

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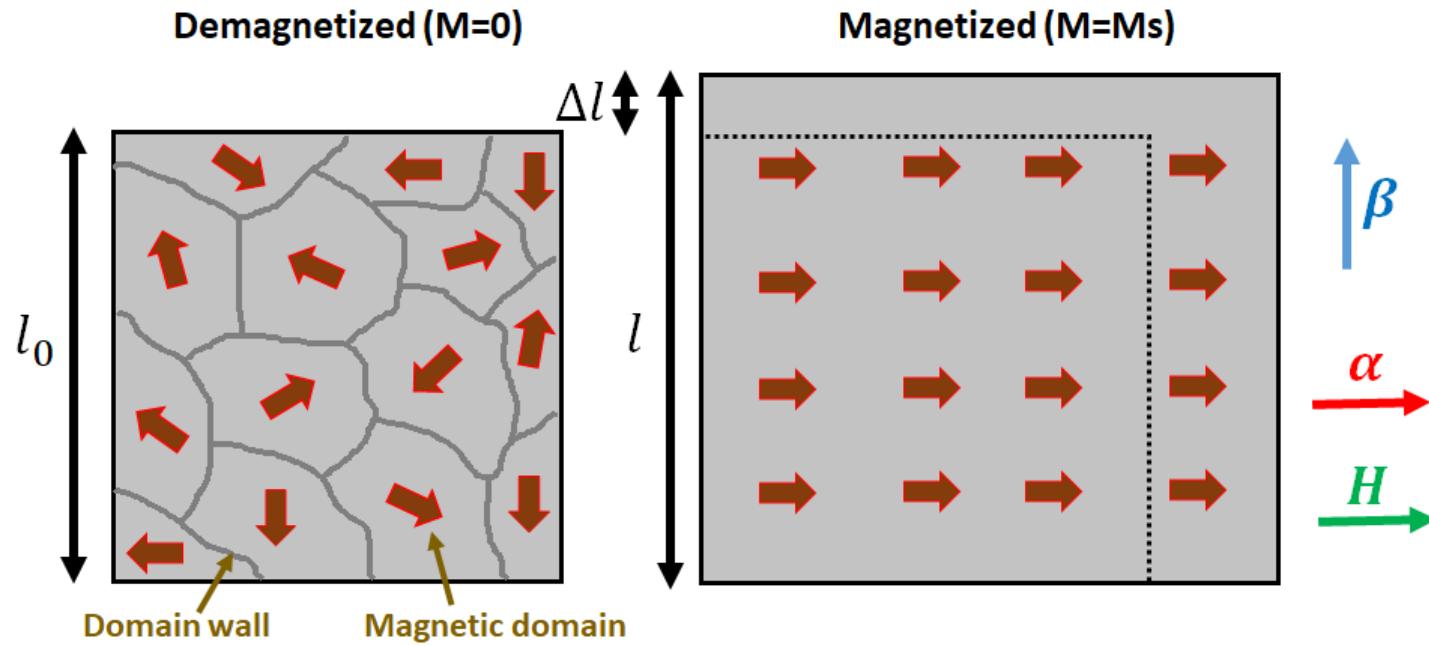
<http://www.md-esg.eu/>

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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.



α =Magnetization direction ($|\alpha|=1$)
 β =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 (λ^{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 (λ^{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 (λ^{iso}) and spontaneous volume magnetostriiction (ω_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 quadratic 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 and spontaneous volume magnetostriiction.
- 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 β for λ_{12} in trigonal (I) symmetry has been changed.
- We also corrected the theoretical relations between $\lambda^{Y,1}$, $\lambda^{Y,2}$ and λ_{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)
```

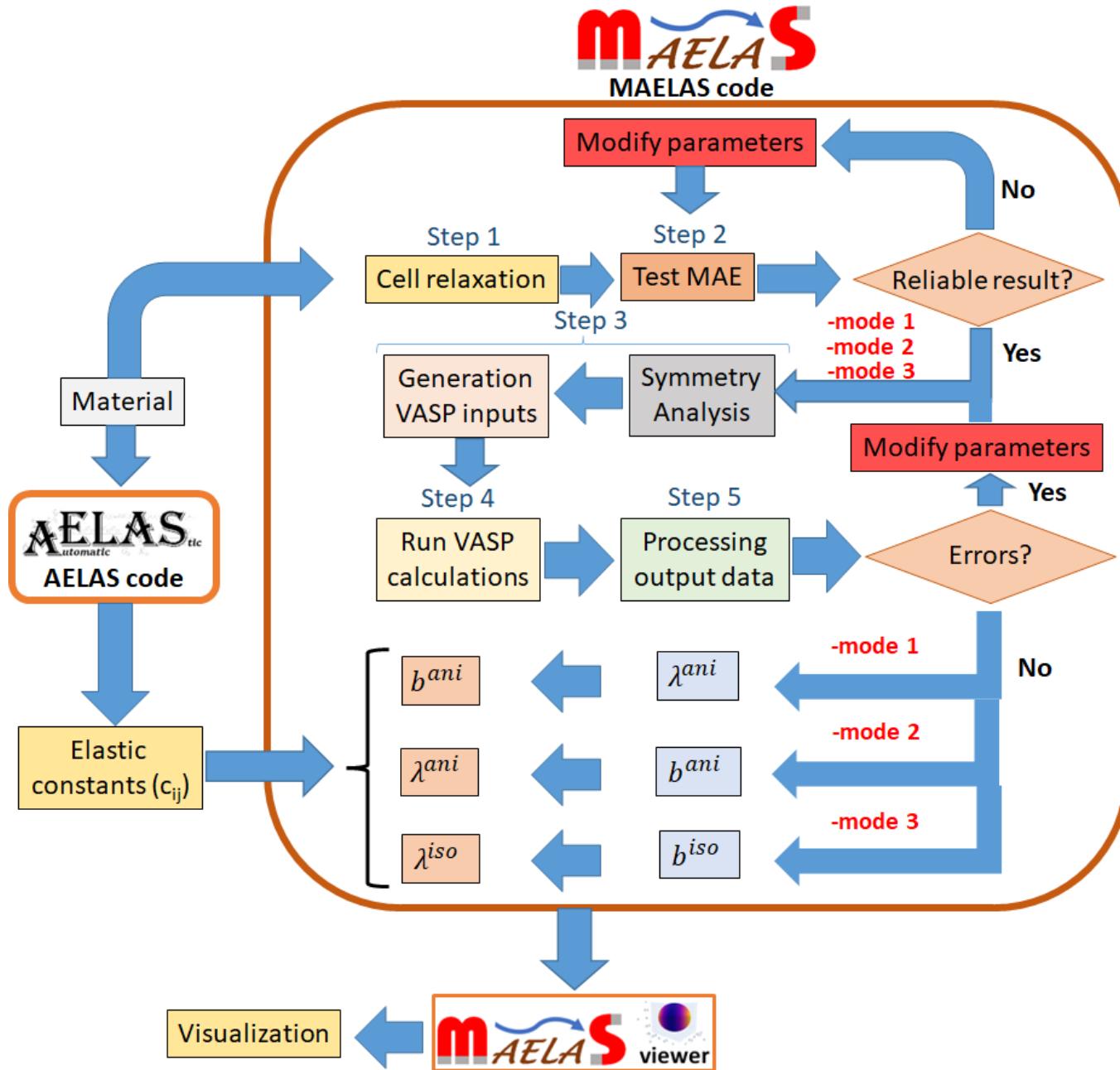
More available options for the installation can be found in the file INSTALL. By default, the executable file "maelas" is installed in the folder /home/\$USER/.local/bin/ where \$USER is the name of your username folder. This folder should be included to the PATH variable by adding in the file /home/\$USER/.bashrc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

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

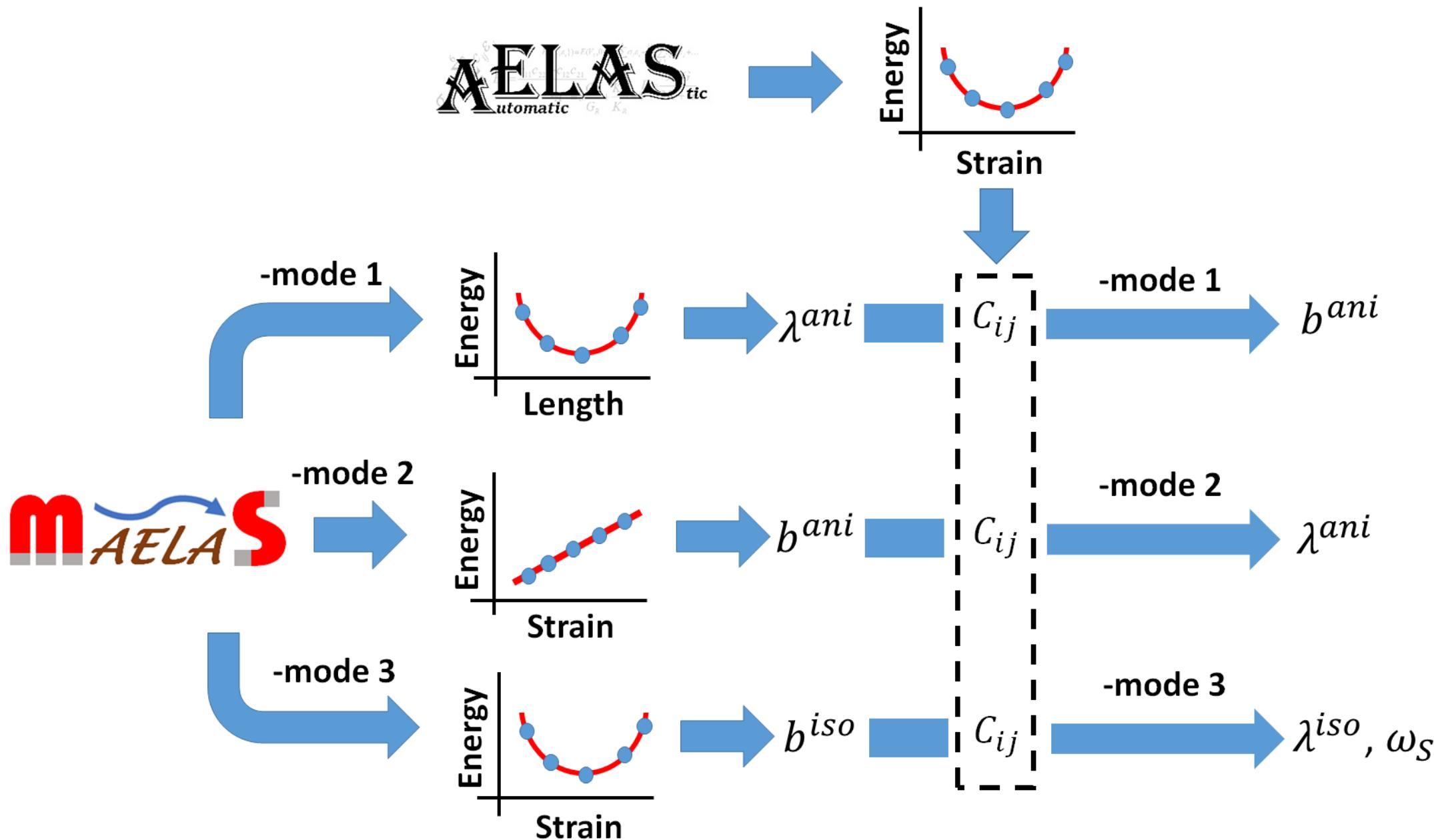
Then you should close the terminal and open the terminal again. If you need to install pip3 in Ubuntu Linux, then type

```
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.

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.

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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
```

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

Format of the
elastic tensor file

Elastic tensor:

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

HOW TO USE MAELAS CODE

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
```

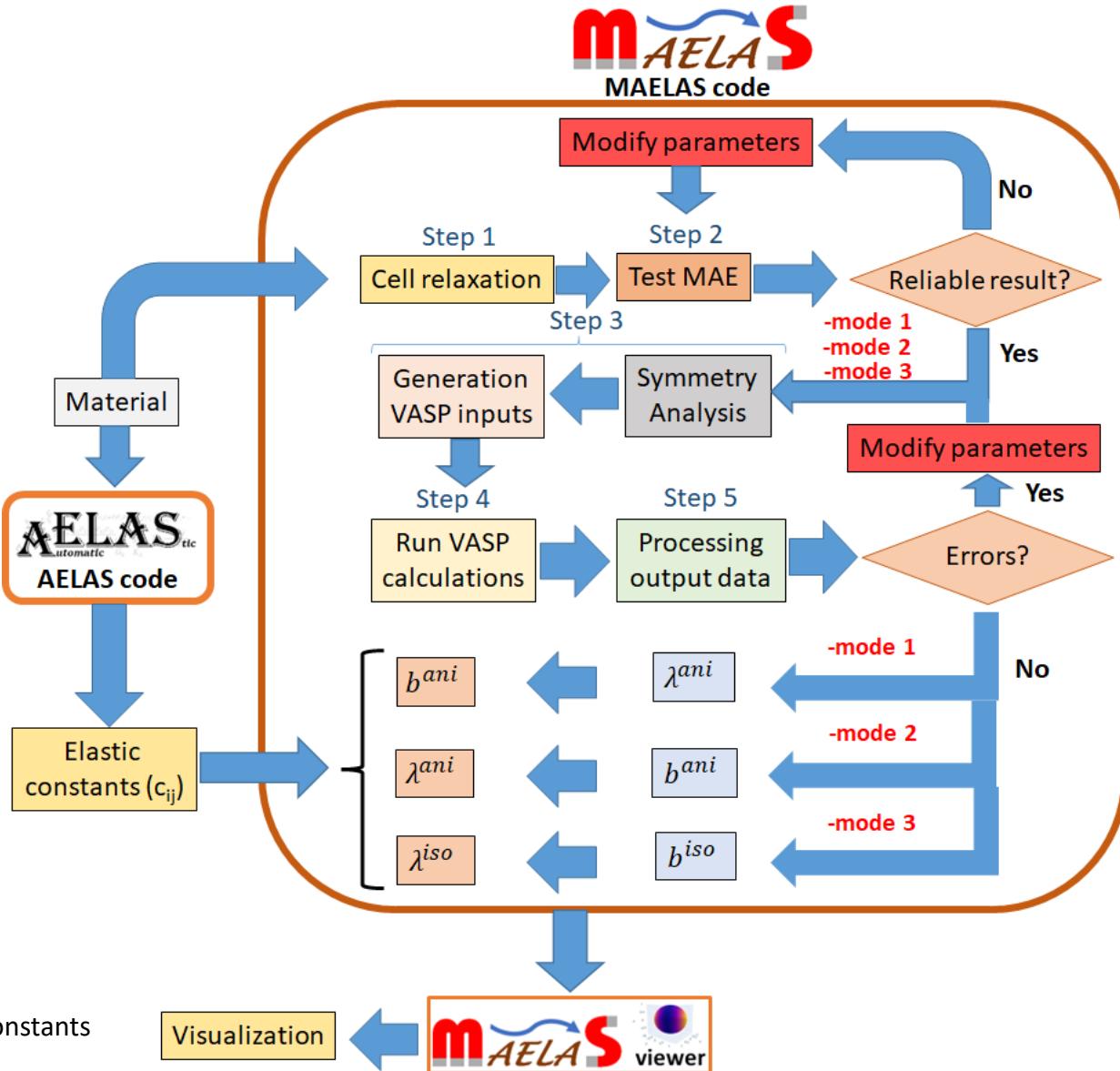
Step 5a: Derivation of anisotropic magnetostrictive coefficients

```
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

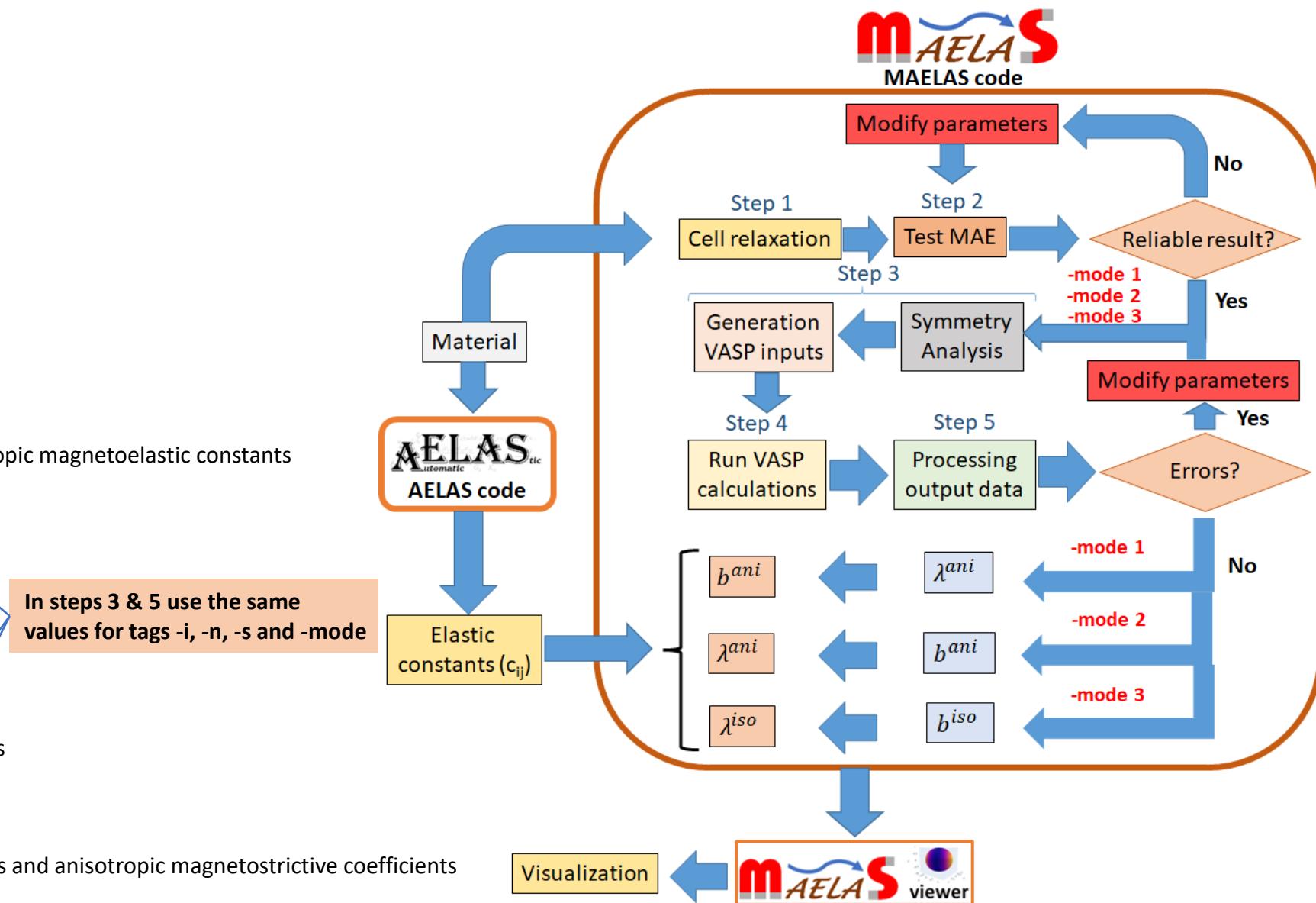
Step 5a: Derivation of anisotropic magnetoelastic constants

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
```

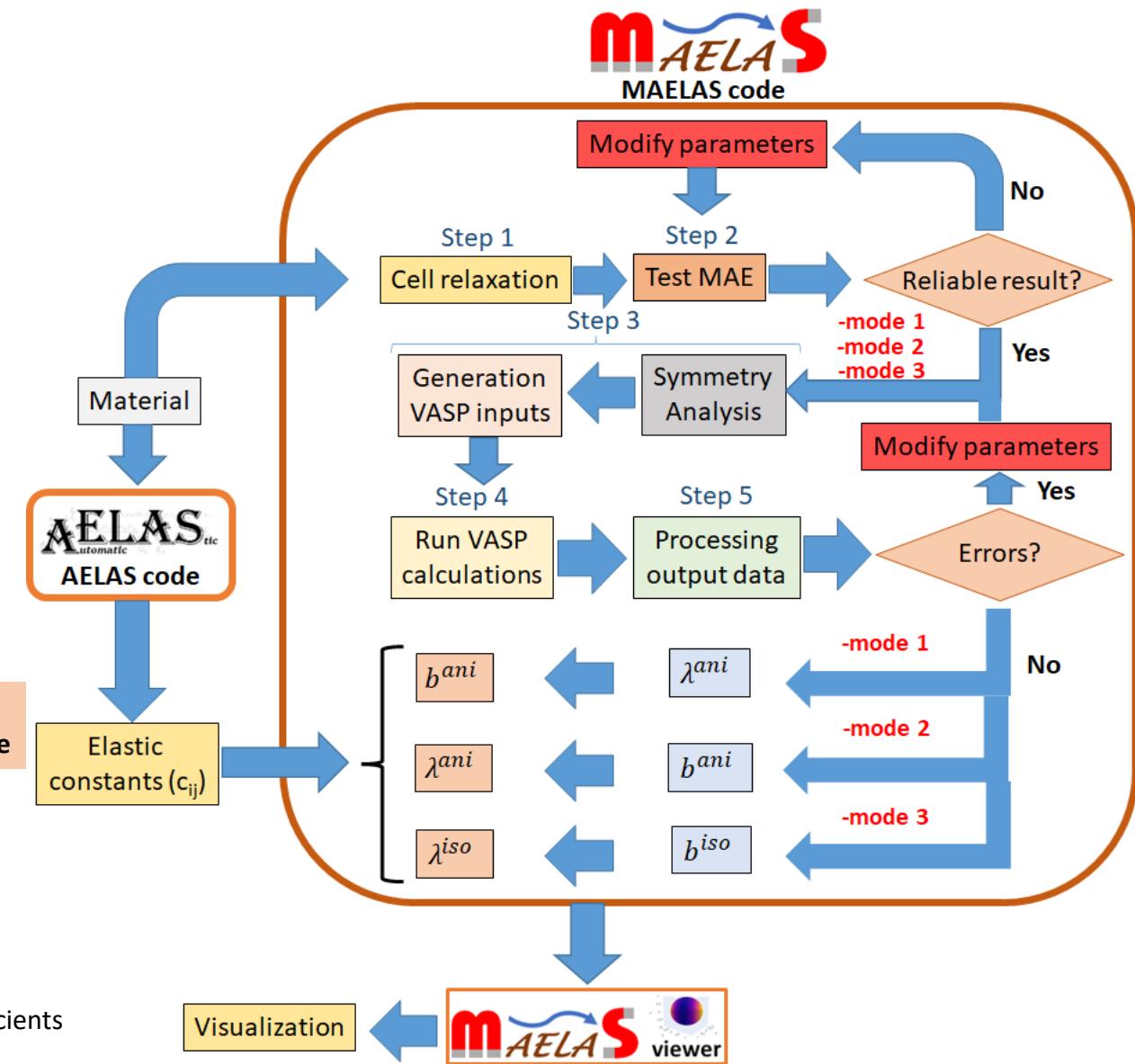
Step 5a: Derivation of isotropic magnetoelastic constants

```
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

User can see all possible optional arguments by typing

maelas -h

The optional arguments are the following:

- h, --help Show this help message and exit
- 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.
- 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

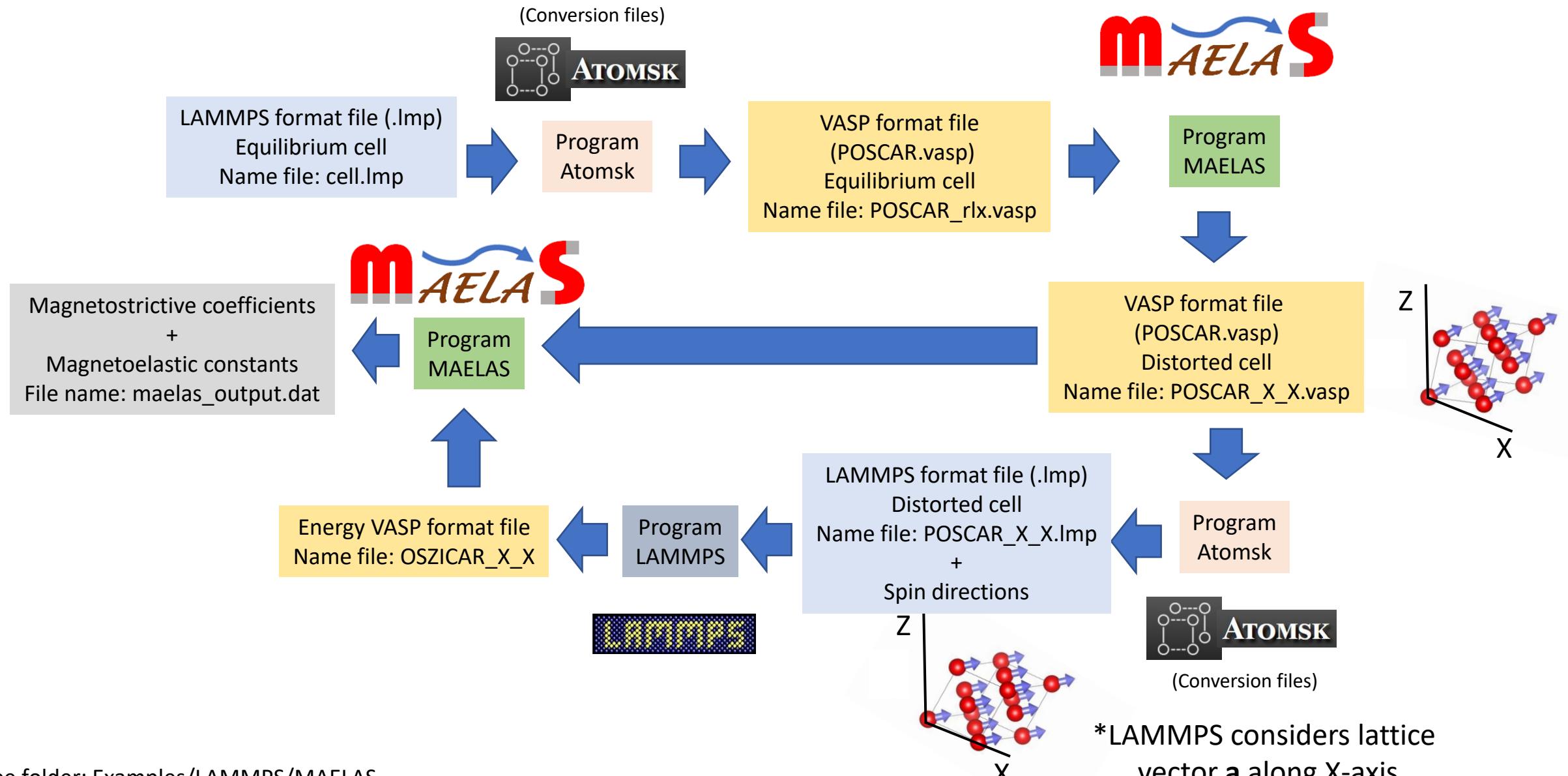
Using MAELAS with other codes instead of VASP

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

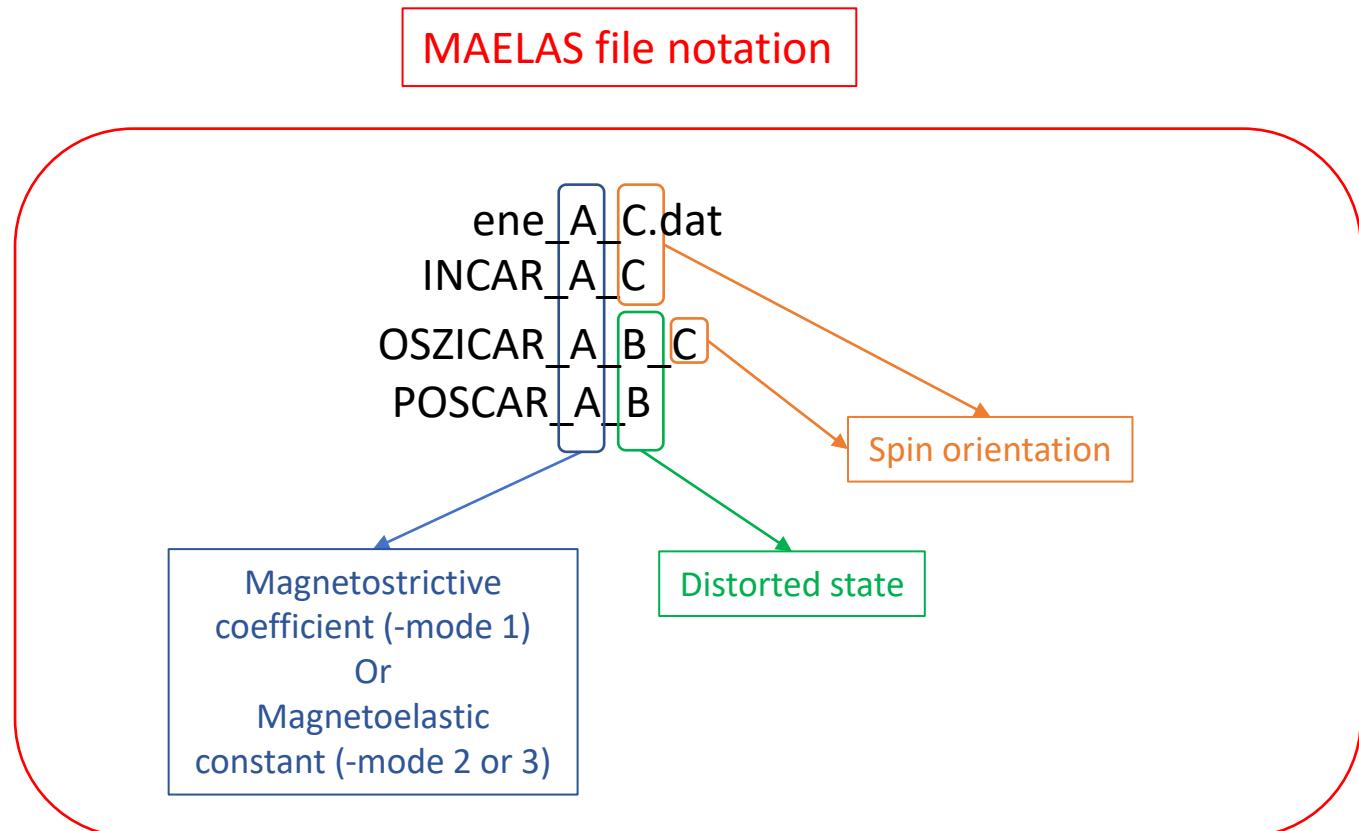
Crystal systems supported by MAELAS v3.0

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 (λ)	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)

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

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

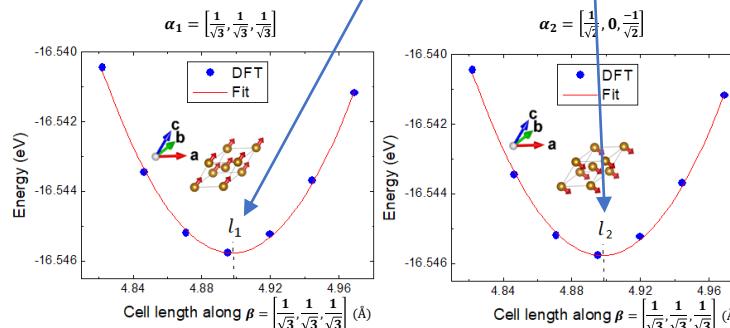
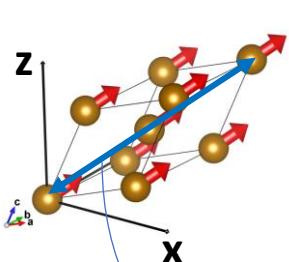
Spin-polarized calculation with SOC

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

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 (β) and magnetization directions (α_1, α_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 ρ 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	β	α_1	α_2	ρ
Cubic (I)	Eq.17	λ_{001}	$(0, 0, 1)$	$(0, 0, 1)$	$(1, 0, 0)$	$\frac{3}{2}$
$a \parallel \hat{x}, b \parallel \hat{y}, c \parallel \hat{z}$		λ_{111}	$\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)$	$\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right)$	$\left(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}} \right)$	$\frac{3}{2}$
Hexagonal (I)	Eq.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
$a = b \neq c$		$\lambda^{\gamma,2}$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}})$	$\frac{ac}{a^2+c^2}$
λ_{12}	$v2.0$		$(1, 0, 0)$	$\left(\frac{a,0,c}{\sqrt{a^2+c^2}} \right)$	$\left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right)$	$v1.0$
λ_{21}	$v1.0$		$\left(\frac{a,0,c}{\sqrt{a^2+c^2}} \right)$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$	$\left(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, 0 \right)$	$\frac{1}{2}$
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
		$\lambda^{\epsilon,2}$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$(\frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}})$	$\frac{2ac}{a^2+c^2}$
		$\lambda^{\delta,2}$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$	$\left(\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$	1
Orthorhombic	Eq.44	λ_1	$(1, 0, 0)$	$(1, 0, 0)$	$(0, 0, 1)$	1
$a \parallel \hat{x}, b \parallel \hat{y}, c \parallel \hat{z}$		λ_2	$(1, 0, 0)$	$(0, 1, 0)$	$(0, 0, 1)$	1
$c < a < b$		λ_3	$(0, 1, 0)$	$(1, 0, 0)$	$(0, 0, 1)$	1
		λ_4	$(0, 1, 0)$	$(0, 1, 0)$	$(0, 0, 1)$	1
		λ_5	$(0, 0, 1)$	$(1, 0, 0)$	$(0, 0, 1)$	1
		λ_6	$(0, 0, 1)$	$(0, 1, 0)$	$(0, 0, 1)$	1
		λ_7	$\frac{(a,b,0)}{\sqrt{a^2+b^2}}$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right)$	$(0, 0, 1)$	$\frac{(a-b)(a[\lambda_1+\lambda_2]-b[\lambda_3+\lambda_4])+4ab\lambda_7}{2(a^2+b^2)\lambda_7}$
		λ_8	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$\left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right)$	$(0, 0, 1)$	$\frac{(a-c)(a[\lambda_1-\lambda_5]+4ac\lambda_8)}{2(a^2+c^2)\lambda_8}$
		λ_9	$\frac{(0,b,c)}{\sqrt{b^2+c^2}}$	$\left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right)$	$(0, 0, 1)$	$\frac{(b-c)(b[\lambda_4-\lambda_6]+4bc\lambda_9)}{2(b^2+c^2)\lambda_9}$

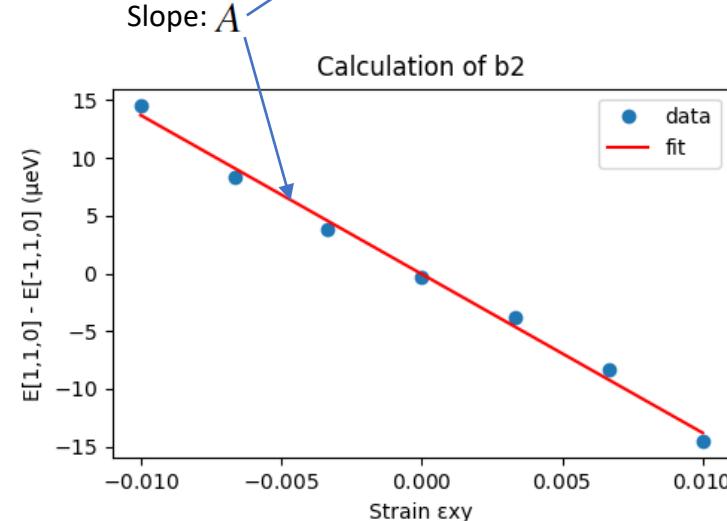
Spin-polarized calculation with SOC

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

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

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 Γ and Φ 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.

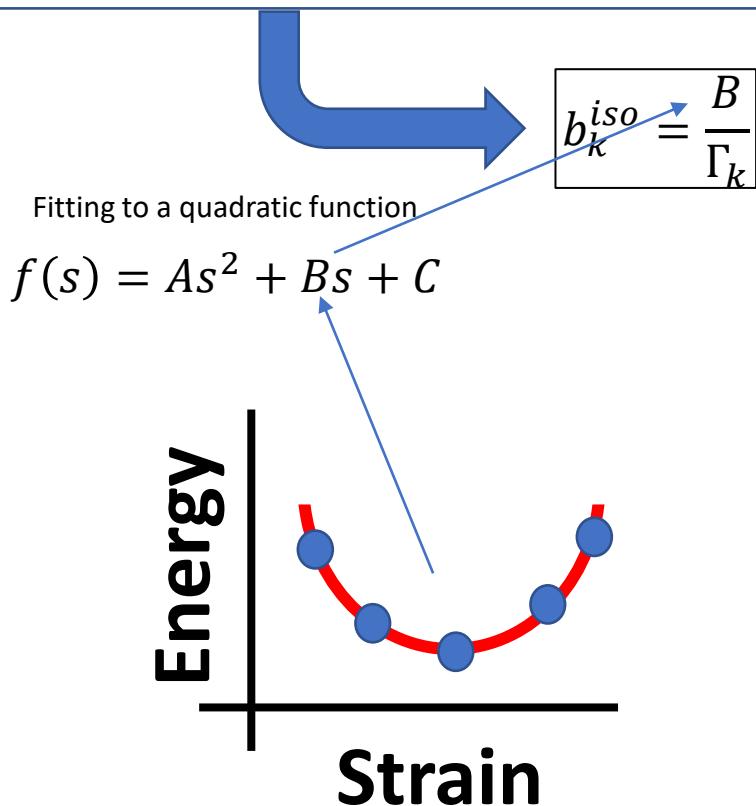
Crystal system	Magnetoelastic constant	$\boldsymbol{\alpha}_1$	$\boldsymbol{\alpha}_2$	Γ	Φ	F
Cubic (I)	b_1	$(1, 0, 0)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$	$\frac{1}{2}$	$-\frac{K_1}{4}$	Eq.A.4
$\boldsymbol{a} \parallel \hat{x}, \boldsymbol{b} \parallel \hat{y}, \boldsymbol{c} \parallel \hat{z}$	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)

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

$$E(\boldsymbol{\epsilon}^k(s)) = \Phi_k(C_{ij})s^2 + \Gamma_k b_k^{iso}s + E_0$$



$$b_k^{iso}$$

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

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.

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

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

The diagram illustrates the workflow. It starts with the 'Elastic energy' section on the left, which contains the equation for the cubic elastic energy. A blue arrow points down to a central rounded rectangle containing two equations. The top equation is $\frac{\partial(E_{el} + E_{me})}{\partial \epsilon_{ij}} = 0$, with an orange arrow pointing down to the bottom equation $\frac{\Delta l}{l_0} \Big|_{\beta}^{\alpha} = \sum_{i,j=x,y,z} \epsilon_{ij}^{eq}(\alpha) \beta_i \beta_j$. Another blue arrow points from the central rectangle to the 'Magnetoelastic energy' section on the right.

$$\begin{aligned}\frac{\partial(E_{el} + E_{me})}{\partial \epsilon_{ij}} &= 0 \\ \frac{\Delta l}{l_0} \Big|_{\beta}^{\alpha} &= \sum_{i,j=x,y,z} \epsilon_{ij}^{eq}(\alpha) \beta_i \beta_j\end{aligned}$$

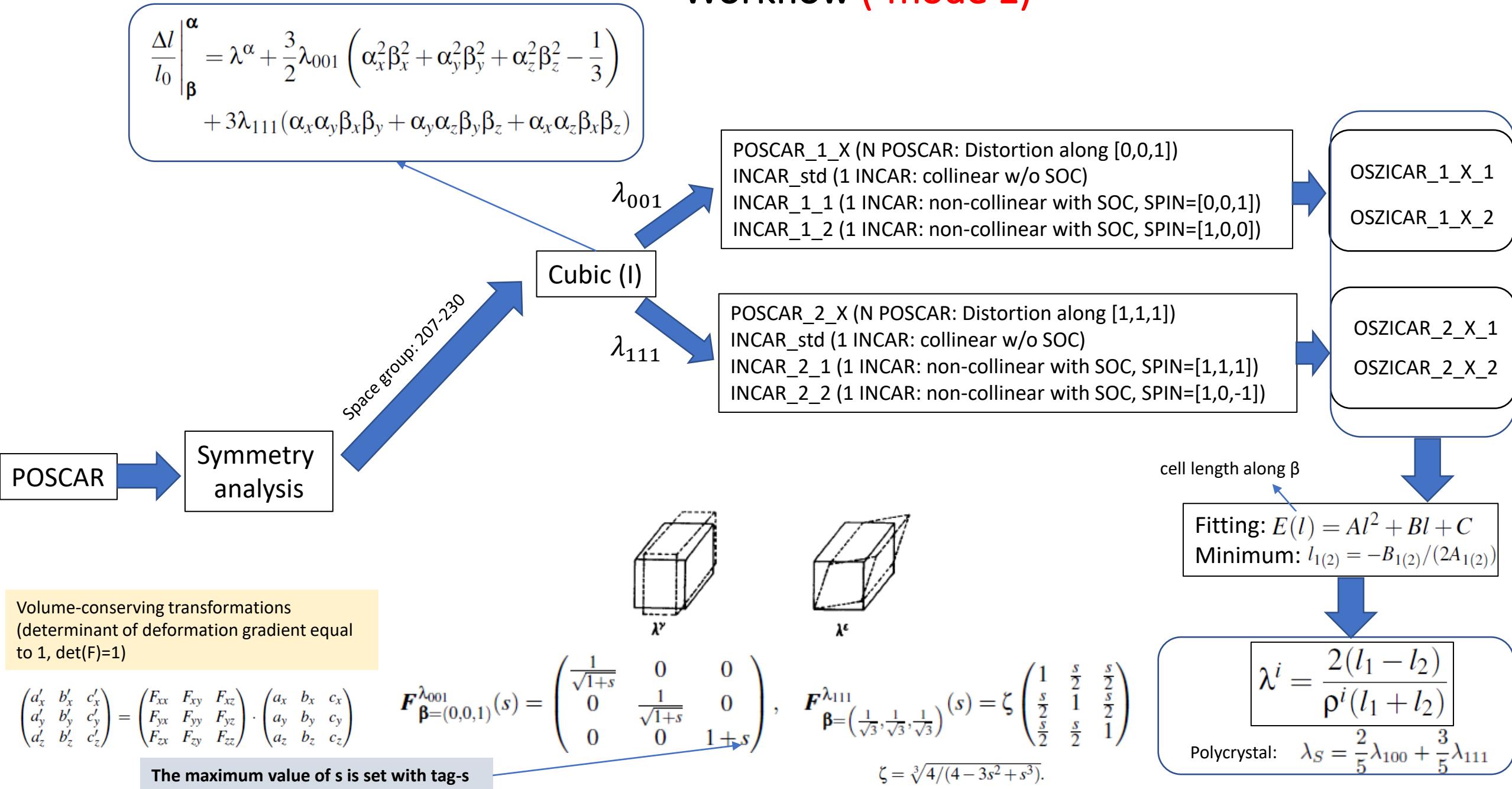
$$\begin{aligned}\frac{\Delta l}{l_0} \Big|_{\beta}^{\alpha} &= \lambda^{\alpha} + \frac{3}{2}\lambda_{001} \left(\alpha_x^2\beta_x^2 + \alpha_y^2\beta_y^2 + \alpha_z^2\beta_z^2 - \frac{1}{3} \right) \\ &\quad + 3\lambda_{111} (\alpha_x\alpha_y\beta_x\beta_y + \alpha_y\alpha_z\beta_y\beta_z + \alpha_x\alpha_z\beta_x\beta_z)\end{aligned}$$

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

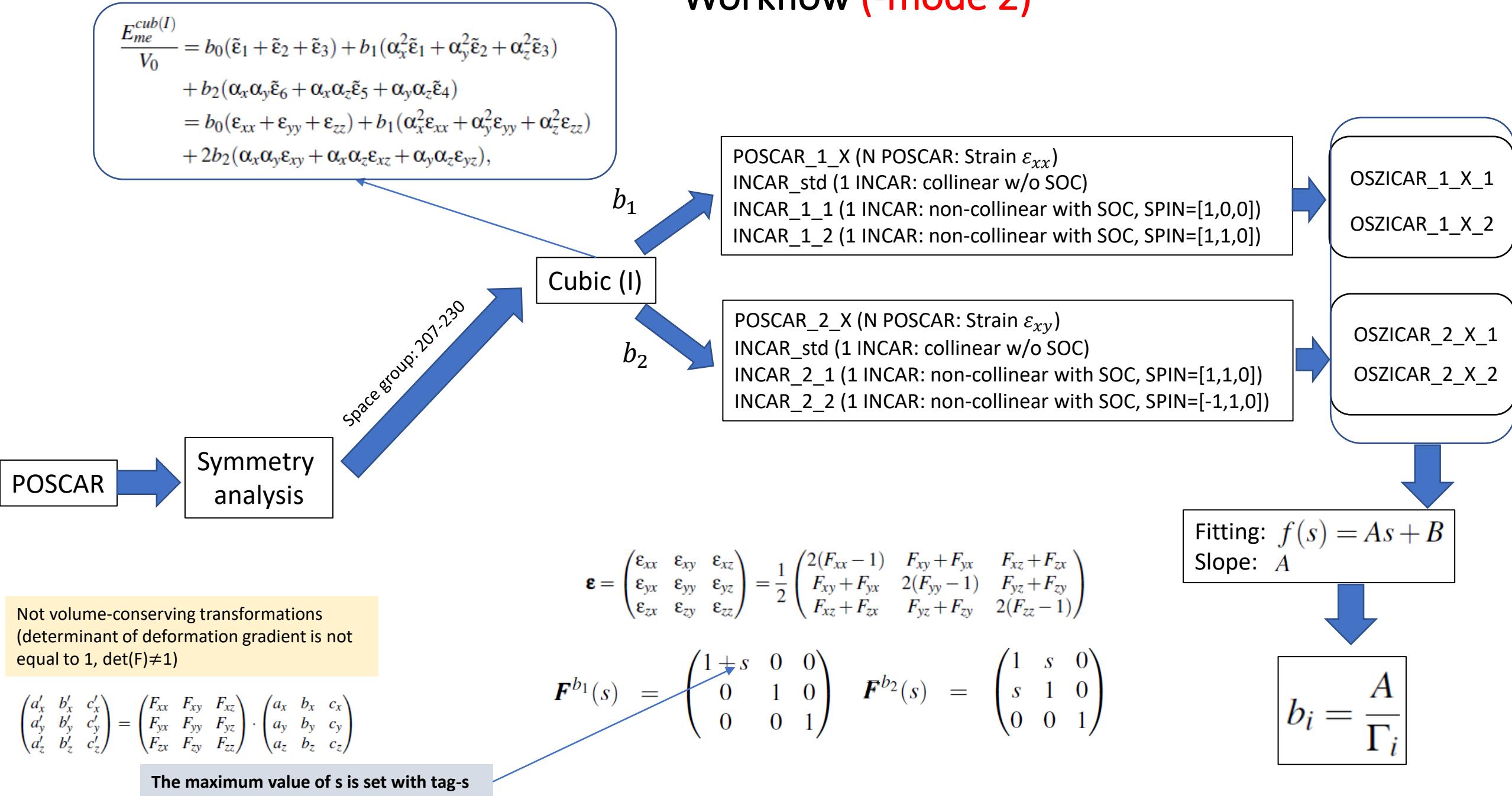
$$\lambda_{001} = \frac{-2b_1}{3(c_{11} - c_{12})},$$

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

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: $f(s) = As^2 + Bs + C$

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

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

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

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

Spontaneous volume magnetostriiction: $\omega_S \simeq \lambda^{\alpha,2} = \frac{-b^{\alpha,2}}{c_{11}+2c_{12}}$

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

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

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

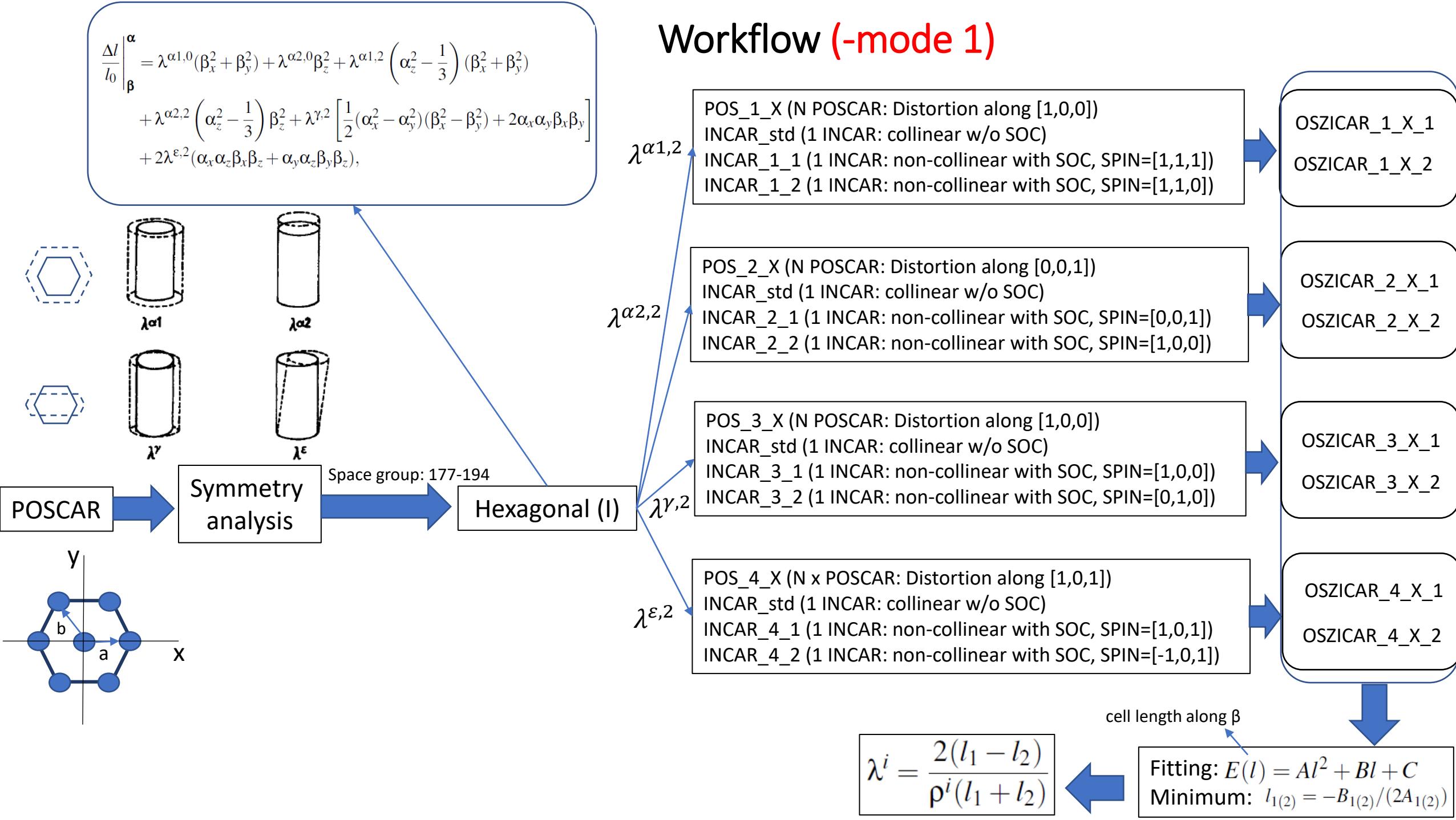
\downarrow

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

\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)

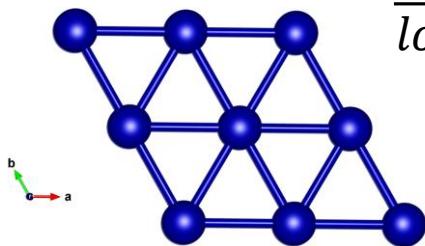
Distorted states (-mode 1)

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

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

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

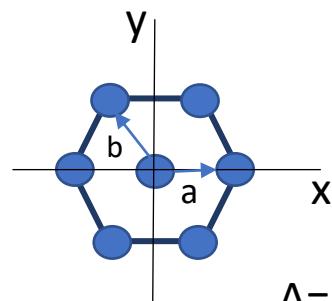
$$\mathbf{F} \Big|_{\beta=(1,0,0)}^{\lambda^{\alpha 1,2}}(s) = \begin{pmatrix} 1+s & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+s}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+s}} \end{pmatrix}$$



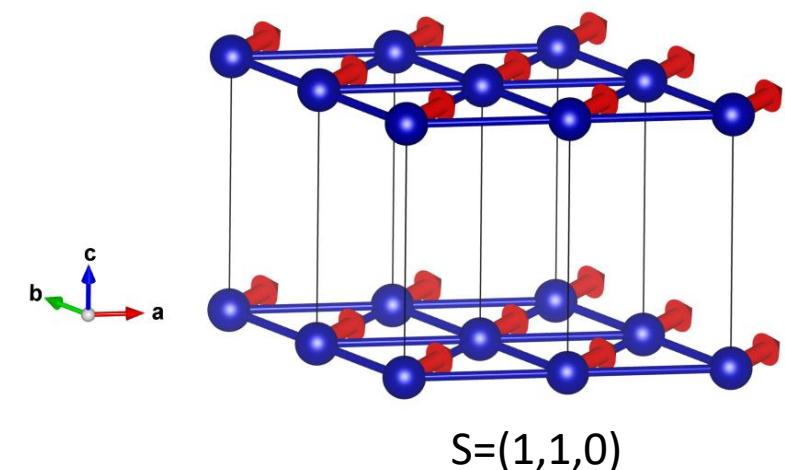
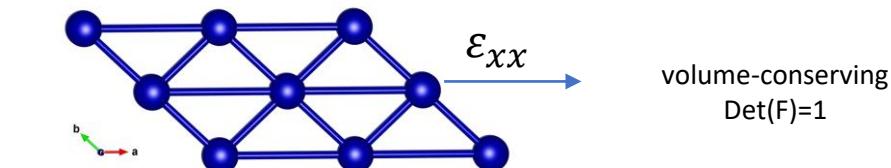
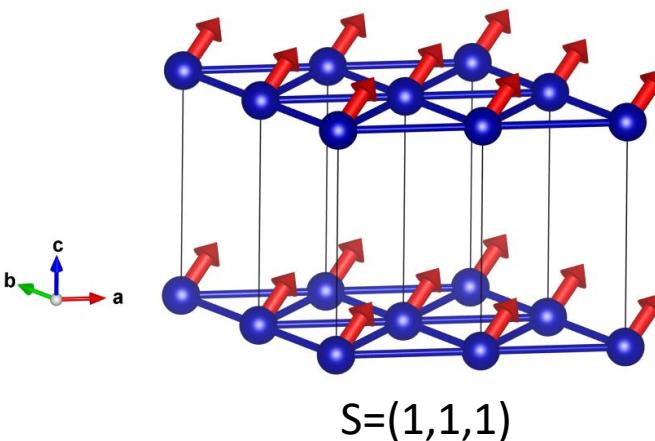
$$\lambda^{\alpha 1,2}$$

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

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



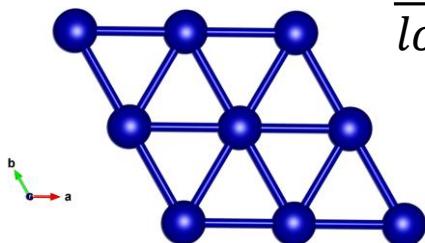
$$\mathbf{A} = \begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$



Hexagonal (I)

Distorted states (-mode 1)

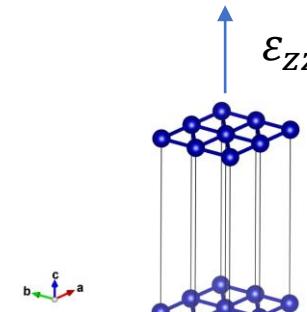
$$\frac{\Delta l^\alpha}{l o_\beta}$$



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

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

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

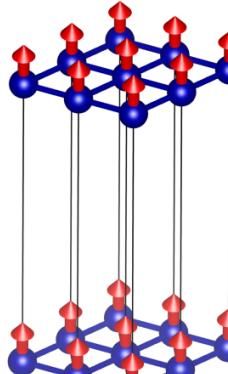
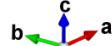


volume-conserving
 $\text{Det}(F)=1$

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

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

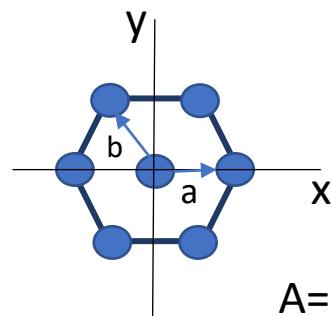
$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx} \\ F_{xy}+F_{yx} & 2(F_{yy}-1)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



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



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



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

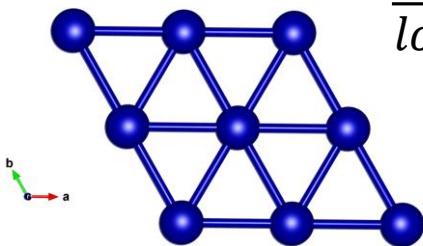
Hexagonal (I)

Distorted states (-mode 1)

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

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

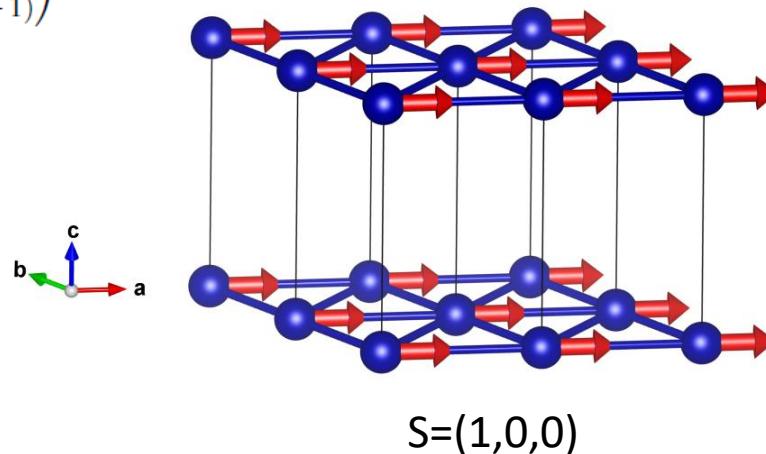
$$\mathbf{F}^{\lambda \gamma^2}_{\beta=(1,0,0)}(s) = \begin{pmatrix} 1+s & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+s}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+s}} \end{pmatrix}$$



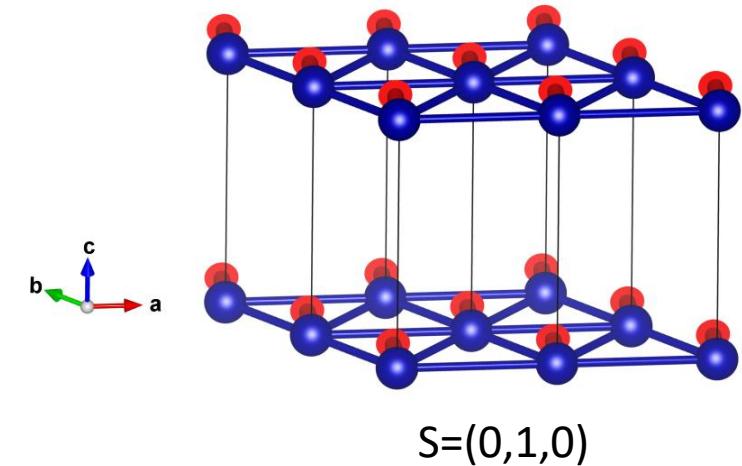
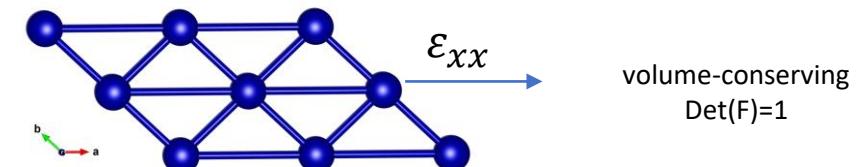
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

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

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



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

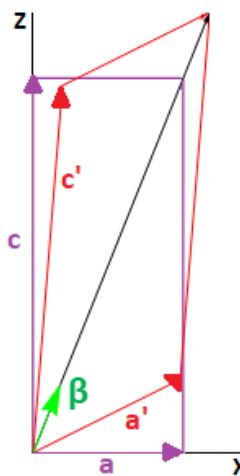


Hexagonal (I)

Distorted states (-mode 1)

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

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

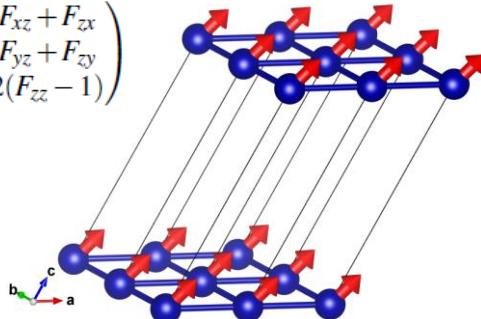


$$A = \begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

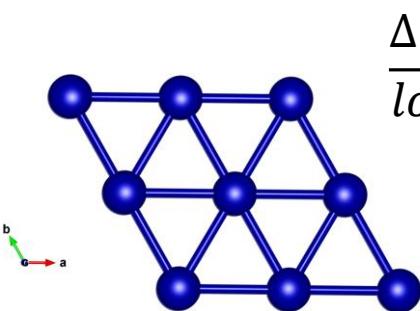
$$\lambda^{\varepsilon,2}$$

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

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



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



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

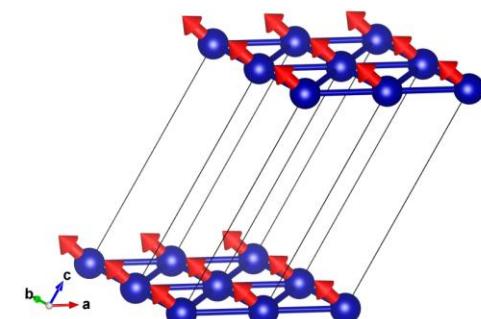
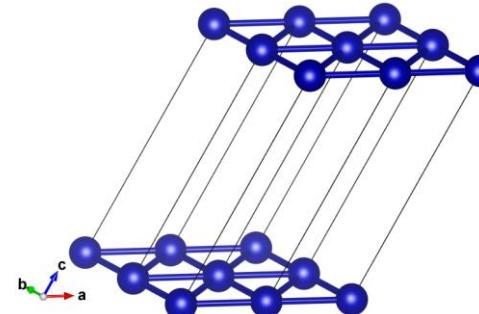
$$|\alpha| = 1, |\beta| = 1$$

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

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

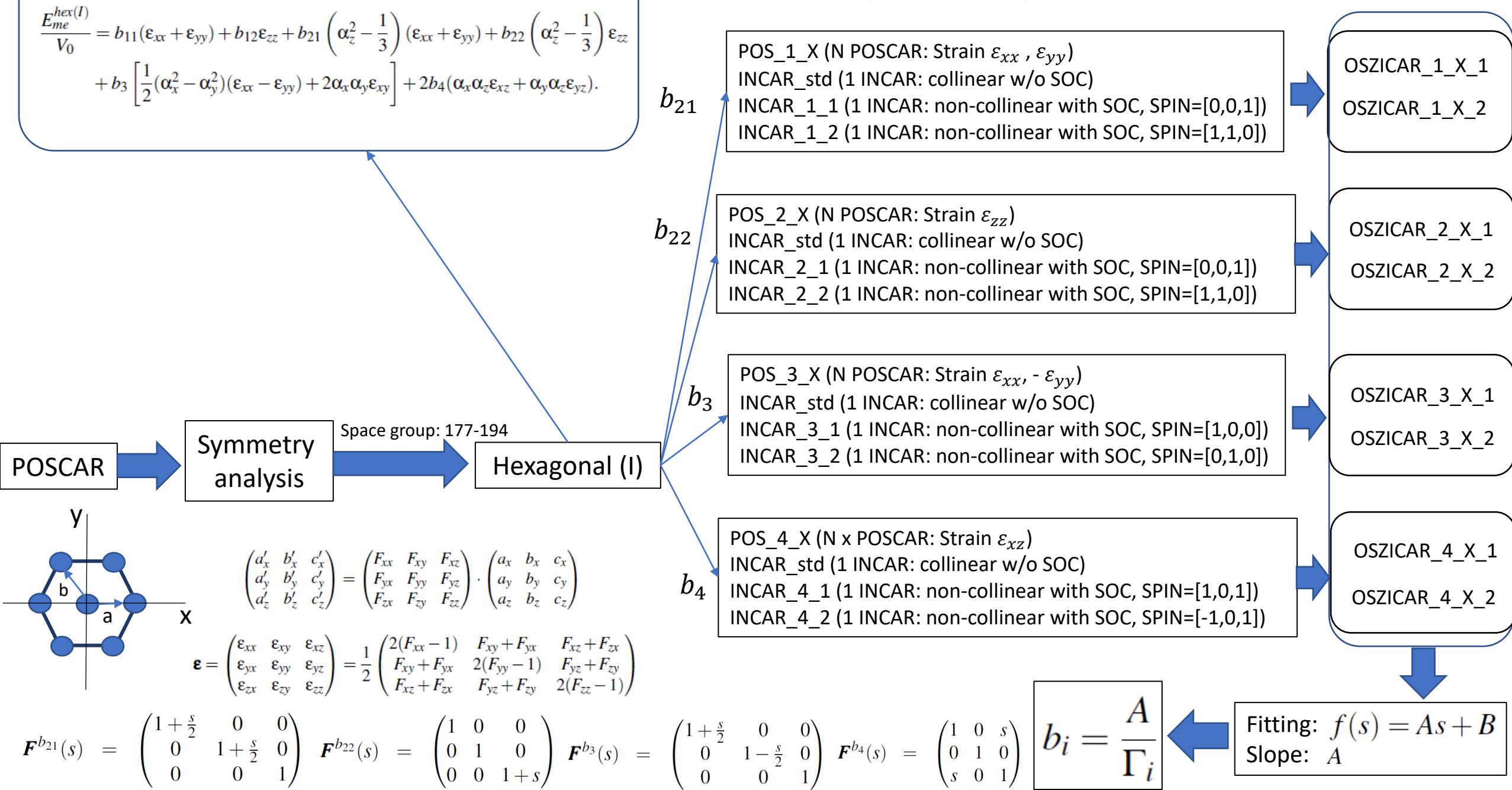
$$\varepsilon_{xz}$$

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



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

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 ^a	Birss ^b
β_x	β_y	β_z	α_x	α_y	α_z	α_x	α_y	α_z					
1	0	0	1	0	0	0	1	0	$\lambda(a,a) - \lambda(b,a)$	$\lambda_A - \lambda_B$	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	$\lambda(a,a) - \lambda(c,a)$	λ_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					

^a W. P. Mason, Phys. Rev. 96, 302 (1954).

^b R. R. Birss, *Advances in Physics* (Francis & Taylor, Ltd., London, 1959), Vol. 8, p. 252.

MAELAS notation

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19 JULY 1965

Callen

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

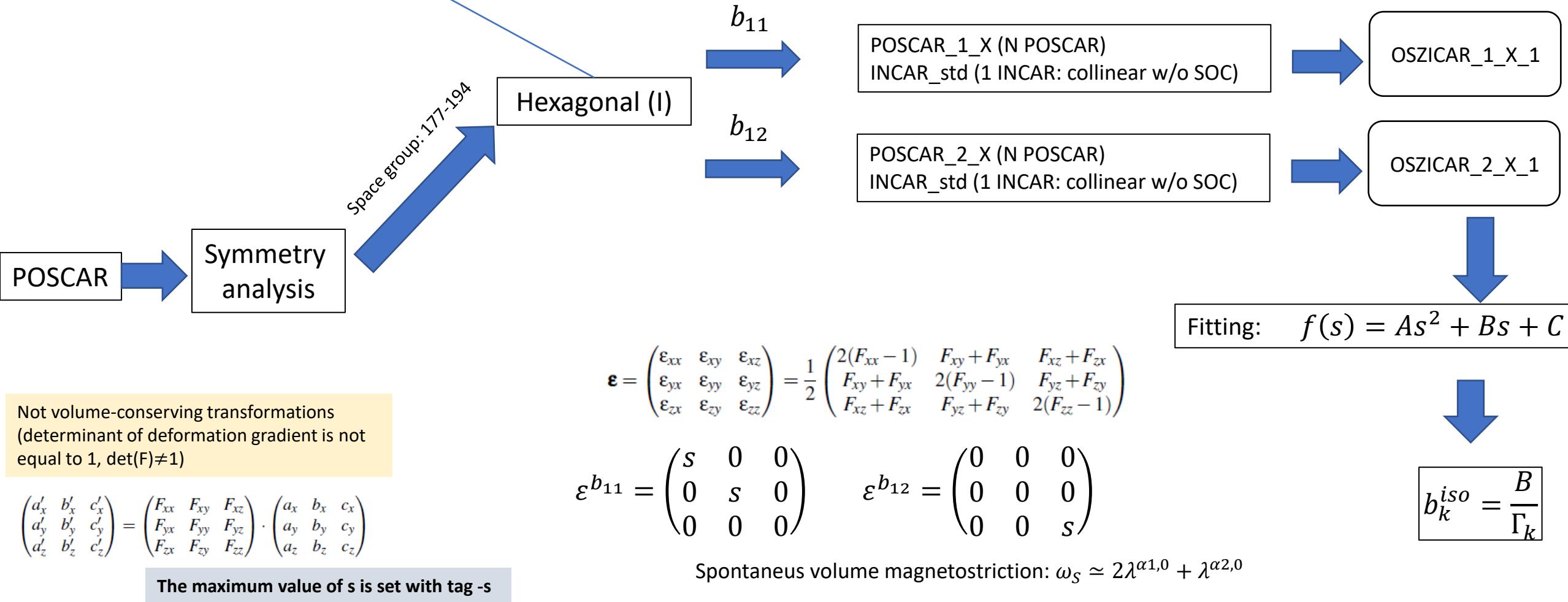
$$\lambda^{\epsilon} = \lambda^{\epsilon,2}$$

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

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

Spin-polarized calculation without SOC

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



Workflow

TRIGONAL (I)

SG 149-167

Trigonal (I)

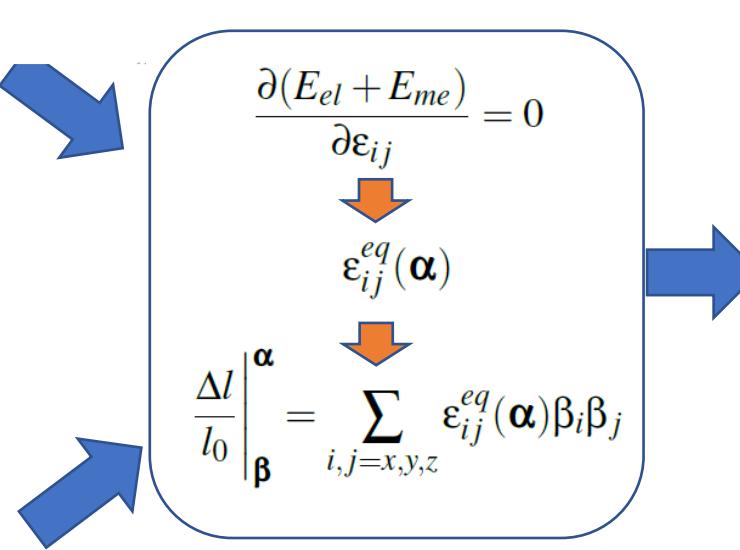
Workflow

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)

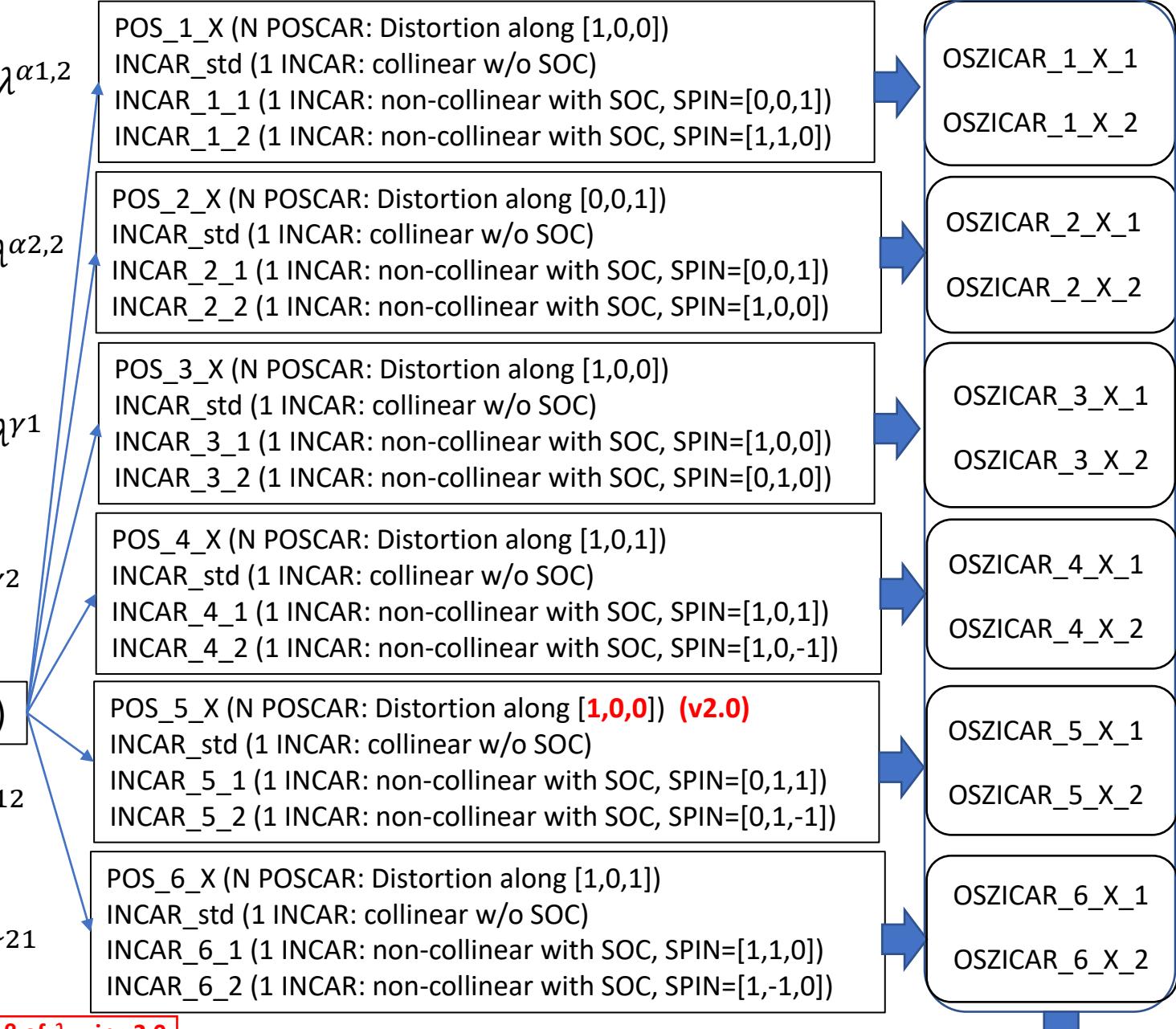
$$\frac{\Delta l}{l_0} \Bigg|_{\beta}^{\alpha} = \lambda^{\alpha 1,0} (\beta_x^2 + \beta_y^2) + \lambda^{\alpha 2,0} \beta_z^2 + \lambda^{\alpha 1,2} \left(\alpha_z^2 - \frac{1}{3} \right) (\beta_x^2 + \beta_y^2) \\ + \lambda^{\alpha 2,2} \left(\alpha_z^2 - \frac{1}{3} \right) \beta_z^2 \\ + \lambda^{\gamma,1}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



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

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

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



We have replaced the deformation gradient (F) and measuring length direction β of λ_{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)

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

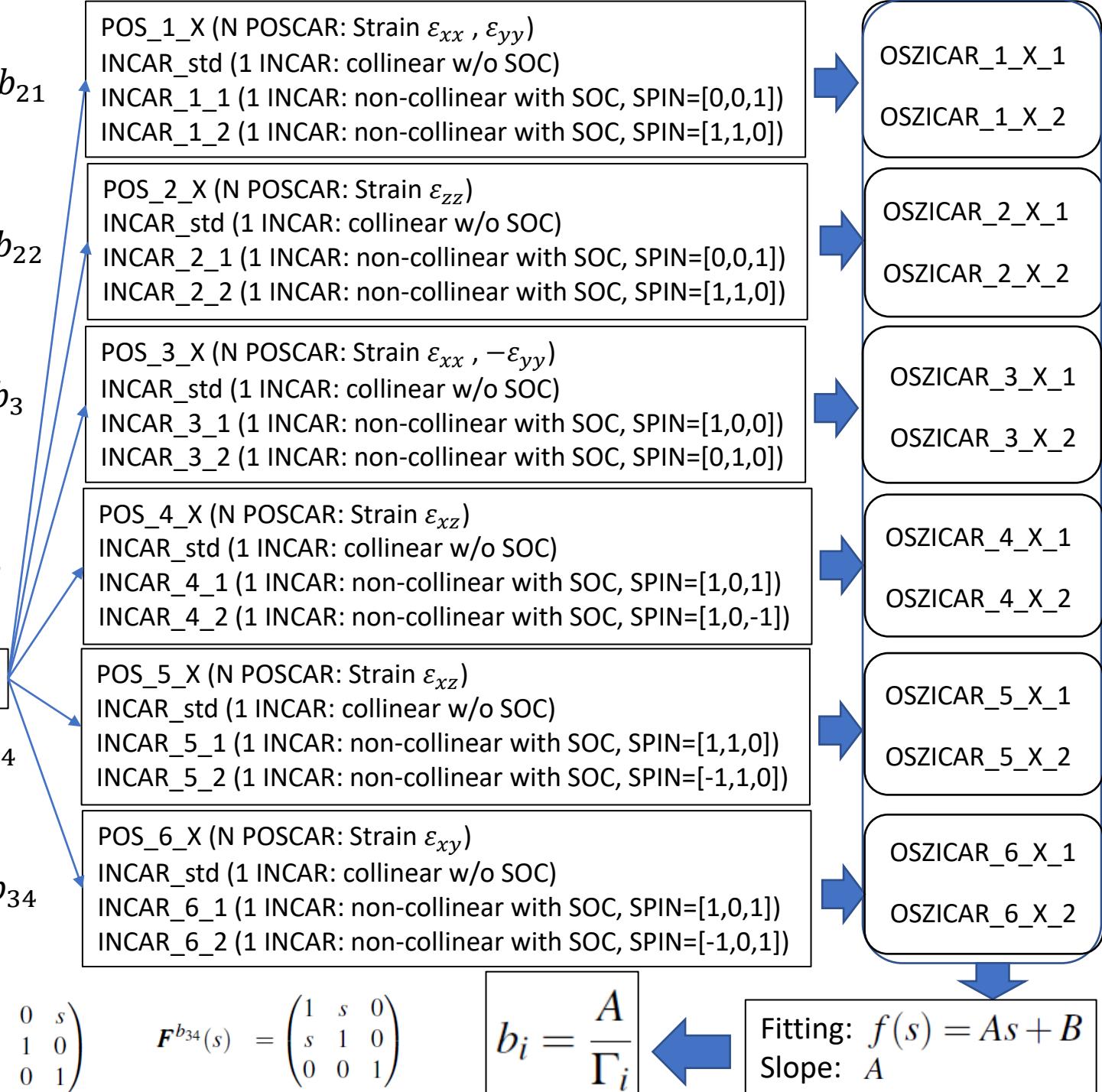
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$



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

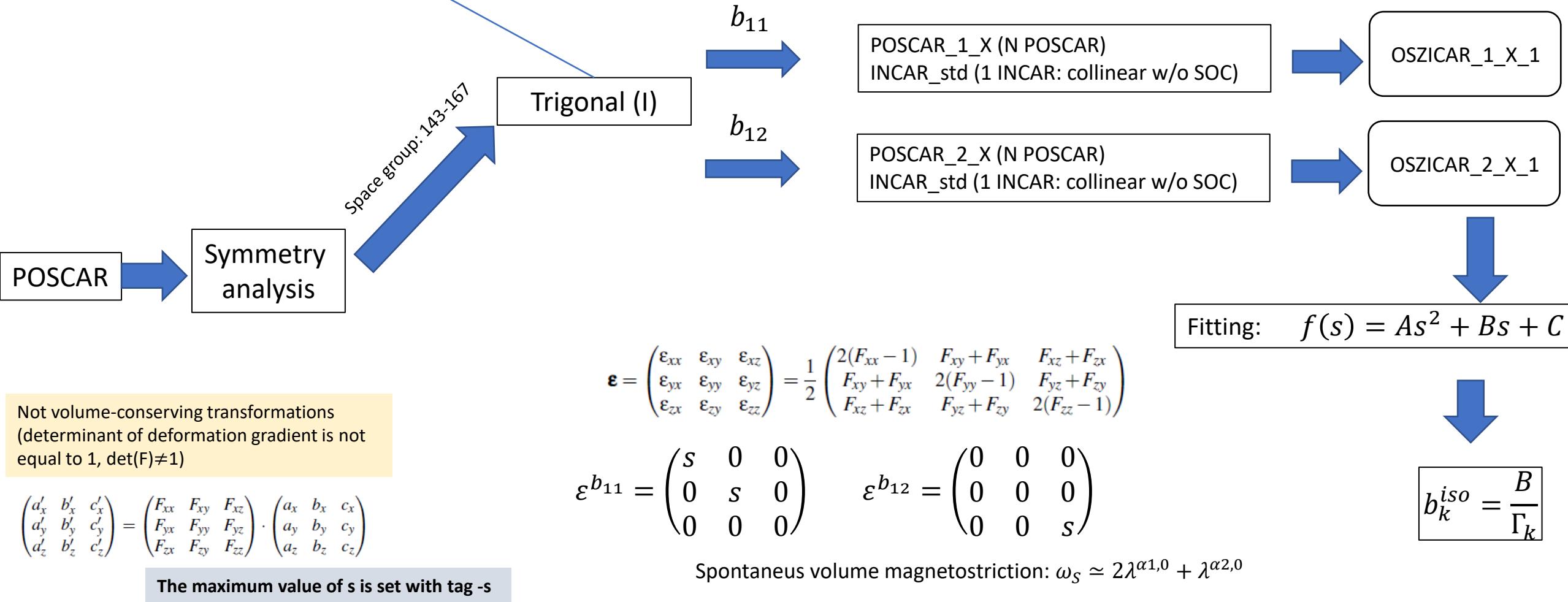
$$\mathbf{F}^{b_{21}}(s) = \begin{pmatrix} 1 + \frac{s}{2} & 0 & 0 \\ 0 & 1 + \frac{s}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_{22}}(s) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+s \end{pmatrix}$$

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



Spin-polarized calculation without SOC

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



Workflow

TETRAGONAL (I)

SG 89-142

Workflow

Tetragonal (I)

Elastic energy

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

Magnetoelastic energy

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

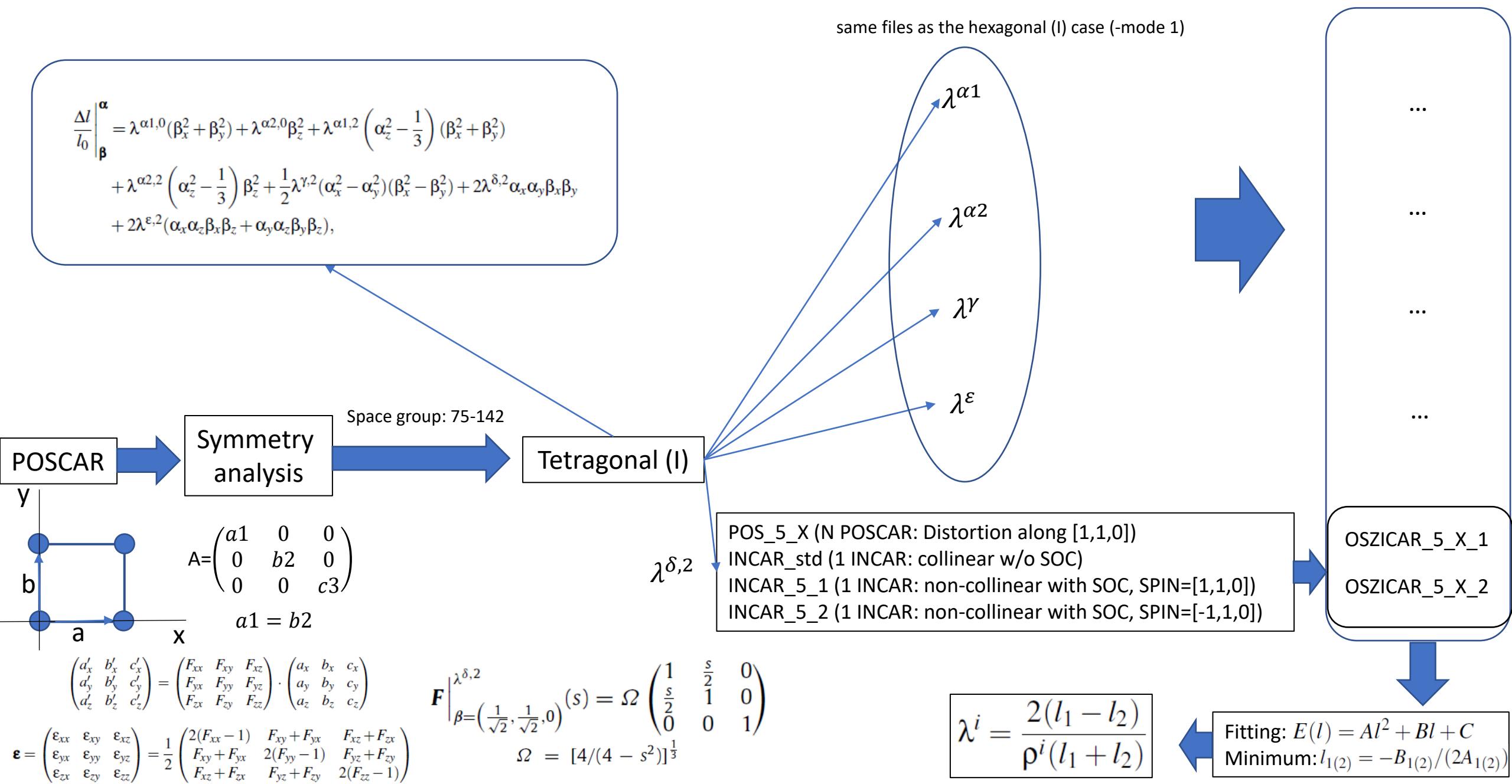
$$\frac{\partial(E_{el} + E_{me})}{\partial\epsilon_{ij}} = 0$$

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

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

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

Workflow (-mode 1)



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

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

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

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

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

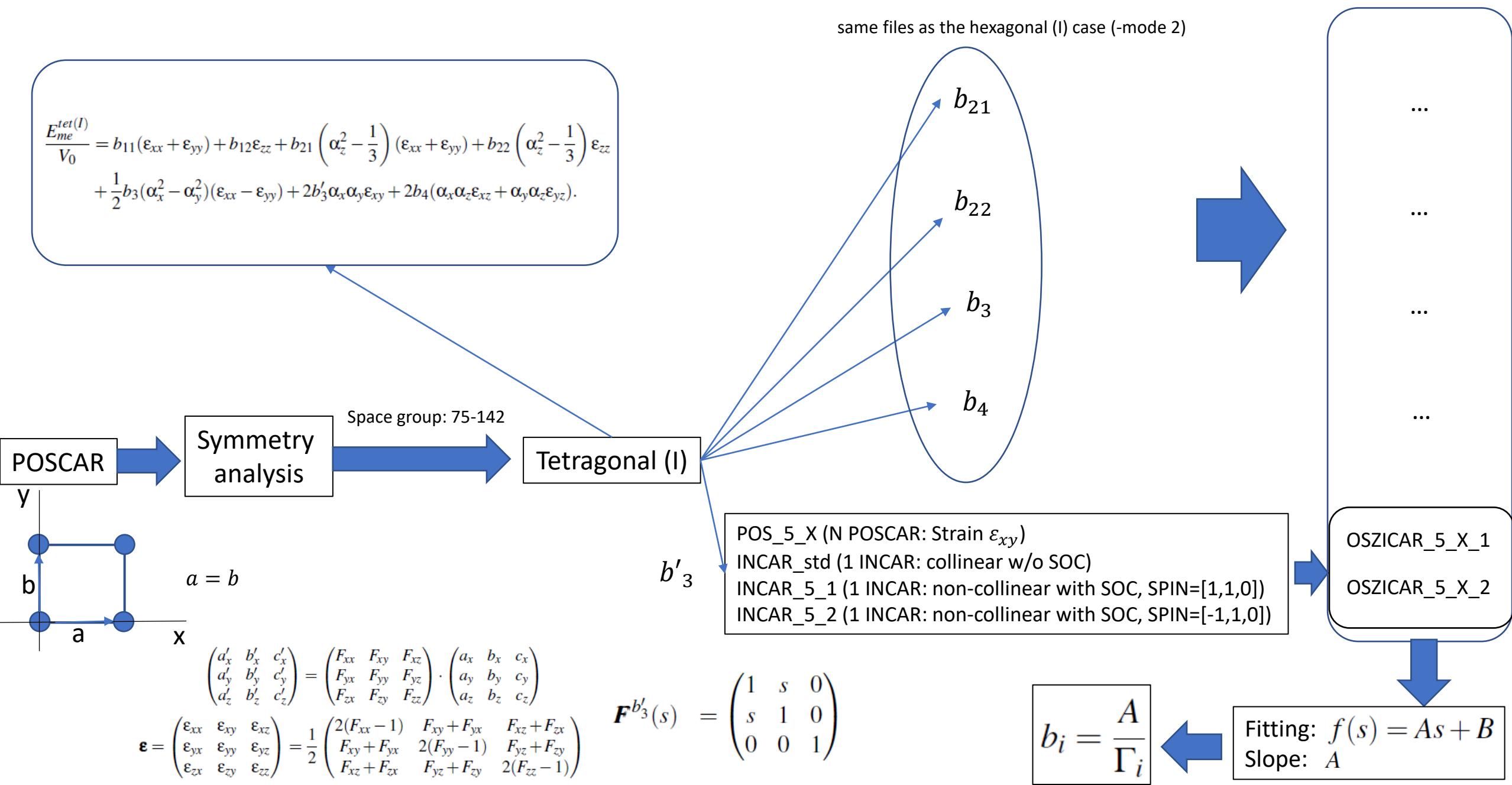
$$\lambda_2 = \frac{1}{2} \lambda^{\varepsilon,2} - \frac{1}{4} \lambda^{\alpha 2,2} - \frac{1}{4} \lambda^{\alpha 1,2} + \frac{1}{8} \lambda^{\gamma,2}$$

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

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

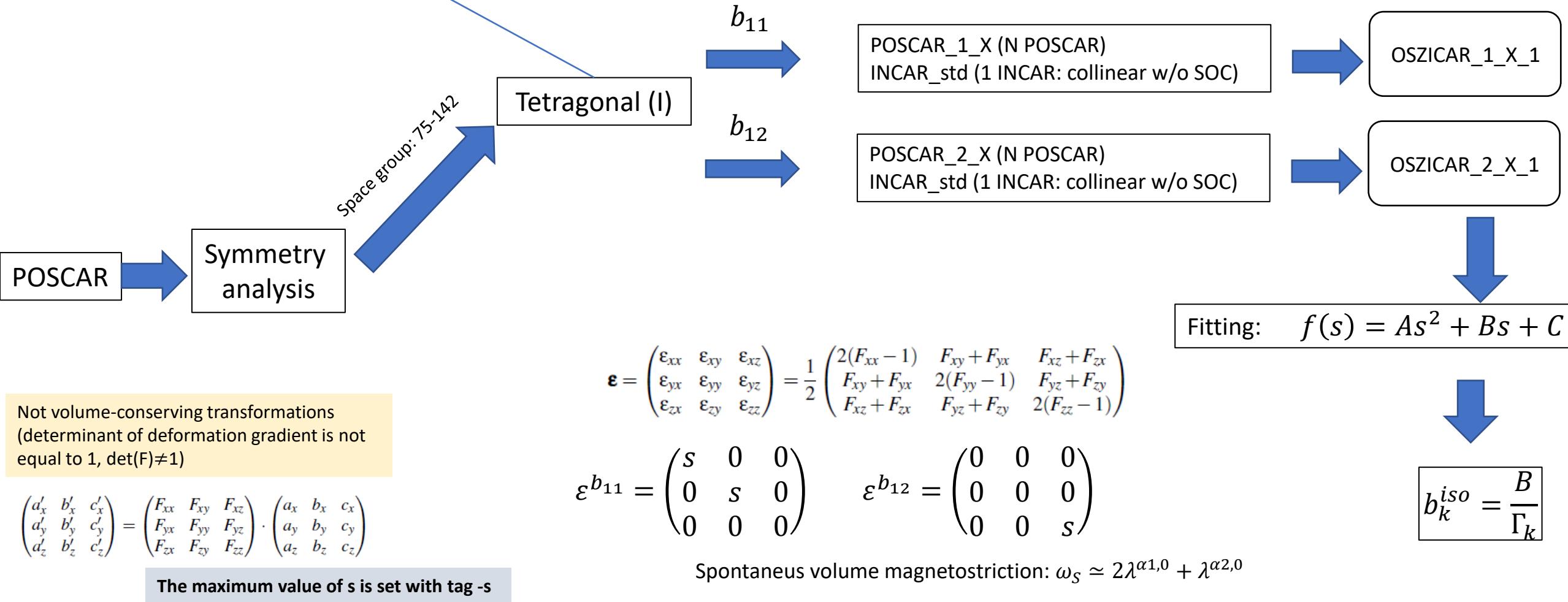
$$\lambda_5 = -\lambda^{\alpha 1,2} - \frac{1}{2} \lambda^{\gamma,2}.$$

Workflow (-mode 2)



Spin-polarized calculation without SOC

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



Workflow

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:

$$c < a < b$$

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

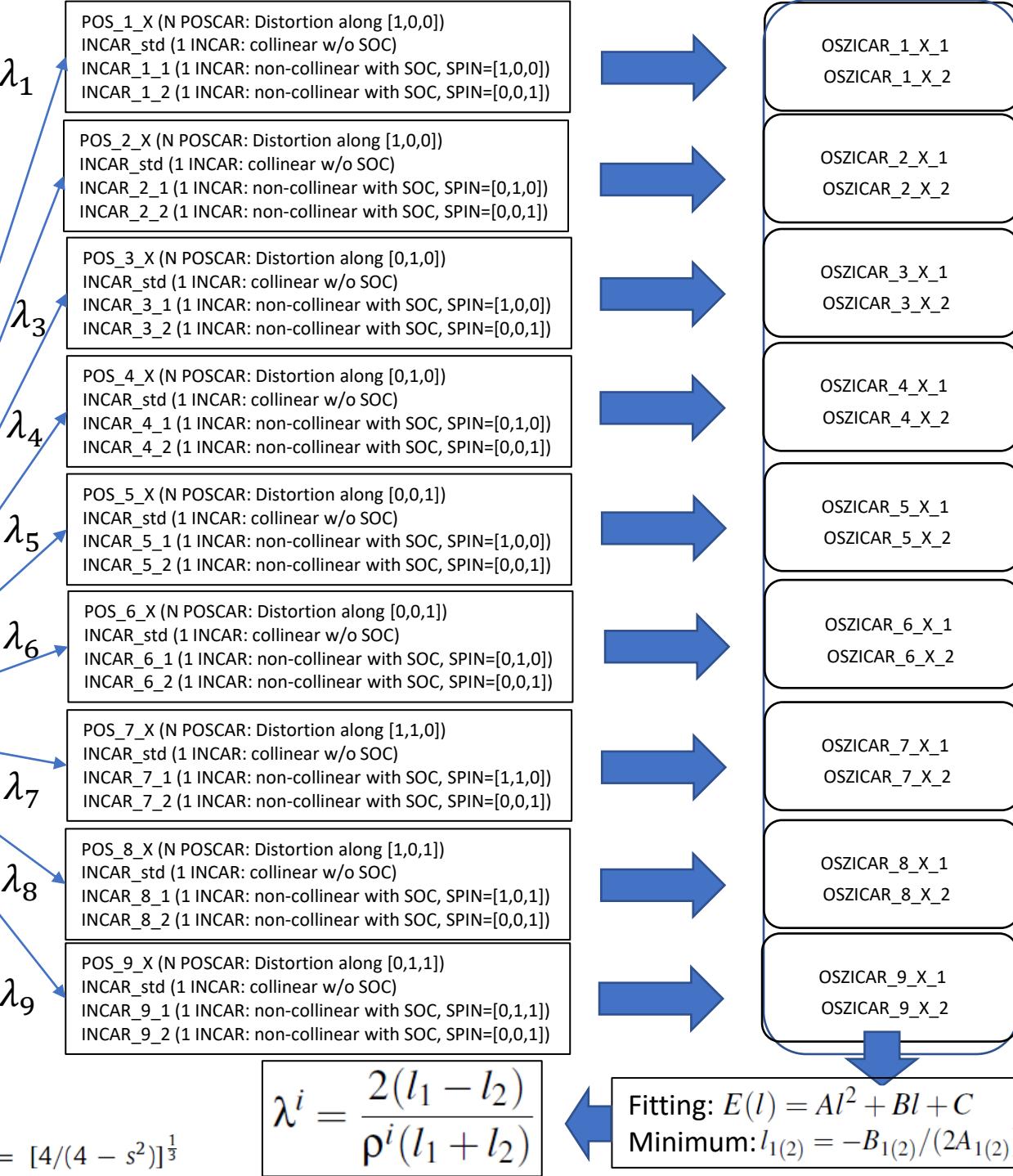
$$\mathbf{F} \Big|_{\beta=(0,1,0)}^{\lambda_4}(s) = \mathbf{F} \Big|_{\beta=(0,1,0)}^{\lambda_3}(s) = \begin{pmatrix} \frac{1}{\sqrt{1+s}} & 0 & 0 \\ 0 & 1+s & 0 \\ 0 & 0 & \frac{1}{\sqrt{1+s}} \end{pmatrix}$$

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

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

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

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



Orthorhombic

Workflow (-mode 2)

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

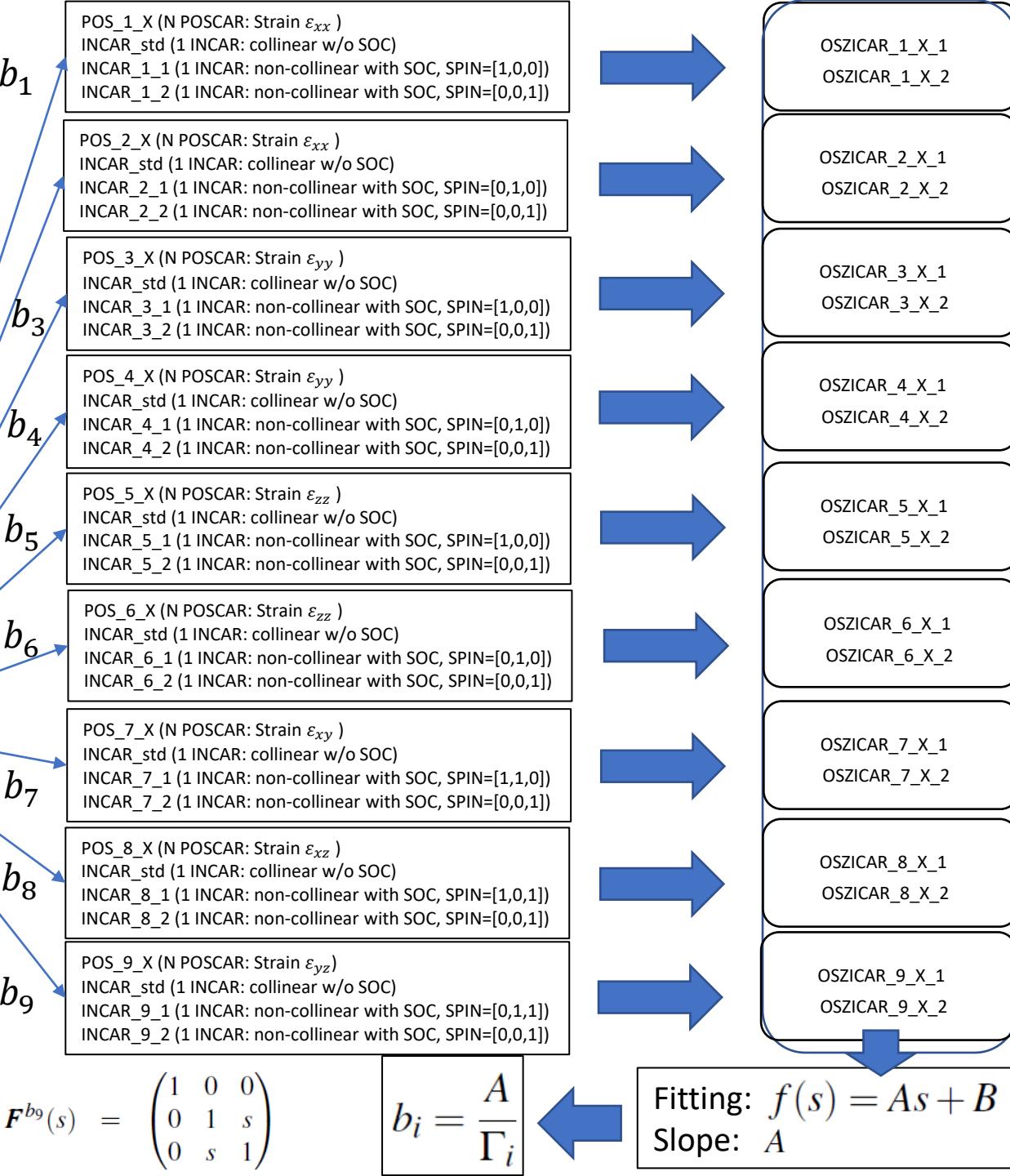


MAELAS uses the same lattice convention as AELAS code:

$$c < a < b$$

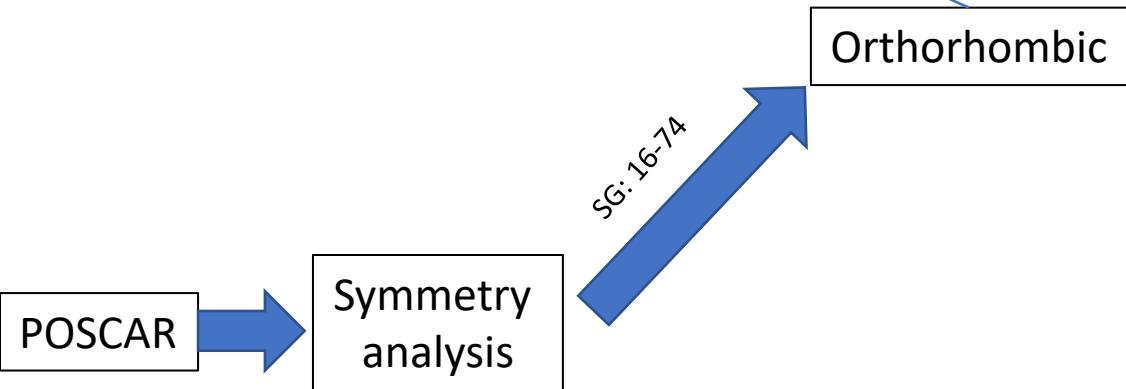
$$\mathbf{F}^{b_1}(s) = \mathbf{F}^{b_2}(s) = \begin{pmatrix} 1+s & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{F}^{b_5}(s) = \mathbf{F}^{b_6}(s) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+s \end{pmatrix}$$

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



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, $\det(F) \neq 1$)

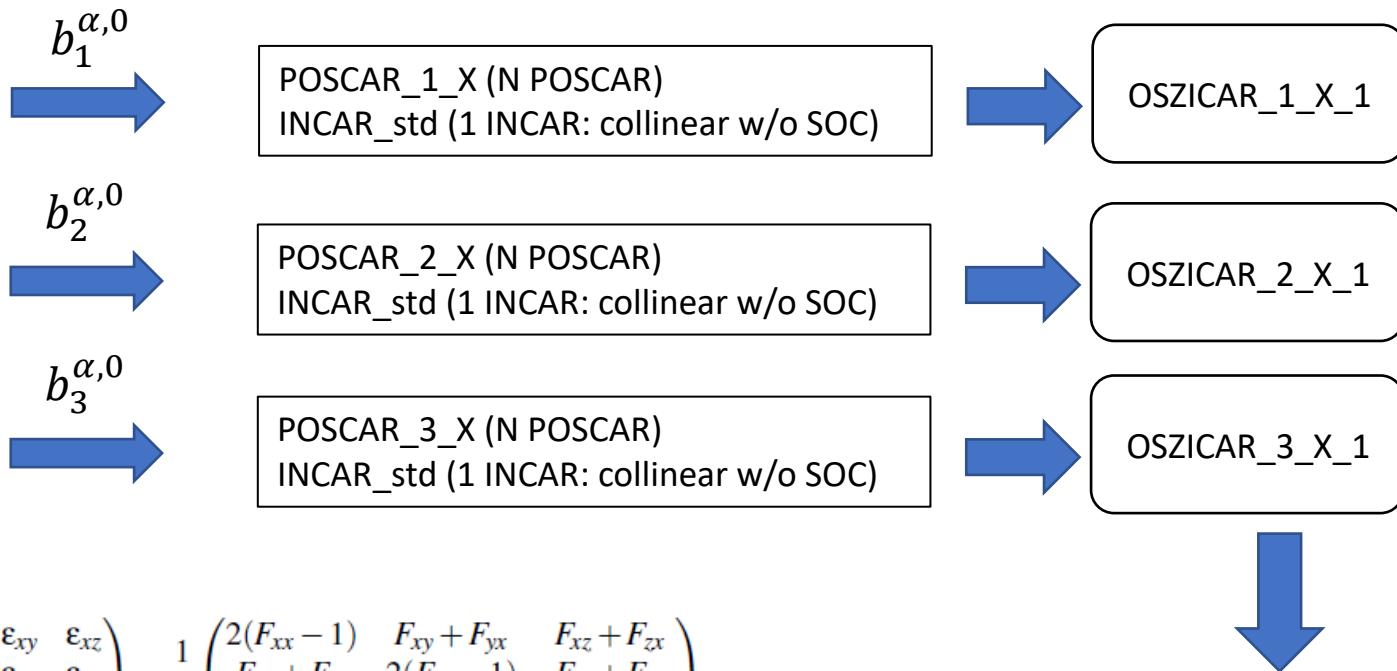
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

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)



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

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

$$\text{Spontaneous volume magnetostriiction: } \omega_S \simeq \lambda_a + \lambda_b + \lambda_c = \lambda_1^{\alpha,0} + \frac{1}{3} \lambda_2^{\alpha,0} \quad \xleftarrow{\text{Lacheisserie convention}}$$

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

BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

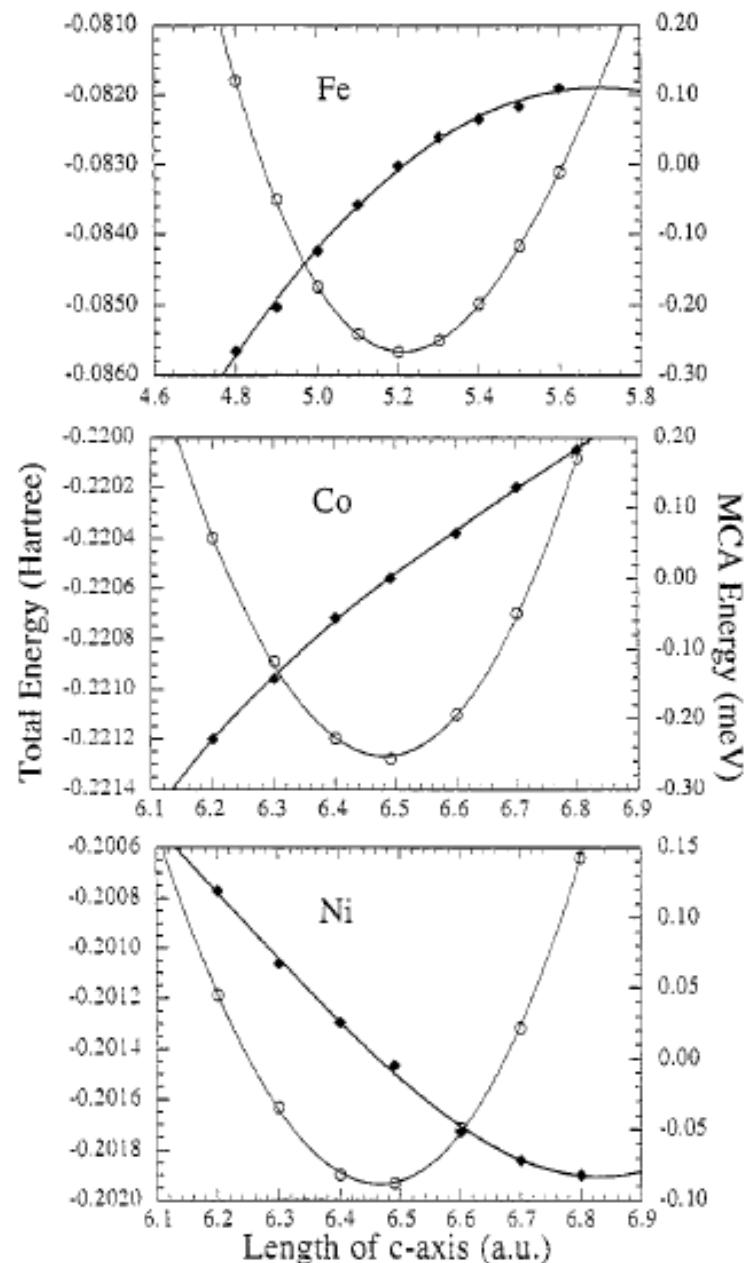
Cubic systems: Itinerant magnets

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

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

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

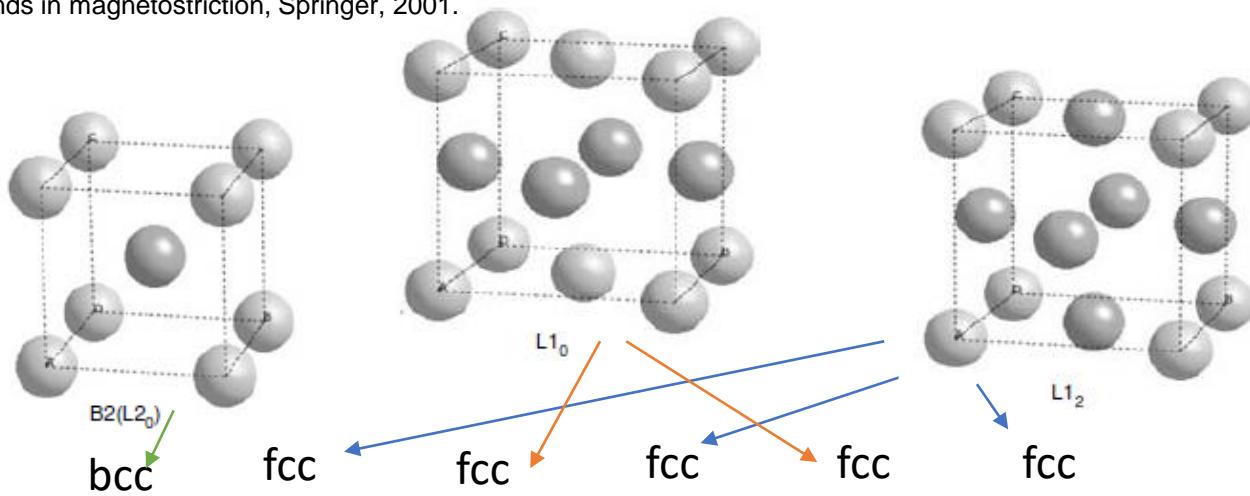
	$T = 4.2\text{ K}$		Room Temperature		
	$\lambda_{100}(\lambda^{z,2})$	$\lambda_{111}(\lambda^{z,2})$	$\lambda_{100}(\lambda^{z,2})$	$\lambda_{111}(\lambda^{z,2})$	Polycrystal λ_s
<i>3d Metals</i>					
BCC-Fe	26	-30	21	-21	-7
HCP-Co ^a	(-150)	(45)	(-140)	(50)	(-62)
FCC-Ni	-60	-35	-46	-24	-34
BCC-FeCo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



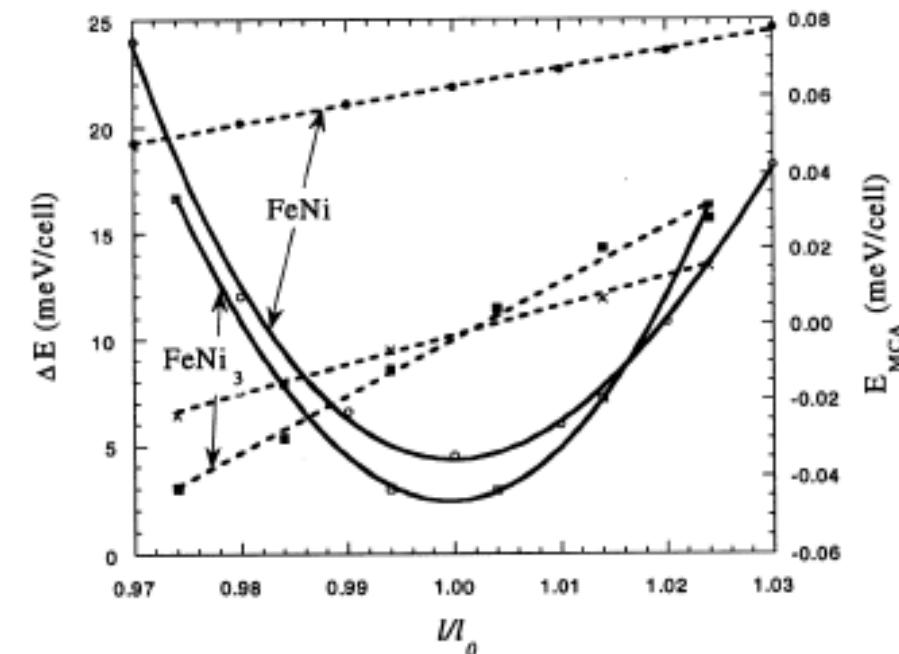
BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

Cubic systems: Itinerant magnets

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



	FeCo	FeCo ₃	FeNi	FeNi ₃	CoNi	CoNi ₃
a (a.u.)	5.38 (5.39)	6.70	6.76 (6.76)	6.70 (6.71)	6.62 (6.67)	6.66 (6.65)
c (a.u.)	5.38 (5.39)	6.70	6.76 (6.76)	6.70 (6.71)	6.78 (6.67)	6.66 (6.65)
$E_{MCA}(\mu\text{eV})$	0	0	63	0	143	0
σ	-0.35	-0.36	-0.33	-0.35	-0.34	-0.36
$\lambda_{001}(10^{-6})$	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
λ_{001} (GdCo_2)	-407	-1200
λ_{111} (GdCo_2)	19	< 10
λ_{001} (SmCo_2)	-290	---
λ_{001} (ErCo_2)	-516	-1000
λ_{001} (GdFe_2)	44	39

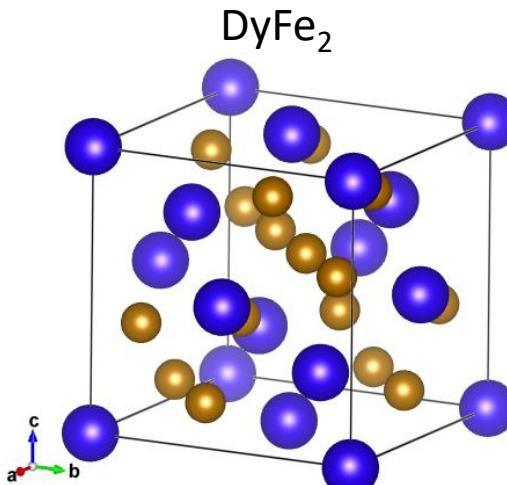
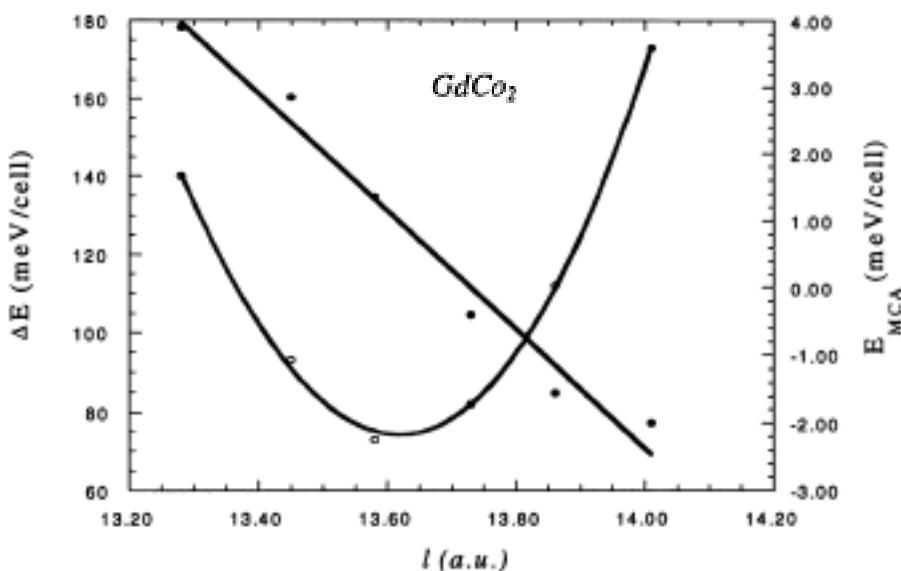


Table 16-10. Low-temperature magnetostriction constants for RCO_2 crystals [from Levitin and Markosyan (1990) unless otherwise noted].

R in RCO_2	$10^6 \lambda_{111}$	$10^6 \lambda_{100}$	T_c (K) ^a
Gd	$< 10^{-5}$	-1200	409
Tb	4500	-1200 ^b	256
Dy	5000 ^{b, c}	-2000 ^d -1300 ^e	159
Ho	300, 600 ^c	-2000	85
Er	-2500	-1000	36
Tm	-4100 ^b	750 ^c	18

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

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

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

Compound	$\frac{1}{2}\lambda_{111} (10^{-6})$ (calculated at 0 K)	$\frac{1}{2}\lambda_{111} (10^{-6})$ (measured at room temperature)	T_c
SmFe_2	-4800	-3150	676
TbFe_2	6600	3690	697, 711
DyFe_2	6300	1890	635
HoFe_2	2400	288	606
ErFe_2	-2250	-450	590, 597
TmFe_2	-5550	-315	560

BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

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

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

^{a)} After Mishima et al. (1976).

^{b)} After Rhyne (1972).

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

Table 14.4. Magnetostriiction constants of spinel-type ferrites (mainly after Tsuya⁴⁹).

Composition	λ_{100}	λ_{111}	Temp.	Ref.
MnFe ₂ O ₄	-31×10^{-6}	6.5×10^{-6}		38
Fe ₃ O ₄	-20	78	20°C	39
Co _{0.8} Fe _{2.2} O ₄	-590	120	20°C	40
NiFe ₂ O ₄	-42	-14		41
CuFe ₂ O ₄	-57.5	4.7		42
MgFe ₂ O ₄	-10.5	1.7		41
Li _{0.5} Fe _{2.5} O ₄	-26	-3.8		38
Mn _{0.6} Fe _{2.4} O ₄	-5	45	20°C	43
Mn _{0.28} Zn _{0.16} Fe _{2.37} O ₄	-0.5	36		44
Mn _{1.04} Zn _{0.22} Fe _{1.82} O ₄	-22	3		44
Mg _{0.63} Fe _{1.26} Mn _{1.11} O ₄	49.5	-2.6		45
Co _{0.32} Zn _{0.22} Fe _{2.2} O ₄	-210	110		40
Co _{0.1} Ni _{0.9} Fe ₂ O ₄	-109	-38.6		46
Li _{0.43} Zn _{0.14} Fe _{2.07} O ₄	-27.1	3.2		41
Li _{0.5} Al _{0.35} Fe _{2.15} O ₄	-19.1	0.2		47
Li _{0.56} Ti _{0.10} Fe _{2.35} O ₄	-16.0	4.3		47
Li _{0.5} Ga _{1.4} Fe _{1.1} O ₄	-12.3	2.9		47
Ti _{0.18} Fe _{2.82} O ₄	47	109	290 K	48
		142	80 K	48
Ti _{0.56} Fe _{2.44} O ₄	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}^{exact} (GPa)	b	b^{exact} (MPa)	λ	λ^{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	λ_{001}	26.0317	0.015	0.013	$7 \cdot 10^{-6}$	$8 \cdot 10^{-6}$
	C_{12}	138	b_2	10.9	λ_{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	$\lambda^{\varepsilon,2}$	-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	λ_{12}	-377.9282	-28.1	46.8	$1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
	C_{44}	118	b_{34}	55.4	λ_{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	$\lambda^{\varepsilon,2}$	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	λ_1	-632.9614	37.4	24.7	$7 \cdot 10^{-6}$	$5 \cdot 10^{-6}$
	C_{12}	45	b_2	-34.2	λ_2	681.5787	6.9	7.9	$6 \cdot 10^{-6}$	$6 \cdot 10^{-6}$
	C_{13}	48	b_3	60.7	λ_3	-752.4503	19.6	0.03	$7 \cdot 10^{-6}$	$7 \cdot 10^{-6}$
	C_{23}	55	b_4	-34.3	λ_4	471.7839	-11.6	-18.5	$6 \cdot 10^{-6}$	$6 \cdot 10^{-6}$
	C_{22}	102	b_5	-42.4	λ_5	809.6944	-46.8	-10.8	$7 \cdot 10^{-6}$	$5 \cdot 10^{-6}$
	C_{33}	141	b_6	55.4	λ_6	-808.9638	-7.6	-5.6	$6 \cdot 10^{-6}$	$6 \cdot 10^{-6}$
	C_{44}	40	b_7	35.4	λ_7	-284.9353	47.3	54.3	$6 \cdot 10^{-6}$	$7 \cdot 10^{-6}$
	C_{55}	27	b_8	-22.6	λ_8	253.4425	43.2	11.6	$9 \cdot 10^{-6}$	$8 \cdot 10^{-6}$
	C_{66}	39	b_9	38.7	λ_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 Fe_2Si 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	λ_{001}	-78.4 ^b	-72.7	-60 ^a	b_1	15.5 ^b	14.4	9.9 ^b
			λ_{111}	-46.1 ^b	-44.0	-35 ^a	b_2	19.4 ^b	18.5	13.9 ^b
BCC Fe	Cubic (I) SG 229	GGA	λ_{001}	25.7 ^b	29.1	26 ^a	b_1	-5.2 ^b	-5.9	-4.1 ^b
			λ_{111}	17.2 ^b	15.7	-30 ^a	b_2	-5.3 ^b	-4.9	10.9 ^b
HCP Co	Hexagonal (I) SG 194	LSDA+U $J = 0.8\text{eV}$ $U = 3\text{eV}$	$\lambda^{a1,2} (\lambda_A)$	111 (-109) ^b	75 (-74)	95 (-66) ^c	b_{21}	-21.3 ^b	-16.2	-31.9 ^b
			$\lambda^{a2,2} (\lambda_B)$	-251 (-114) ^b	-156 (-77)	-126 (-123) ^c	b_{22}	48.3 ^b	28.4	25.5 ^b
			$\lambda^{c1,2} (\lambda_C)$	4 (251) ^b	2 (156)	57 (126) ^c	b_3	-0.7 ^b	-0.4	-8.1 ^b
			$\lambda^{c2,2} (\lambda_D)$	-51 (10) ^b	-57 (-8)	-286 (-128) ^c	b_4	7.1 ^b	7.9	42.9 ^b
Fe_2Si	Trigonal (I) SG 164	GGA	$\lambda^{a1,2}$	-9 ^b [v1.0]	-5		b_{21}	3.1 ^b [v1.0]	0.7	
			$\lambda^{a2,2}$	15 ^b [v1.0]	17		b_{22}	-4.2 ^b [v1.0]	-6.2	
			$\lambda^{c1,2}$	8 ^b [v1.0]	6		b_3	-0.7 ^b [v1.0]	-1.9	
			$\lambda^{c2,2}$	29 ^b [v1.0]	29		b_4	3.3 ^b [v1.0]	-3.5	
			λ_{12}	-3 ^b [v1.0]	-5		b_{14}	-1.4 ^b [v1.0]	1.9	
		GGA	λ_{21}	-13 ^b [v1.0]	-14		b_{34}	-0.4 ^b [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 ₀ FePd	Tetragonal (I) SG 123	GGA	λ_{12}	-11 [v2.0]			b_{14}	2.0 [v2.0]		
			λ_{21}	-13 [v2.0]			b_{34}	2.2 [v2.0]		
			$\lambda^{a1,2}$	-21 ^b	-41		b_{21}	-2.4 ^b	5.1	
			$\lambda^{a2,2}$	79 ^b	82		b_{22}	-15.2 ^b	-10.7	
			$\lambda^{c1,2}$	31 ^b	27		b_3	-7.9 ^b	-6.9	
YCo	Orthorhombic SG 63	LSDA+U $J = 0.8\text{eV}$ $U = 1.9\text{eV}$	$\lambda^{c2,2}$	28 ^b	26		b_4	-5.6 ^b	-5.3	
			$\lambda^{c3,2}$	106 ^b	106		b'_3	-7.9 ^b	-7.9	
			λ_1	-11 ^b	-36		b_1	-1.7 ^b	0.8	
			λ_2	32 ^b	57		b_2	1.2 ^b	-2.9	
			λ_3	70 ^b	75		b_3	-3.8 ^b	-2.2	
			λ_4	-74 ^b	-64		b_4	4.3 ^b	0.6	
			λ_5	-30 ^b	-35		b_5	-0.1 ^b	1.7	
			λ_6	7 ^b	24		b_6	2.3 ^b	-2.2	
			λ_7	36 ^b	38		b_7	-4.4 ^b	-4.2	
			λ_8	-20 ^b	-34		b_8	1.1 ^b	1.8	
			λ_9	35 ^b	-7		b_9	-8.7 ^b	-0.5	

^aRef.[9], ^bRef.[1], ^cRef.[10]

MAELAS TESTS: FCC Ni (-mode 1)

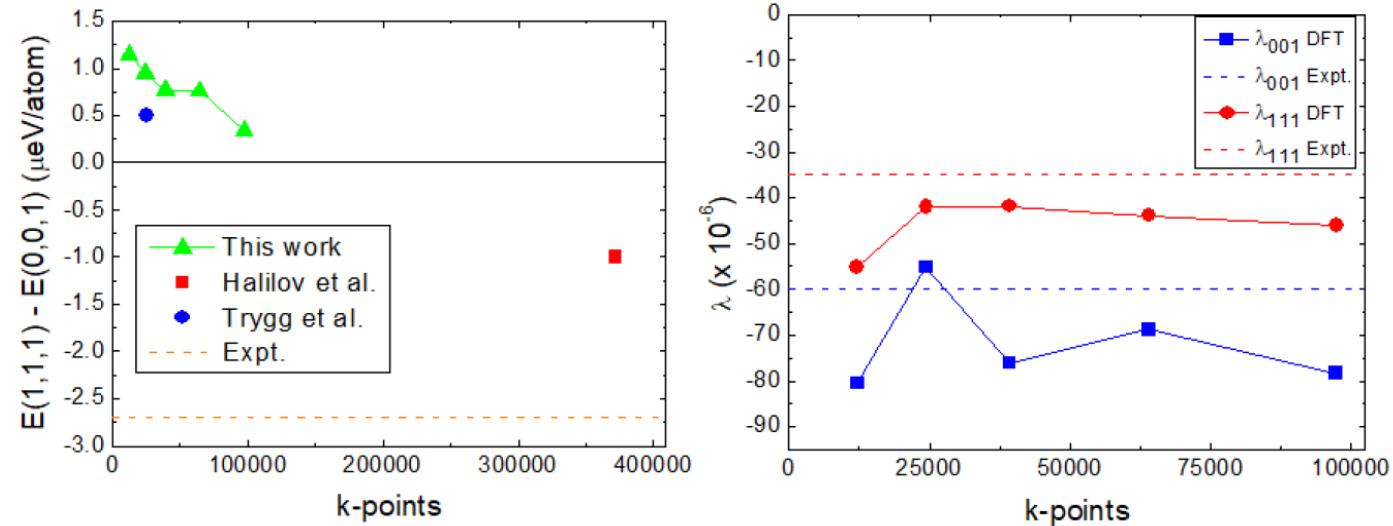


Figure 3: Calculation of (left) MAE of the unstrained unit cell and (right) magnetostrictive coefficients for FCC Ni as a function of k-points.

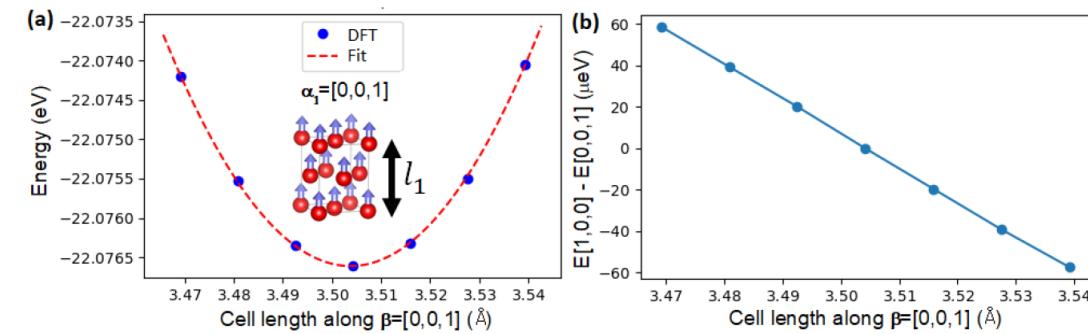


Figure 4: Calculation of λ_{001} for FCC Ni using MAELAS. (Left) Quadratic curve fit to the energy versus cell length along $\beta = (0, 0, 1)$ with spin direction $\alpha_1 = (0, 0, 1)$. (Right) Energy difference between states with spin directions $\alpha_2 = (1, 0, 0)$ and $\alpha_1 = (0, 0, 1)$ against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

MAELAS TESTS: FCC Ni (-mode 2)

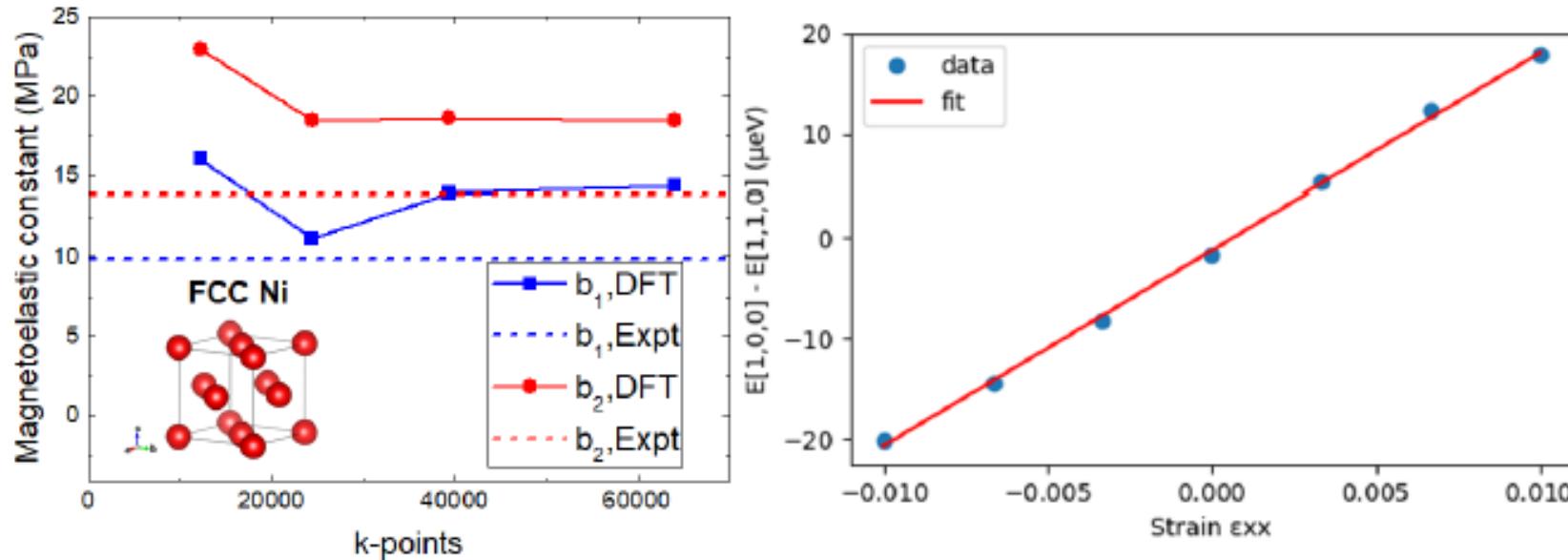


Figure 3: (Left) Calculated magnetoelastic constants for FCC Ni with the new method implemented in MAELAS v2.0 (-mode 2). (Right) Calculation of b_1 for FCC Ni through a linear fitting of the energy difference between magnetization directions $\alpha_1 = (1, 0, 0)$ and $\alpha_2 = (1/\sqrt{2}, 1/\sqrt{2},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

MAELAS TESTS: BCC Fe (-mode 1)

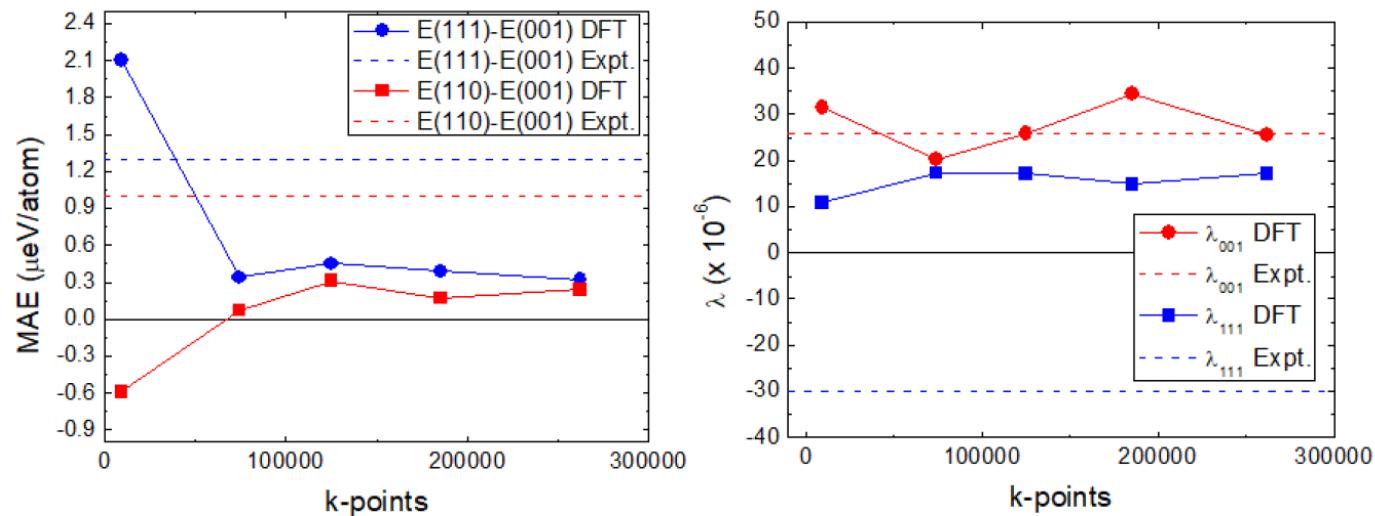


Figure 5: Calculation of (left) MAE of the unstrained unit cell and (right) magnetostrictive coefficients for BCC Fe as a function of k-points.

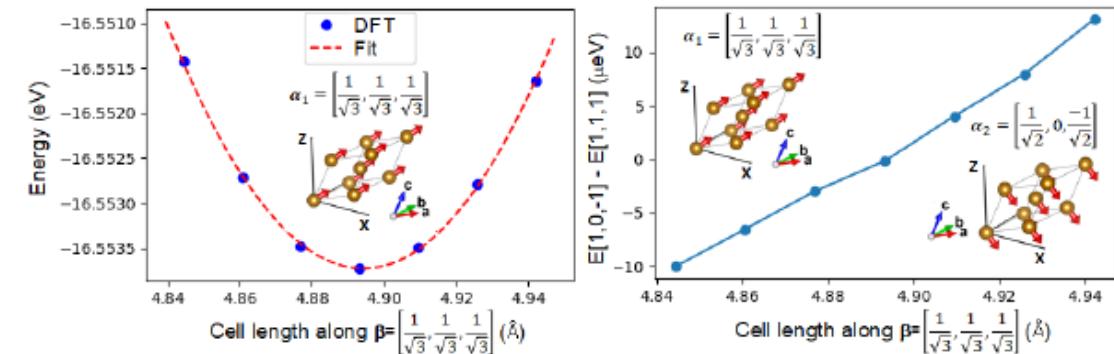


Figure 6: Calculation of λ_{111} for BCC Fe using MAELAS. (Left) Quadratic curve fit to the energy versus cell length along $\beta = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$ with spin direction $\alpha_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$. (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)

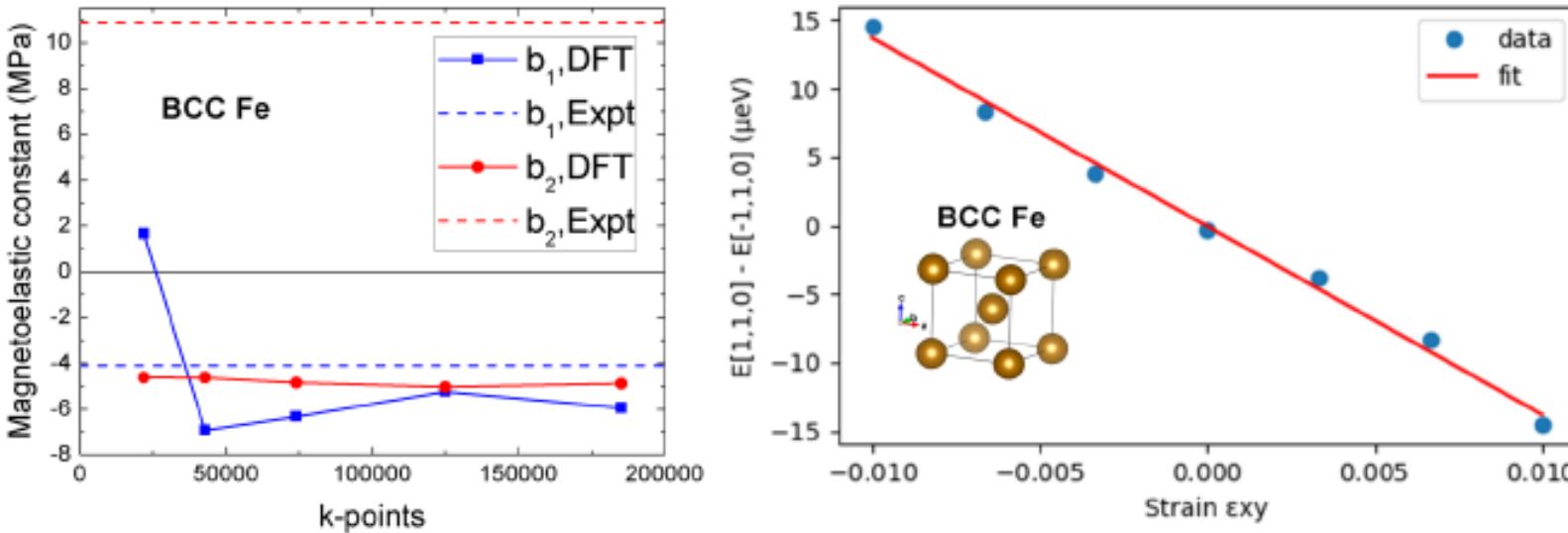


Figure 4: (Left) Calculated magnetoelastic constants for BCC Fe with the new method implemented in MAELAS v2.0 (-mode 2). (Right) Calculation of b_2 for BCC Fe through a linear fitting of the energy difference between magnetization directions $\alpha_1 = (1/\sqrt{2}, 1/\sqrt{2}, 0)$ and $\alpha_2 = (-1/\sqrt{2},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

MAELAS TESTS: HCP Co (-mode 1)

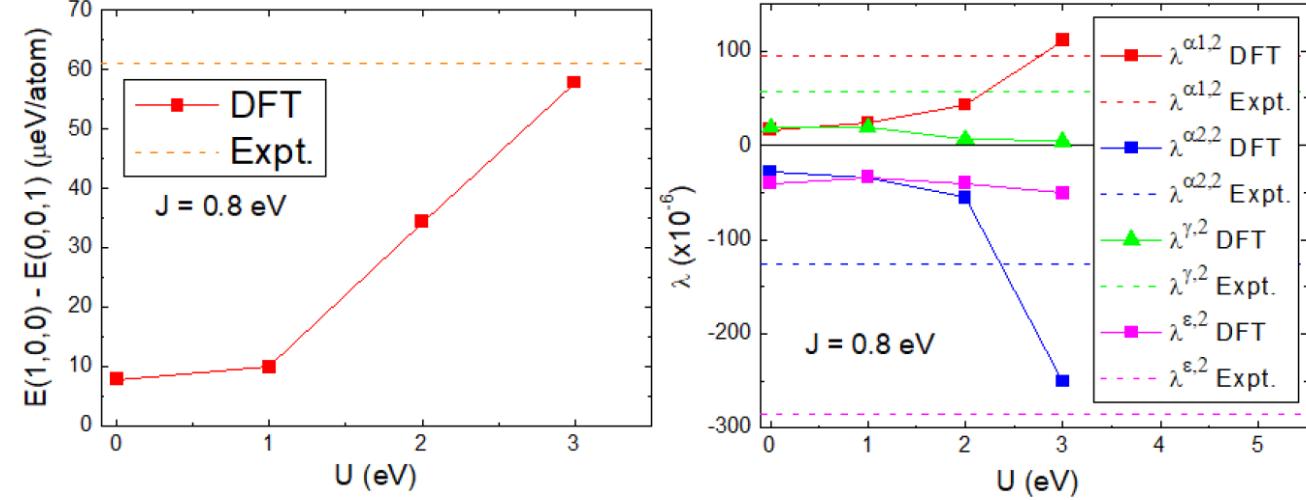


Figure 8: Calculation of (left) MAE of the unstrained unit cell and (right) magnetostrictive coefficients for HCP Co using the LSDA+U approach with different values of parameter U .

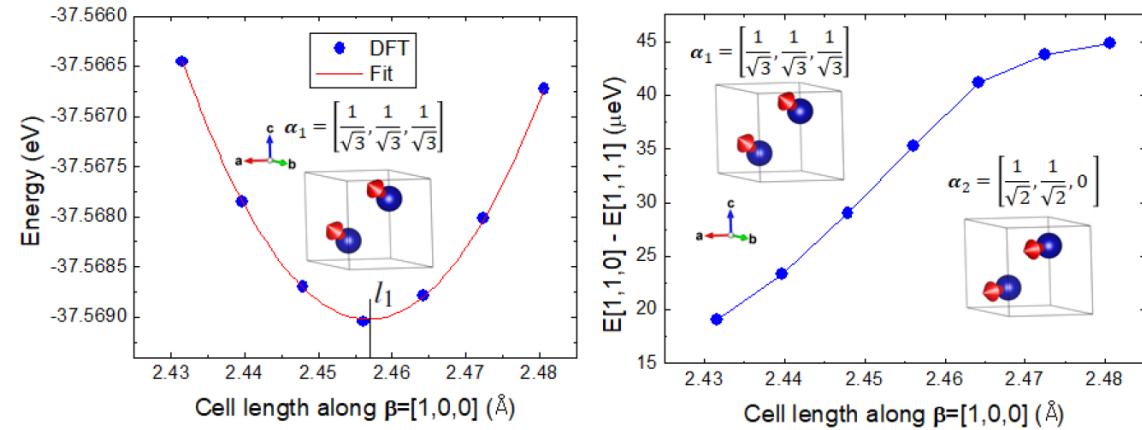


Figure 7: Calculation of $\lambda^{\alpha_{1,2}}$ for HCP Co using MAELAS with the meta-GGA functional SCAN. (Left) Quadratic curve fit to the energy versus cell length along $\beta = (1, 0, 0)$ with spin direction $\alpha_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$.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

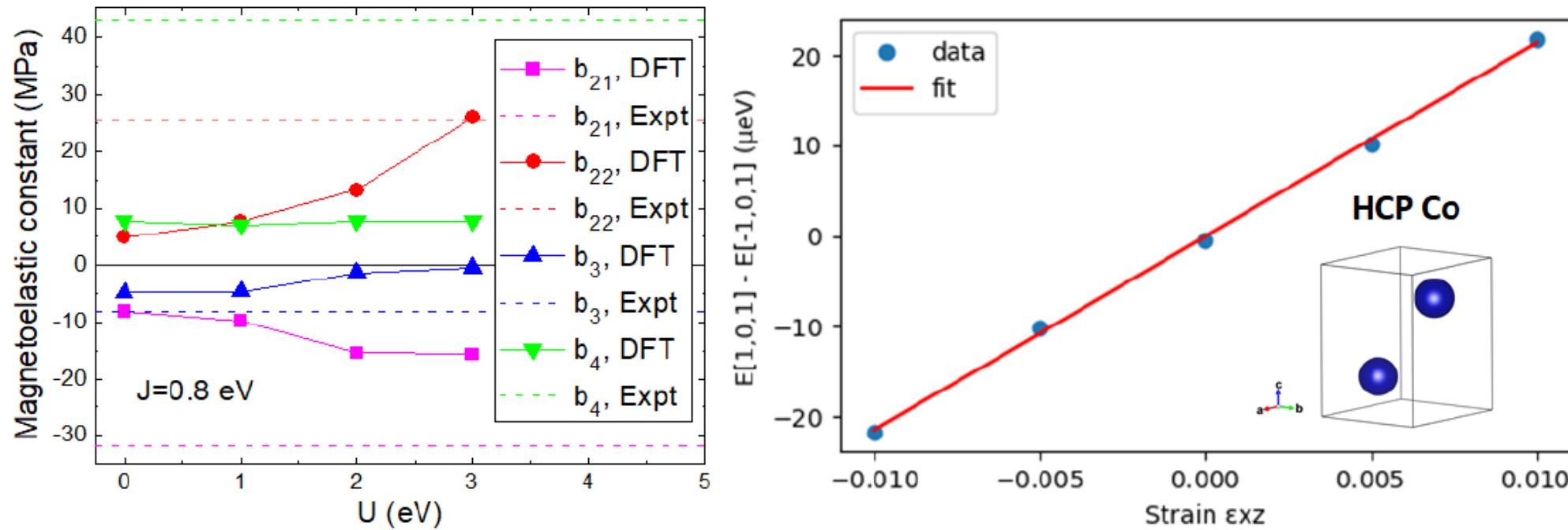


Figure 5: (Left) Calculated magnetoelastic constants for HCP Co with the new method implemented in MAELAS v2.0 (-mode 2) for different values of the Hubbard U parameter. (Right) Calculation of b_4 for HCP Co through a linear fitting of the energy difference between magnetization directions $\alpha_1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

Visualization tool MAELASviewer

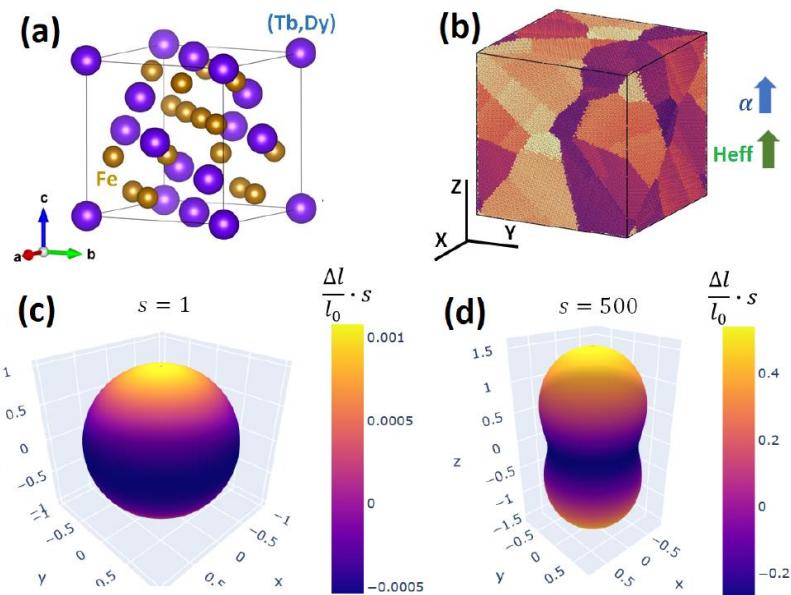
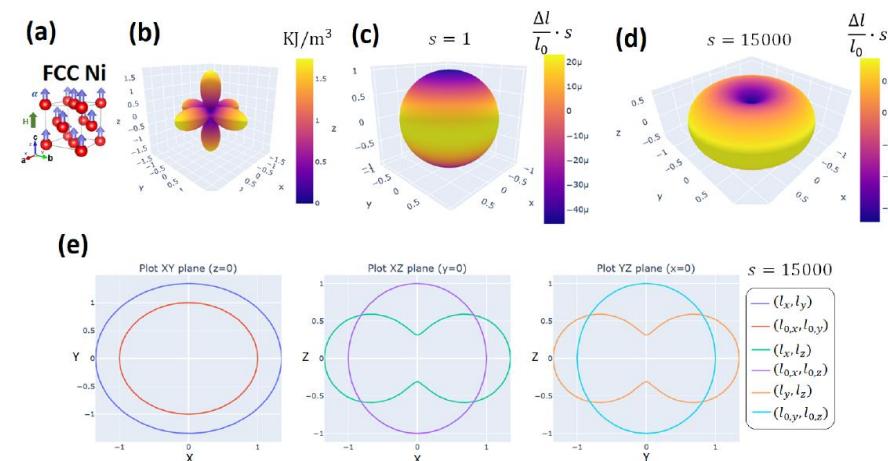
We have also developed an online visualization tool called MAELASviewer that is available at

<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.



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