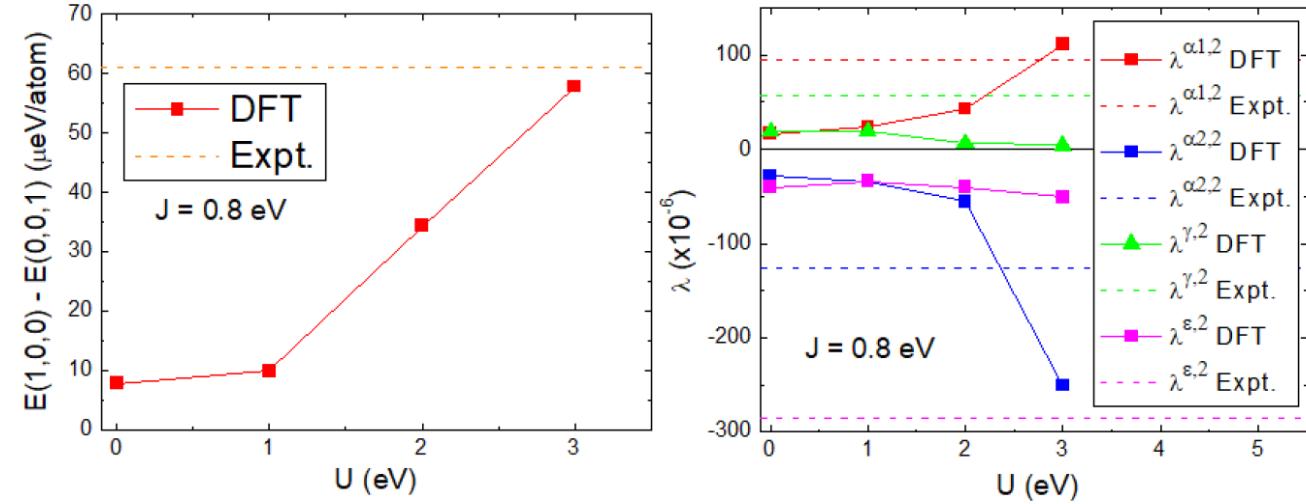


Figure 8: Calculation of (left) MAE of the unstrained unit cell and (right) magnetostrictive coefficients for HCP Co using the LSDA+U approach with different values of parameter  $U$ .

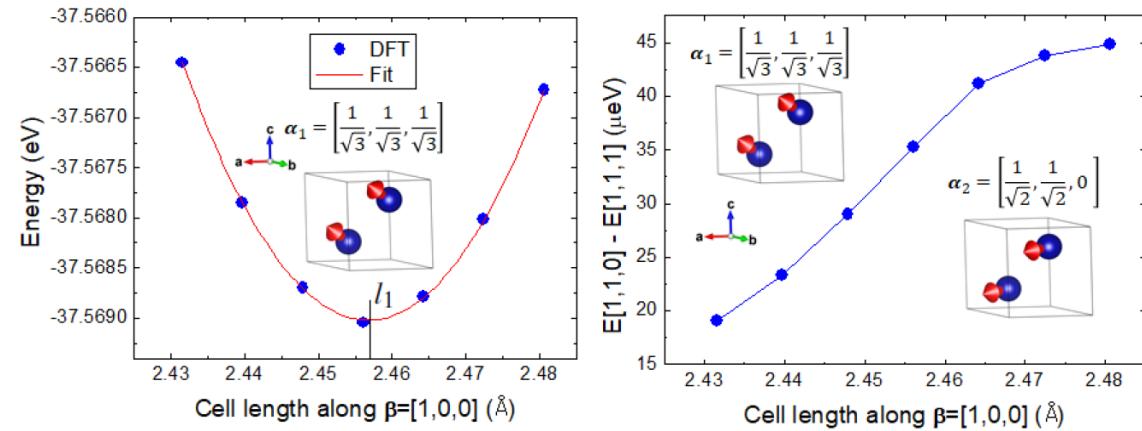


Figure 7: Calculation of  $\lambda^{\alpha_{1,2}}$  for HCP Co using MAELAS with the meta-GGA functional SCAN. (Left) Quadratic curve fit to the energy versus cell length along  $\beta = (1, 0, 0)$  with spin direction  $\alpha_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$ . (Right) Energy difference between states with spin directions  $\alpha_2 = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$  and  $\alpha_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$  against the cell length along  $\beta = (1, 0, 0)$ .

# MAELAS TESTS: HCP Co (-mode 2)

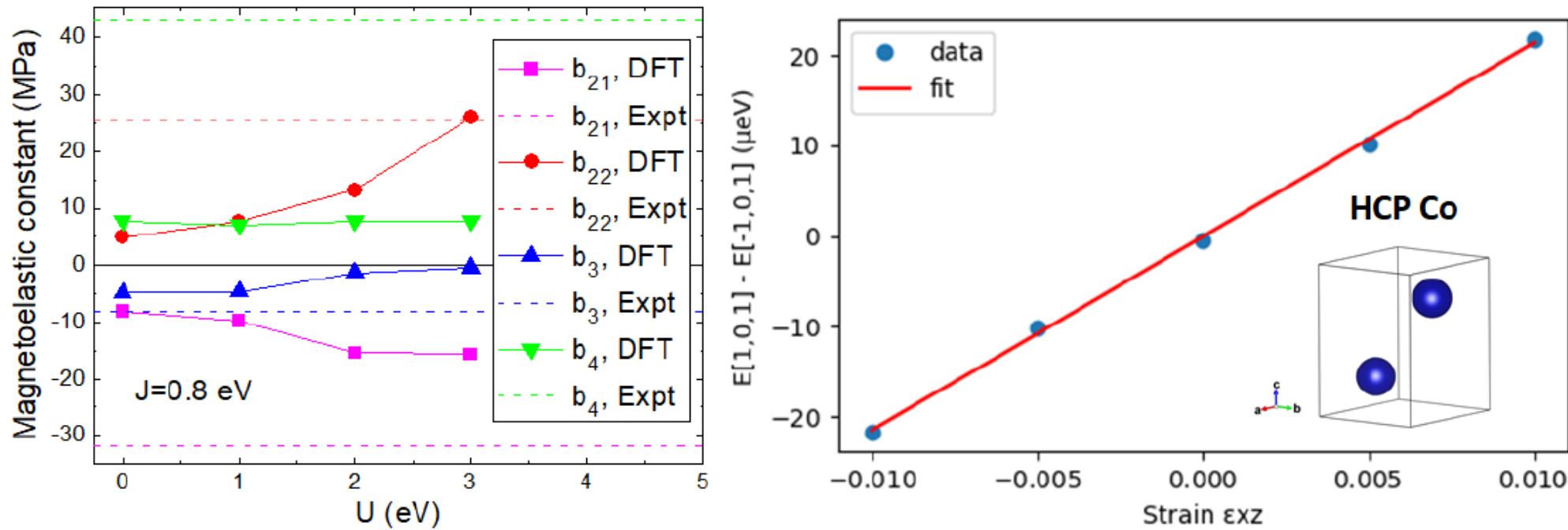


Figure 5: (Left) Calculated magnetoelastic constants for HCP Co with the new method implemented in MAELAS v2.0 (-mode 2) for different values of the Hubbard U parameter. (Right) Calculation of  $b_4$  for HCP Co through a linear fitting of the energy difference between magnetization directions  $\alpha_1 = (1/\sqrt{2}, 0, 1/\sqrt{2})$  and  $\alpha_2 = (-1/\sqrt{2}, 0, 1/\sqrt{2})$  versus strain ( $\epsilon_{xz}$ ) data.

# MAELAS TESTS: bcc Fe (-mode 3)

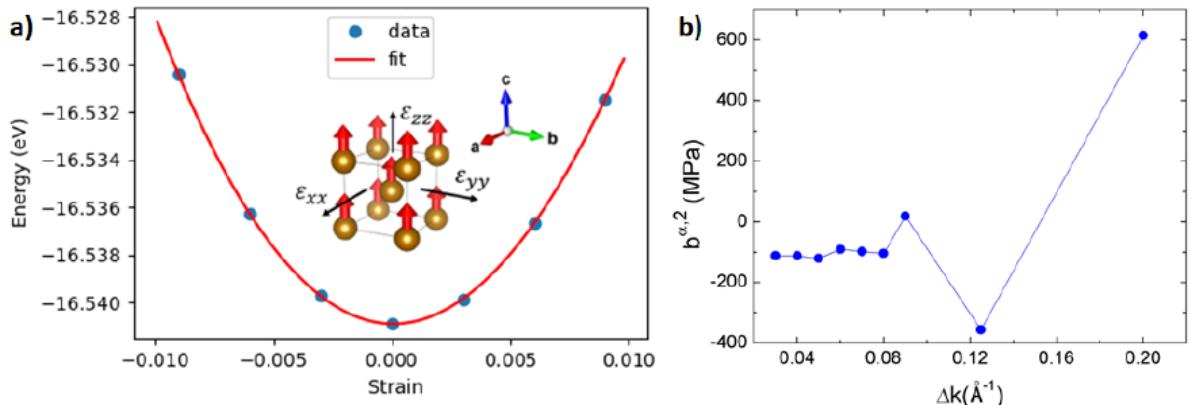


Figure 4: (a) Fitting procedure to extract  $b^{\alpha,2}$  for bcc Fe. The unit cell is deformed according to the parameterized strain tensor  $\boldsymbol{\epsilon}(s)$  given in Table 1. Blue circles give the DFT data, while the red solid line shows the fitting to a third order polynomial Eq.3. (b) Analysis of the convergence of  $b^{\alpha,2}$  with respect to the smallest allowed spacing between k-points ( $\Delta k$ ) in the mesh of the Brillouin zone.

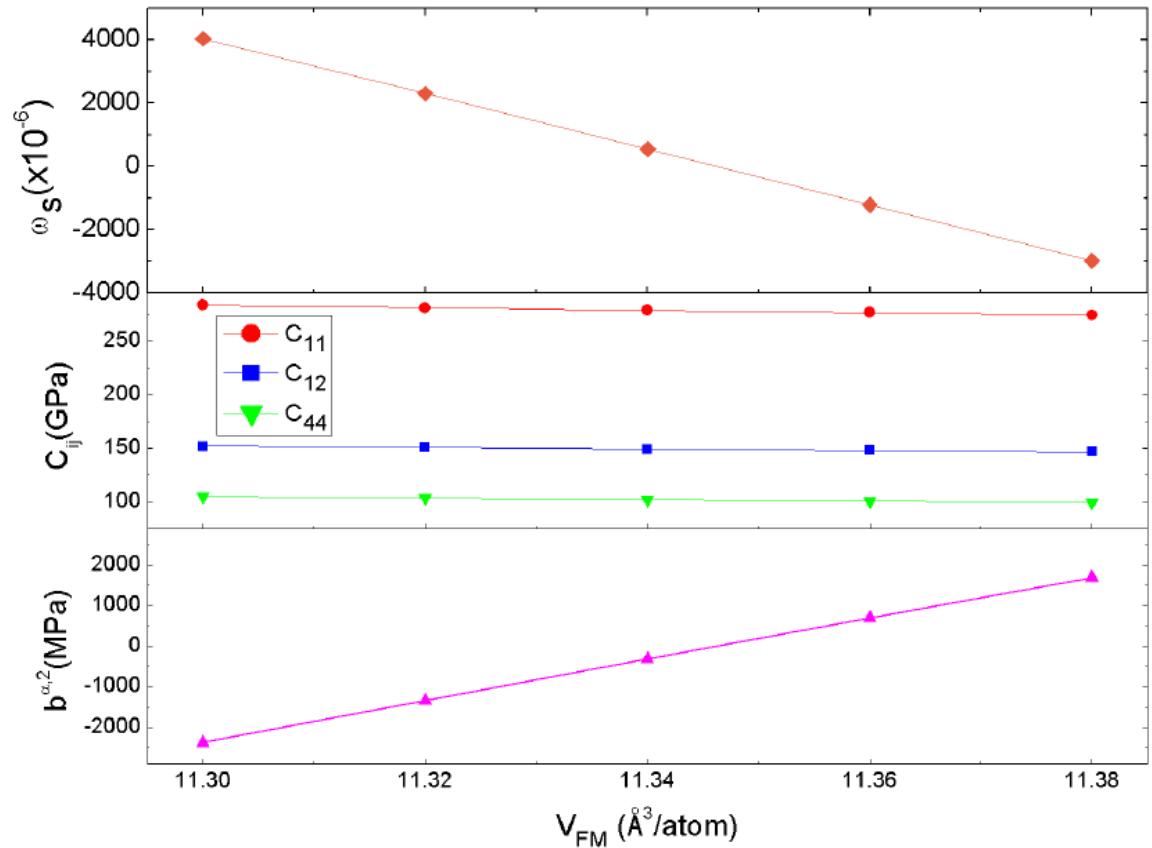


Figure 5: Calculated isotropic magnetoelastic constant  $b^{\alpha,2}$ , elastic constants  $C_{ij}$  and spontaneous volume magnetostriction  $\omega_s$  for bcc Fe using different equilibrium volumes of the ferromagnetic state  $V_{FM}$ .

# Visualization tool MAELASviewer

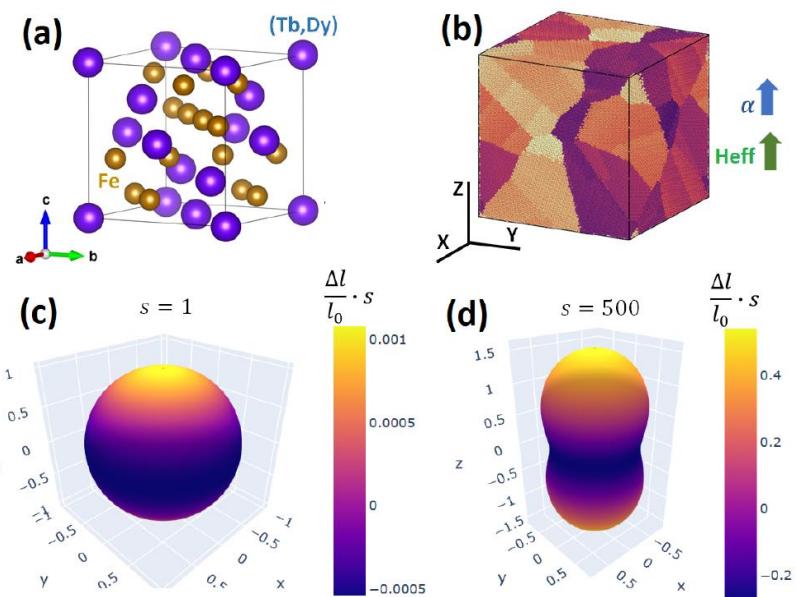
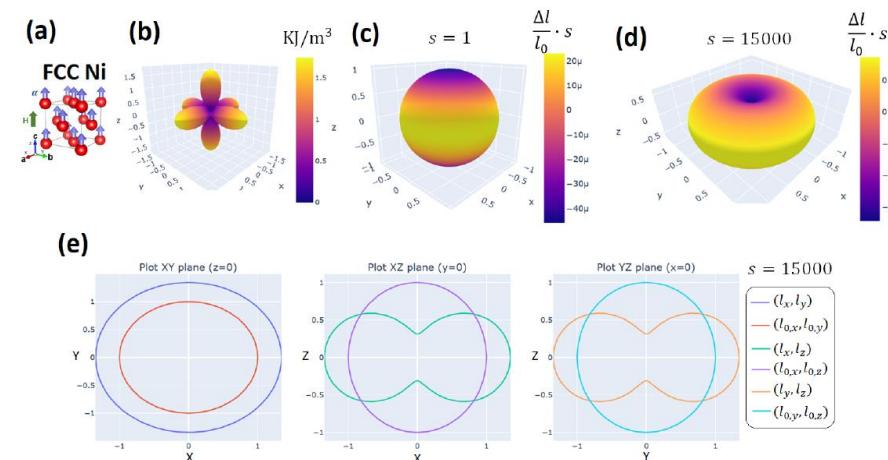
We have also developed an online visualization tool called MAELASviewer that is available at

<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.; Kądzielawa, A.P.; Legut, D. MAELASviewer: An Online Tool to Visualize Magnetostriction. Sensors 2020, 20, 6436.



# Bibliography

- MAELAS version 1.0:

P. Nieves, S. Arapan, S.H. Zhang, A.P. Kądzielawa, R.F. Zhang and D. Legut, "MAELAS: MAgneto-ELASTic properties calculation via computational high-throughput approach", *Comput. Phys. Commun.* 264, 107964 (2021).

- MAELAS version 2.0:

P. Nieves, S. Arapan, S.H. Zhang, A.P. Kądzielawa, R.F. Zhang and D. Legut, "MAELAS 2.0: A new version of a computer program for the calculation of magneto-elastic properties", *Computer Physics Communications* 271 (2022) 108197

- MAELAS version 3.0 (Preprint):

P. Nieves, S. Arapan, S.H. Zhang, A.P. Kądzielawa, R.F. Zhang and D. Legut, "Automated calculations of exchange magnetostriction", arXiv (2022) 2210.00791

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

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

- M.R.J.Gibbs, *Modern Trends in Magnetostriction*, Springer Netherlands (2001).

- Göran Engdahl, Isaak D. Mayergoyz, *Handbook of Giant Magnetostrictive Materials*, Academic Press (1999).