MAELAS code

User manual v1.0

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MAELAS: MAgneto-ELAStic properties calculation via computational high-throughput approach

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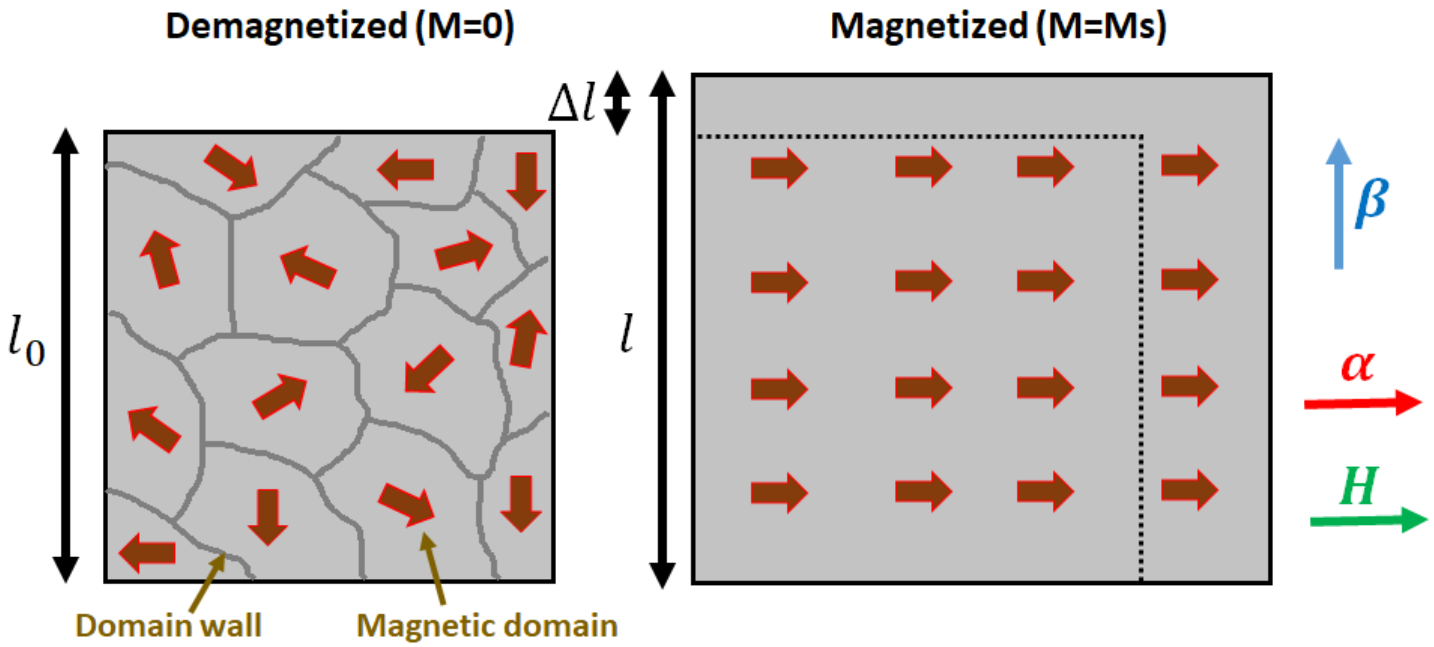
WHAT IS MAGNETOSTRICTION?

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 (|**α**|=1)
β=Measured length direction (|**β**|=1)
H=External magnetic field

relative length change

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

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

WHAT IS MAELAS CODE?

- MAELAS code is a software to calculate anisotropic magnetostrictive coefficients and magnetoelastic constants up to second order.
- It generates required input files for VASP code to perform Density Functional Theory calculations, and it deduces the value of magnetostrictive coefficients from the calculated energies given by VASP.
- If the elastic tensor is provided, then it can also calculate the magnetoelastic constants.
- MAELAS can also be used with other DFT codes instead of VASP, after file conversion to VASP format files.

INSTALLATION

The MAELAS code requires to have Python3(>=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)

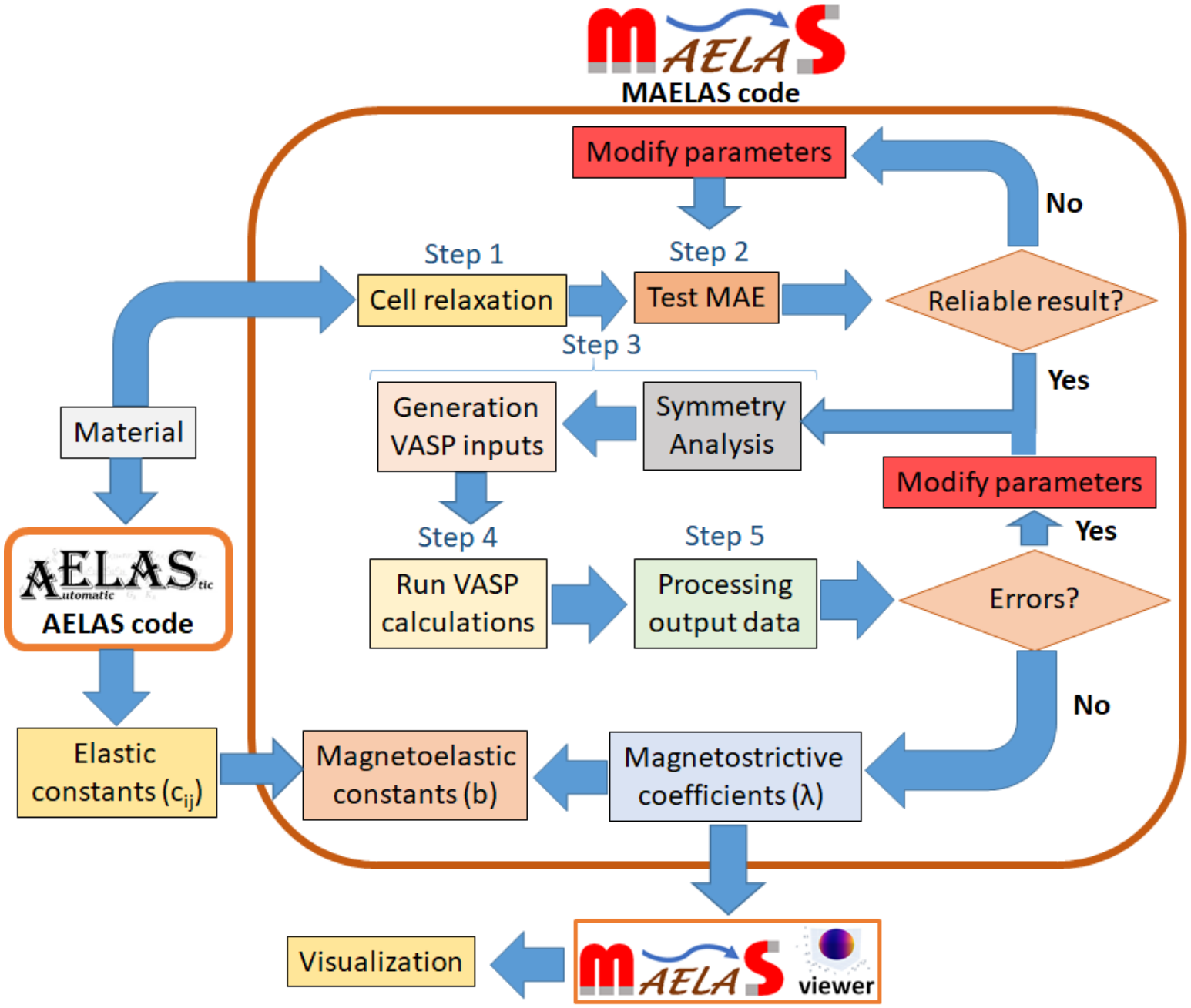
More available options for the installation can be found in the file INSTALL. By default, the executable file "maelas" is installed in the folder /home/$USER/.local/bin/ where $USER is the name of your username folder. This folder should be included to the PATH variable by adding in the file /home/$USER/.bashrc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

Step 1: Cell relaxation

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

maelas -r -i POSCAR0 -k 40

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

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

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

qsub vasp_jsub_rlx

This procedure might be helpful for high-throughput routines. Note that the user might need to modify vasp_jsub_rlx (it is in PBS Pro format) depending on the cluster or local computer batch scheduling. More options can be added in vasp_jsub_rlx file through the terminal command line, to see them just type

maelas –h

Note that generated INCAR and KPOINTS files contain standard setting for cell relaxation. The user might need to change these files in order to include more advanced settings. In case your structure is already relaxed or you do not want to perform a cell relaxation, then you can skip this step and move to step 2.

HOW TO USE MAELAS CODE

Step 2: Test MAE

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

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

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

POSCAR_0_0 (it is the same POSCAR as)
INCAR_0_C (non-collinear calculation where C=1,2 is the spin orientation case)
INCAR_std (collinear calculation to generate the WAVECAR and CHGCAR files to run non-collinear calculations)
KPOINTS (file for the kpoint generation of VASP)
vasp_mae, vasp_mae_jsub and vasp_mae_0 (interconnected bash scripts to run VASP calculations automatically)
vasp_mae_cp_oszicar (bash script to get the calculated OSZICAR_0_0_C files after VASP calculation is finished)

The generated files vasp_mae, vasp_mae_jsub and vasp_mae_0 are interconnected scripts to submit jobs in HPC facilities. One needs only to execute the file vasp_mae in order to run all VASP jobs automatically. You can specify some job settings in these scripts by adding more tags in the command line. For instance,

maelas -m -i POSCAR_rlx -k 70 -s1 1 0 0 -s2 0 0 1 -t 48 -c 24 -q qprod -a OPEN-00-00 -f /scratch/example_mag

where -t 48 indicates that the number of maximum CPU hours for the VASP calculation is 48 hours,-c 24 means that the number of cores for the VASP calculation is 24, -q qprod set to production queuethe type of queue in HPC facilities, -a OPEN-00-00 is the project identification number for running jobs in HPC facilities and -f /scratch/example_mag is the folder where you want to run VASP calculations. This procedure might be helpful for high-throughput routines. Note that the user might need to modify vasp_mae_jsub (it is in PBS Pro format) depending on the cluster or local computer batch scheduling. More options can be added in these script files through the terminal command line, to see them just type

maelas -h

HOW TO USE MAELAS CODE

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

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

maelas -g -i POSCAR_rlx -k 70 -n 7 -s 0.01

where -g indicates that you want to generate input VASP files for the calculation of anisotropic magnetostrictive coefficients, -i POSCAR_rlx is the initial relaxed POSCAR file (you can name it whatever you want), -k 70 is the length parameter that determines a regular mesh of k-points, -n 7 means that it will generate 7 distorted states for each magentostriction mode and -s 0.01 is the maximum value of parameter s for the deformation gradient Fij(s) to deform the structure. It will generate the following files:

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

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

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

where -t 48 indicates that the number of maximum CPU hours for the VASP calculation is 48 hours,-c 24 means that the number of cores for the VASP calculation is 24, -q qprod set the type of queue in HPC facilities, -a OPEN-00-00 is the project identification number for running jobs in HPC facilities and -f /scratch/example_mag is the folder where you want to run VASP calculations. This procedure might be helpful for high-throughput routines. Note that the user might need to modify vasp_jsub (it is in PBS Pro format) depending on the cluster or local computer batch scheduling. More options can be added in these script files through the terminal command line, to see them just type
maelas –h

HOW TO USE MAELAS CODE

Step 4: Run VASP calculations

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

./vasp_maelas

This will launch independent jobs for each POSCAR_A_B. Each job will run 3 VASP calculations: a collinear one (VASP executable "vasp_std") to generate WAVECAR and CHGCAR files, and two non-collinear (VASP executable "vasp_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 vasp_jsub depending on the cluster or local computer queuing system.

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

./vasp_cp_oszicar

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

<u>VASP executables:</u>

"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 and magnetoelastic constants

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

POSCAR_rlx (the relaxed POSCAR file used as input in step 3)
POSCAR_A_B (distorted POSCAR generated in step 3)
OSZICAR_A_B_C (non-collinear OSZICAR files calculated in step 4 for each POSCAR_A_B and INCAR_A_C)

Next, in the terminal go to this folder a type

maelas -d -i POSCAR_rlx -n 7

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

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

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

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

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

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

Format of the elastic tensor file

```
Elastic tensor:

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

HOW TO USE MAELAS CODE

Full list of arguments in 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
-i POS Name of the initial non-distorted POSCAR file (default: POSCAR)
-n NDIST Number of distorted states for each magnetostriction mode (default: 7)
-s STRAIN Maximum value of the parameter 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.
-d Derivation of magnetostrictive coefficients from the energy written in the OSZICAR files.
-r Generation of required VASP files for the cell relaxation
-m Generation of required VASP files to test MAE
-s1 s1x s1y s1z First spin direction to calculate MAE
-s2 s2x s2y s2z Second spin direction to calculate MAE
-b Calculation of the magnetoelastic constants from the calculated magnetostrictive coefficients and provided elastic tensor.
-e ELAS File with the elastic tensor data in the same format and units (GPa) as it is written by ELAS code (file ELADAT).
-sp SYMPRE Tolerance for symmetry finding (default: 0.01)
-sa SYMANG Angle tolerance for symmetry finding (default: 5.0)
-sg SG0 Space group number 1-230. If it is equal to 0, then it will be determined by a symmetry analysis (default: 0)
-c CORE Number of cores for the VASP calculation (default: 24)
-t TIME Number of maximum CPU hours for the VASP calculation (default: 48)
-f VASP_FOLD Folder where you will run VASP calculations (default: /scratch)
-mp MPI Command for mpi run of VASP (default: mpiexec.hydra)
-a P_ID Project id for running jobs in HPC facilities (default: OPEN-X-X)
-l LOAD_MODULE Module of VASP that should be loaded (default: VASP/5.4.4-intel-2017c-mkl=cluster)
-q QUEUE Type of queue to be used for VASP calculations in HPC facilities (default: qprod)

HOW TO USE MAELAS CODE

Summary: In a nutshell

Step 1: Cell relaxation

maelas -r -i POSCAR0 -k 40

qsub vasp_jsub_rlx

Step 2: Test MAE

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

./vasp_mae

./vasp_mae_cp_oszicar

Step 3: Generate VASP inputs for calculation of magnetostrictive coefficients

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

Step 4: Run VASP calculations

./vasp_maelas

./vasp_cp_oszicar

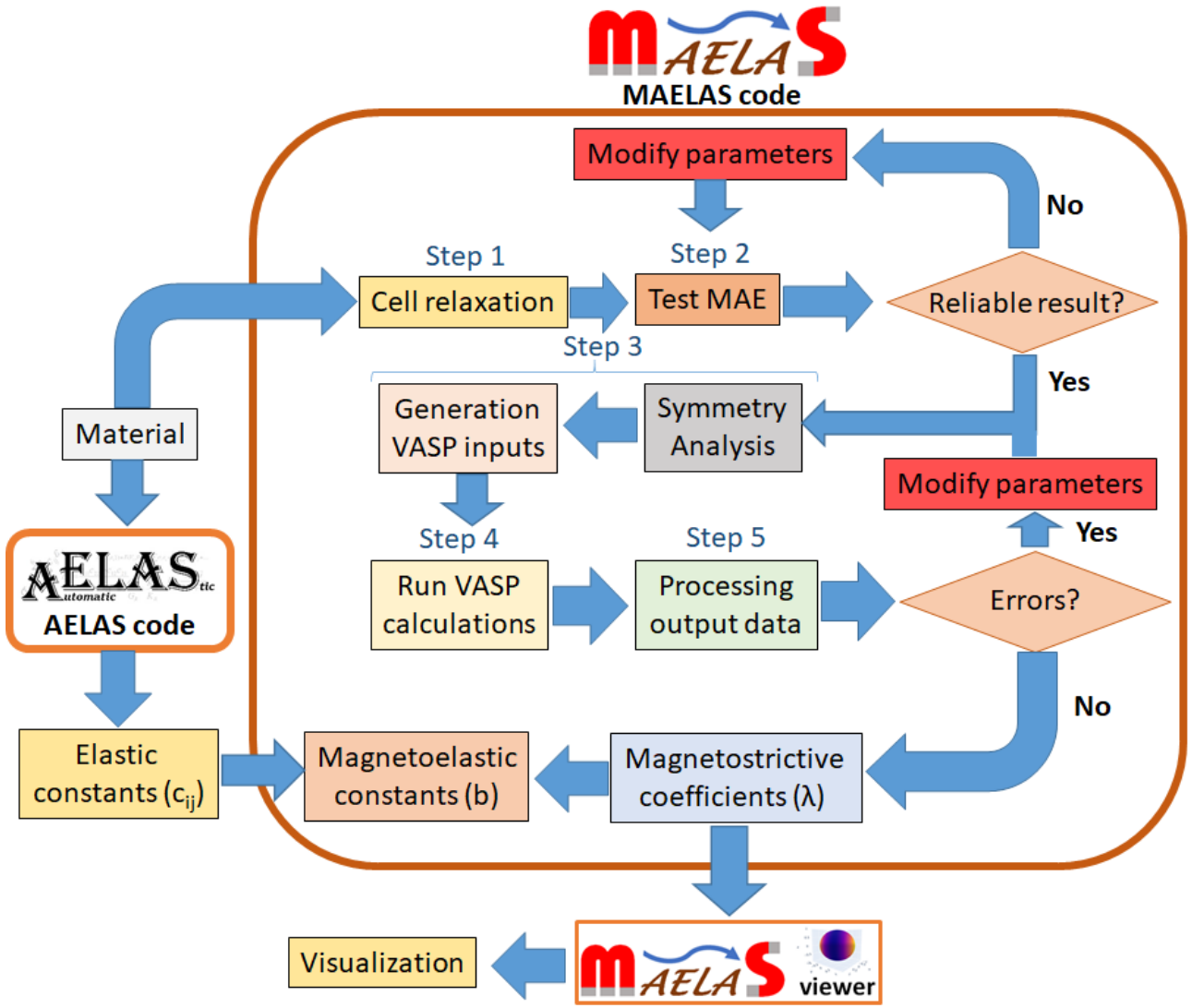
Step 5: Derivation of anisotropic magnetostrictive coefficients

maelas -d -i POSCAR_rlx -n 7

Step 5: Derivation of anisotropic magnetostrictive coefficients and magnetoelastic constants

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

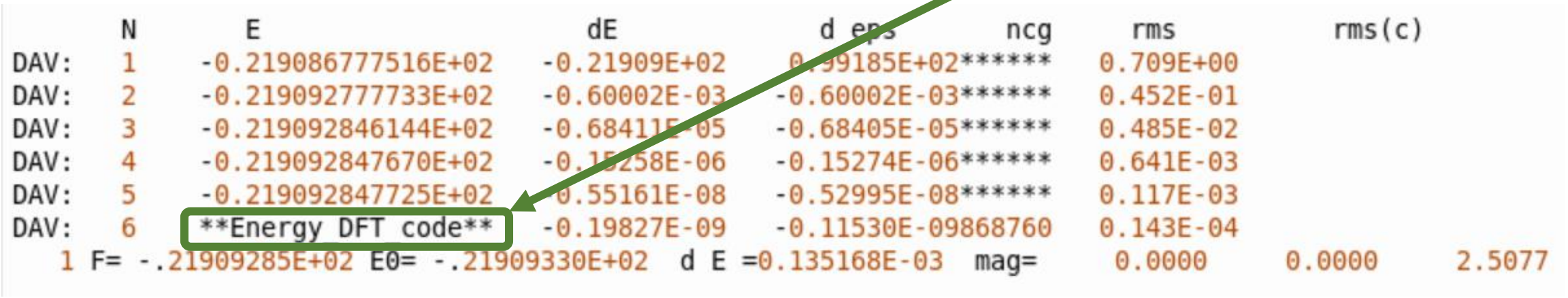
See all optional arguments: maelas -h



HOW TO USE MAELAS CODE

Using MAELAS with other 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**":



HOW TO USE MAELAS CODE

Interface between LAMMPS and MAELAS

(Conversion files)

ATOMSK

LAMMPS format file (.lmp)
Equilibrium cell
Name file: cell.lmp

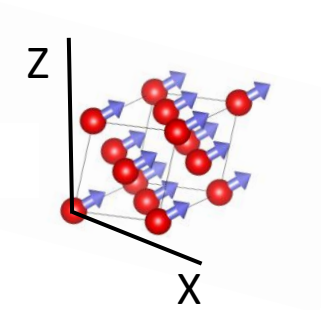
Program
Atomsk

VASP format file
(POSCAR.vasp)
Equilibrium cell
Name file: POSCAR_rlx.vasp

MAELAS

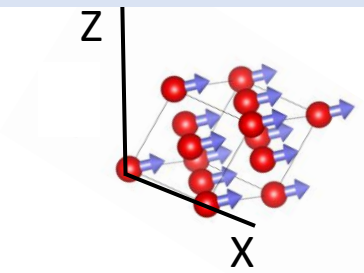
Program
MAELAS

VASP format file
(POSCAR.vasp)
Distorted cell
Name file: POSCAR_X_X.vasp



Program
Atomsk

LAMMPS format file (.lmp)
Distorted cell
Name file: POSCAR_X_X.lmp
+
Spin directions



ATOMSK

(Conversion files)

Program
LAMMPS

LAMMPS

Energy VASP format file
Name file: OSZICAR_X_X

Program
MAELAS

MAELAS

Magnetostrictive coefficients
+
Magnetoelastic constants
File name: maelas_output.dat

*LAMMPS considers lattice vector **a** along X-axis

See folder: Examples/LAMMPS/MAELAS

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

HOW TO USE MAELAS CODE

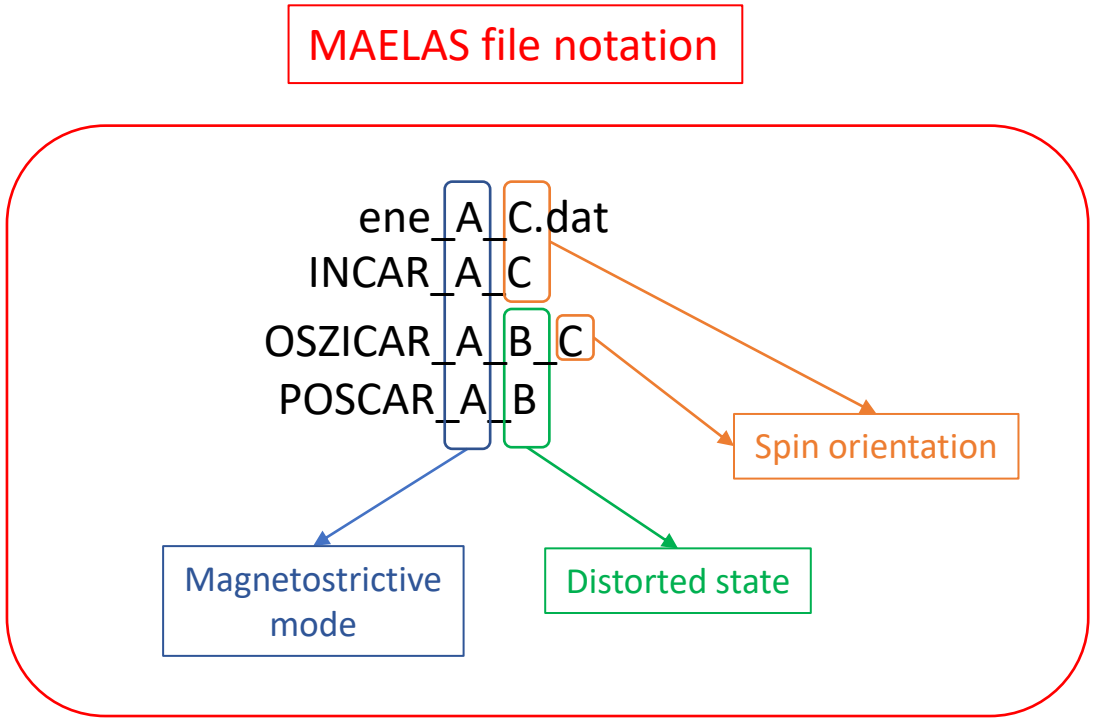
Crystal systems supported by MAELAS v1.0

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

Crystal system	Point groups	Space groups	Elastic constants (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



R. Wu, A. J. Freeman, Journal of Applied Physics 79, 6209–6212 (1996)

Methodology

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

$$\left.\frac{\Delta l}{l_0}\right|_{\beta^i}^{\alpha_1^i} - \left.\frac{\Delta l}{l_0}\right|_{\beta^i}^{\alpha_2^i} = \frac{l_1 - l_0}{l_0} - \frac{l_2 - l_0}{l_0} = \frac{2(l_1 - l_2)}{(l_1 + l_2)\left[1 - \frac{l_1 + l_2 - 2l_0}{l_1 + l_2}\right]}$$

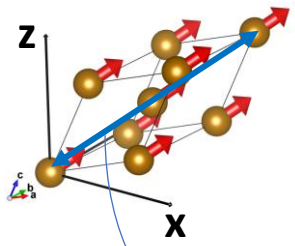
$$= \frac{2(l_1 - l_2)}{l_1 + l_2}\left[1 + \frac{l_1 + l_2 - 2l_0}{l_1 + l_2} + \ldots\right] \approx \frac{2(l_1 - l_2)}{l_1 + l_2}$$

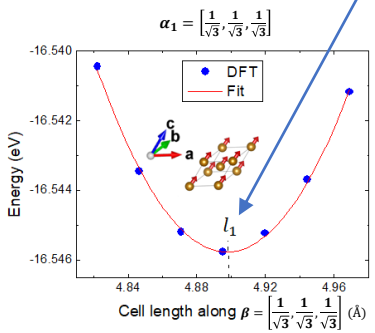
$$\lambda^i = \frac{2(l_1 - l_2)}{\rho^i (l_1 + l_2)}$$

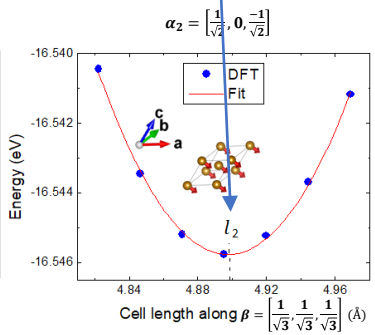
Fitting to a quadratic function

$$E(\boldsymbol{\alpha}_j, l) = A_j l^2 + B_j l + C_j, \quad j = 1, 2$$

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







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

Table 2: Selected cell length ($\boldsymbol{\beta}$) and magnetization directions ($\boldsymbol{\alpha}_1$, $\boldsymbol{\alpha}_2$) in MAELAS to calculate the anisotropic magnetostrictive coefficients according to Eq.48. The first column shows the crystal system and the corresponding lattice convention set in MAELAS based on the IEEE format [44]. The second column presents the equation of the relative length change that we used in Eq.48 for each crystal system. In the last column we show the values of the parameter 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	$\boldsymbol{\beta}$	$\boldsymbol{\alpha}_1$	$\boldsymbol{\alpha}_2$	ρ
Cubic (I)	Eq.17	λ_{001}	$(0,0,1)$	$(0,0,1)$	$(1,0,0)$	$\frac{3}{2}$
$\boldsymbol{a}\|\hat{\boldsymbol{x}}, \boldsymbol{b}\|\hat{\boldsymbol{y}}, \boldsymbol{c}\|\hat{\boldsymbol{z}}$		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	$\lambda^{\alpha 1,2}$	$(1,0,0)$	$\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$	$\frac{1}{3}$
$\boldsymbol{a}\|\hat{\boldsymbol{x}}, \boldsymbol{c}\|\hat{\boldsymbol{z}}$		$\lambda^{\alpha 2,2}$	$(0,0,1)$	$(0,0,1)$	$(1,0,0)$	1
$\boldsymbol{b} = \left(-\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0\right)$		$\lambda^{\gamma,2}$	$(1,0,0)$	$(1,0,0)$	$(0,1,0)$	1
$a = b \neq c$		$\lambda^{\varepsilon,2}$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$\left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)$	$\left(\frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)$	$\frac{2ac}{a^2+c^2}$
Trigonal (I)	Eq.35	$\lambda^{\alpha 1,2}$	$(1,0,0)$	$(0,0,1)$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$	1
$\boldsymbol{a}\|\hat{\boldsymbol{x}}, \boldsymbol{c}\|\hat{\boldsymbol{z}}$		$\lambda^{\alpha 2,2}$	$(0,0,1)$	$(0,0,1)$	$(1,0,0)$	1
$\boldsymbol{b} = \left(-\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0\right)$		$\lambda^{\gamma,1}$	$(1,0,0)$	$(1,0,0)$	$(0,1,0)$	1
$a = b \neq c$		$\lambda^{\gamma,2}$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$\left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)$	$\left(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}}\right)$	$\frac{ac}{a^2+c^2}$
		λ_{12}	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$\left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$	$\left(0, \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}\right)$	$\frac{a^2}{2(a^2+c^2)}$
		λ_{21}	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$	$\left(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, 0\right)$	$\frac{ac}{a^2+c^2}$
Tetragonal (I)	Eq.40	$\lambda^{\alpha 1,2}$	$(1,0,0)$	$\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$	$\frac{1}{3}$
$\boldsymbol{a}\|\hat{\boldsymbol{x}}, \boldsymbol{b}\|\hat{\boldsymbol{y}}, \boldsymbol{c}\|\hat{\boldsymbol{z}}$		$\lambda^{\alpha 2,2}$	$(0,0,1)$	$(0,0,1)$	$(1,0,0)$	1
$a = b \neq c$		$\lambda^{\gamma,2}$	$(1,0,0)$	$(1,0,0)$	$(0,1,0)$	1
		$\lambda^{\varepsilon,2}$	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$\left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)$	$\left(\frac{-1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)$	$\frac{2ac}{a^2+c^2}$
		$\lambda^{\delta,2}$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$	$\left(\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$	1
Orthorhombic	Eq.44	λ_1	$(1,0,0)$	$(1,0,0)$	$(0,0,1)$	1
$\boldsymbol{a}\|\hat{\boldsymbol{x}}, \boldsymbol{b}\|\hat{\boldsymbol{y}}, \boldsymbol{c}\|\hat{\boldsymbol{z}}$		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	$\frac{(a,0,c)}{\sqrt{a^2+c^2}}$	$\left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right)$	$(0,0,1)$	$\frac{(a-c)(a\lambda_1-c\lambda_5)+4ac\lambda_8}{2(a^2+c^2)\lambda_8}$
		λ_9	$\frac{(0,b,c)}{\sqrt{b^2+c^2}}$	$\left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$	$(0,0,1)$	$\frac{(b-c)(b\lambda_4-c\lambda_6)+4bc\lambda_9}{2(b^2+c^2)\lambda_9}$

CUBIC (I)

SG 207-230

Workflow

Cubic (I)

Elastic energy

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

Magnetoelastic energy

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

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

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

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

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

$$\lambda^{\alpha}=\frac{-b_0-\frac{1}{3}b_1}{c_{11}+2c_{12}},$$
$$\lambda_{001}=\frac{-2b_1}{3(c_{11}-c_{12})},$$
$$\lambda_{111}=\frac{-b_2}{3c_{44}}.$$

Workflow

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

POSCAR → Symmetry analysis → Space group: 207-230 → Cubic (I)

Cubic (I) → λ_{001}

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

→ OSZICAR_1_X_1, OSZICAR_1_X_2

Cubic (I) → λ_{111}

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

→ OSZICAR_2_X_1, OSZICAR_2_X_2

cell length along β

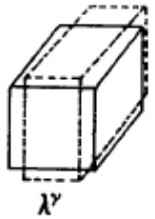
Fitting: $E(l) = Al^2 + Bl + C$
Minimum: $l_{1(2)} = -B_{1(2)}/(2A_{1(2)})$

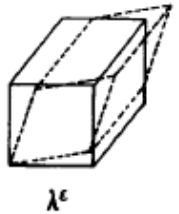
$$\lambda^i = \frac{2(l_1 - l_2)}{\rho^i(l_1 + l_2)}$$

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

Volume-conserving transformations (determinant of deformation gradient equal to 1, det(F)=1)

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





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

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

The maximum value of s is set with tag-s

HEXAGONAL (I)

SG 177-194

Workflow

Hexagonal (I)

Elastic energy

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

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

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

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

$$\begin{aligned}\left.\frac{\Delta l}{l_0}\right|_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} &= \lambda^{\alpha1,0}(\beta_x^2+\beta_y^2)+\lambda^{\alpha2,0}\beta_z^2+\lambda^{\alpha1,2}\left(\alpha_z^2-\frac{1}{3}\right)(\beta_x^2+\beta_y^2)\\ &+\lambda^{\alpha2,2}\left(\alpha_z^2-\frac{1}{3}\right)\beta_z^2+\lambda^{\gamma,2}\left[\frac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2)+2\alpha_x\alpha_y\beta_x\beta_y\right]\\ &+2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z+\alpha_y\alpha_z\beta_y\beta_z),\end{aligned}$$

$$\lambda^{\alpha1,0}=\frac{b_{11}c_{33}+b_{12}c_{13}}{c_{33}(c_{11}+c_{12})-2c_{13}^2},$$

$$\lambda^{\alpha2,0}=\frac{2b_{11}c_{13}-b_{12}(c_{11}+c_{12})}{c_{33}(c_{11}+c_{12})-2c_{13}^2},$$

$$\lambda^{\alpha1,2}=\frac{-b_{21}c_{33}+b_{22}c_{13}}{c_{33}(c_{11}+c_{12})-2c_{13}^2},$$

$$\lambda^{\alpha2,2}=\frac{2b_{21}c_{13}-b_{22}(c_{11}+c_{12})}{c_{33}(c_{11}+c_{12})-2c_{13}^2},$$

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

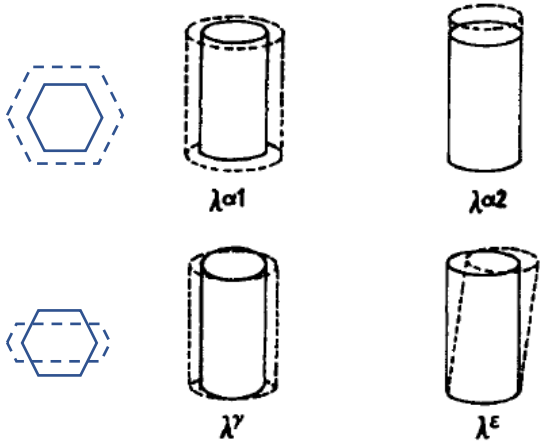
$$\lambda^{\varepsilon,2}=\frac{-b_4}{2c_{44}}.$$

Magnetoelastic energy

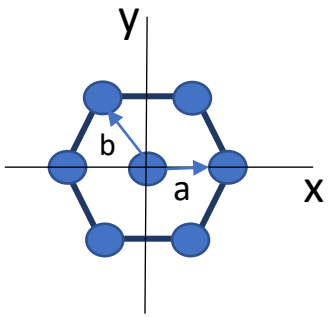
$$\begin{aligned}\frac{E_{me}^{hex(I)}}{V_0} &= b_{11}(\varepsilon_{xx}+\varepsilon_{yy})+b_{12}\varepsilon_{zz}+b_{21}\left(\alpha_z^2-\frac{1}{3}\right)(\varepsilon_{xx}+\varepsilon_{yy})+b_{22}\left(\alpha_z^2-\frac{1}{3}\right)\varepsilon_{zz}\\ &+b_3\left[\frac{1}{2}(\alpha_x^2-\alpha_y^2)(\varepsilon_{xx}-\varepsilon_{yy})+2\alpha_x\alpha_y\varepsilon_{xy}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

Workflow

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



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



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

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

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

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

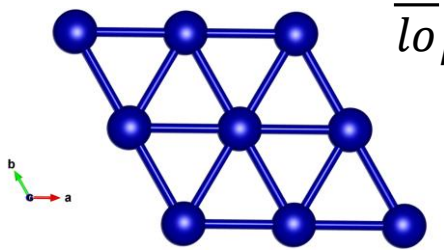
cell length along β

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

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

Hexagonal (I)

Distorted states



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

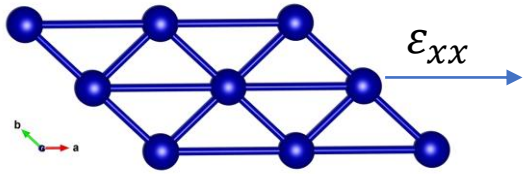
$$|\boldsymbol{\alpha}| = 1, |\boldsymbol{\beta}| = 1$$

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

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

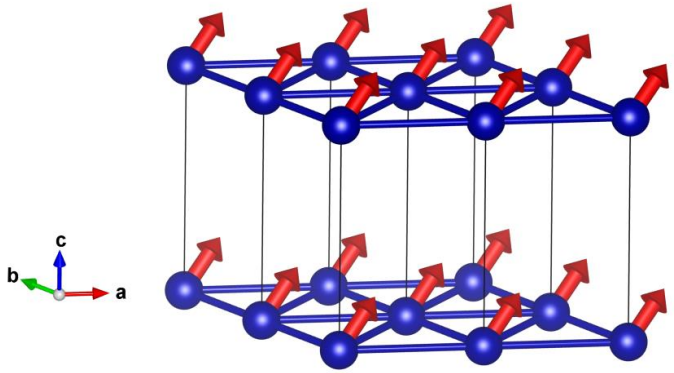
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

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

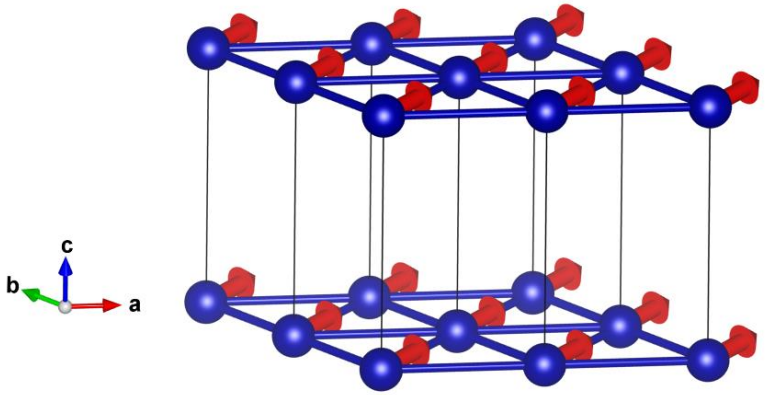


volume-conserving
Det(F)=1

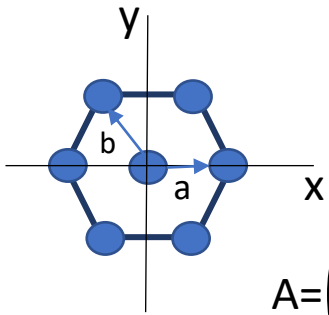
$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx}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



S=(1,1,1)



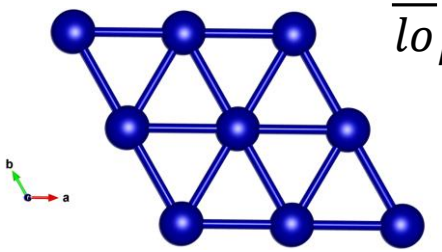
S=(1,1,0)



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

Hexagonal (I)

Distorted states



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

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

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

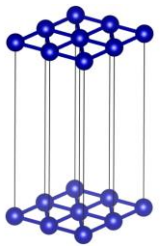
$$\boldsymbol{F}\Big|^{\lambda^{\alpha 2,2}}_{\boldsymbol{\beta}=(0,0,1)}(s) = \begin{pmatrix} \frac{1}{\sqrt{1+s}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+s}} & 0 \\ 0 & 0 & 1+s \end{pmatrix}$$

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

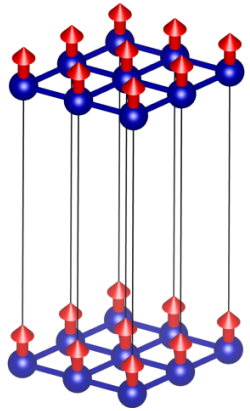
$$\boldsymbol{\lambda^{\alpha 2,2}}$$

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

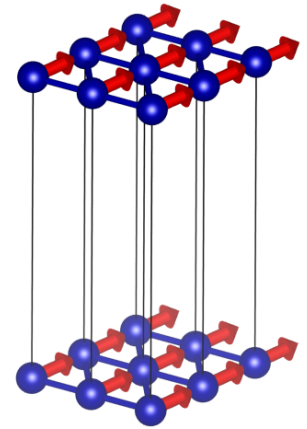
ε_{zz}



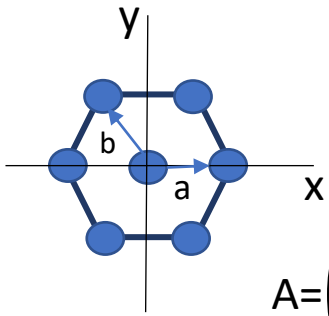
volume-conserving
Det(F)=1



S=(0,0,1)



S=(1,0,0)



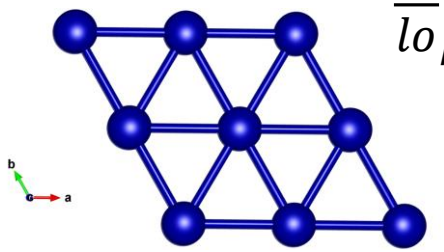
$$A = \begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

Hexagonal (I)

Distorted states

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

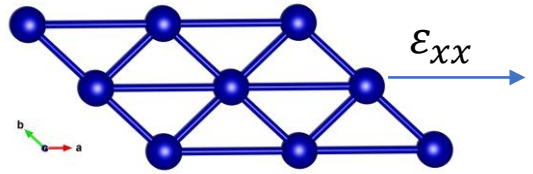
$|\boldsymbol{\alpha}| = 1, |\boldsymbol{\beta}| = 1$



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

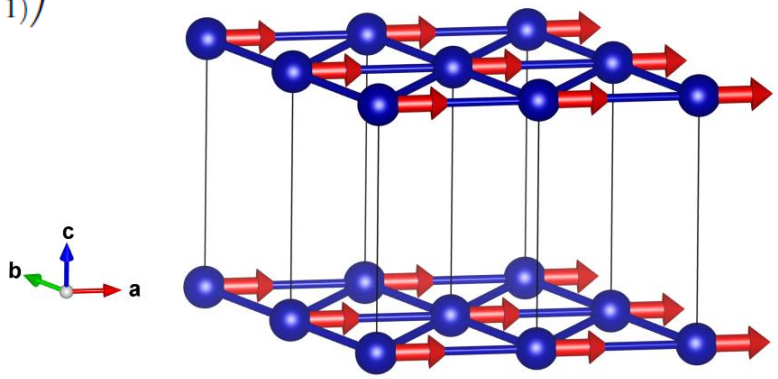
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

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

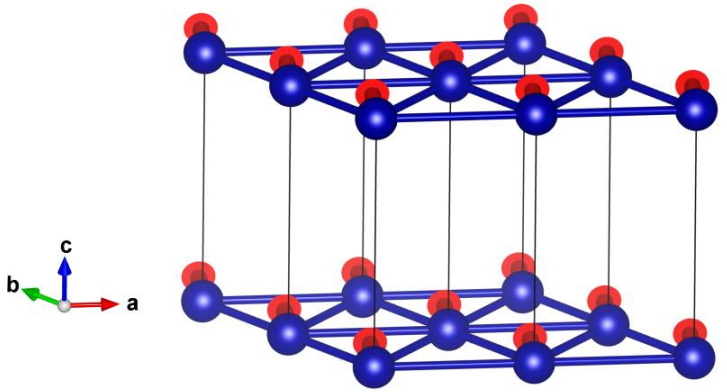


volume-conserving
Det(F)=1

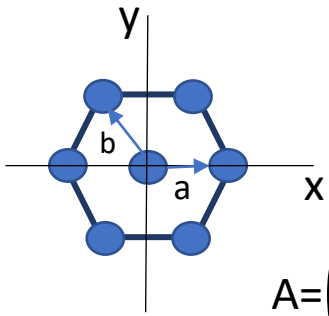
$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2(F_{xx}-1) & F_{xy}+F_{yx} & F_{xz}+F_{zx}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



S=(1,0,0)



S=(0,1,0)

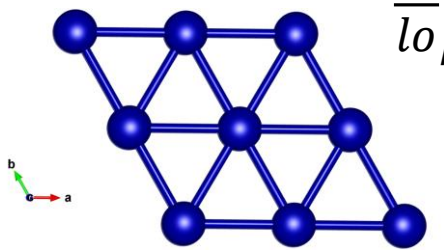


$$A = \begin{pmatrix} a1 & 0 & 0 \\ b1 & b2 & 0 \\ 0 & 0 & c3 \end{pmatrix}$$

Hexagonal (I)

Distorted states

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



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

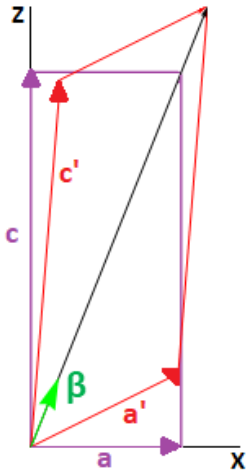
$$|\boldsymbol{\alpha}| = 1, |\boldsymbol{\beta}| = 1$$

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

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

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

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

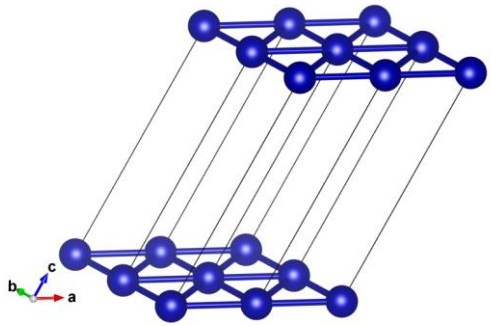


$$\boldsymbol{\lambda}^{\boldsymbol{\varepsilon},2}$$

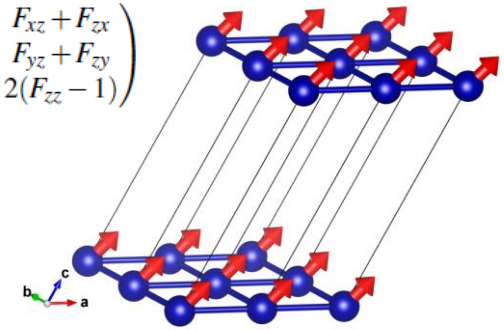
$$\begin{pmatrix} a'_x & b'_x & c'_x \\ a'_y & b'_y & c'_y \\ a'_z & b'_z & c'_z \end{pmatrix} = \begin{pmatrix} F_{xx} & F_{xy} & F_{xz} \\ F_{yx} & F_{yy} & F_{yz} \\ F_{zx} & F_{zy} & F_{zz} \end{pmatrix} \cdot \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$

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

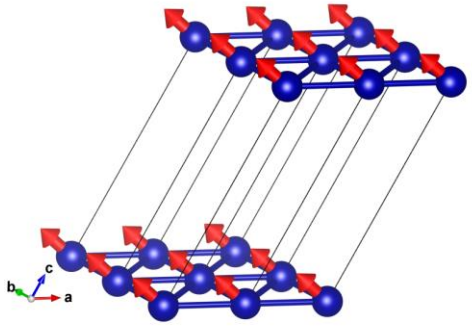
ε_{xz}



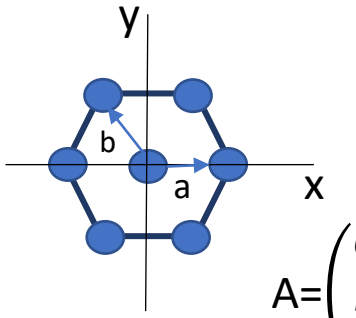
volume-conserving
Det(F)=1



S=(1,0,1)



S=(-1,0,1)



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

Relation between different notations

Clark

Hexagonal system

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

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

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Callen

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

MAELAS notation

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

Workflow

TRIGONAL (I)

SG 149-167

Trigonal (I)

Workflow

Elastic energy

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

Magnetoelastic energy

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

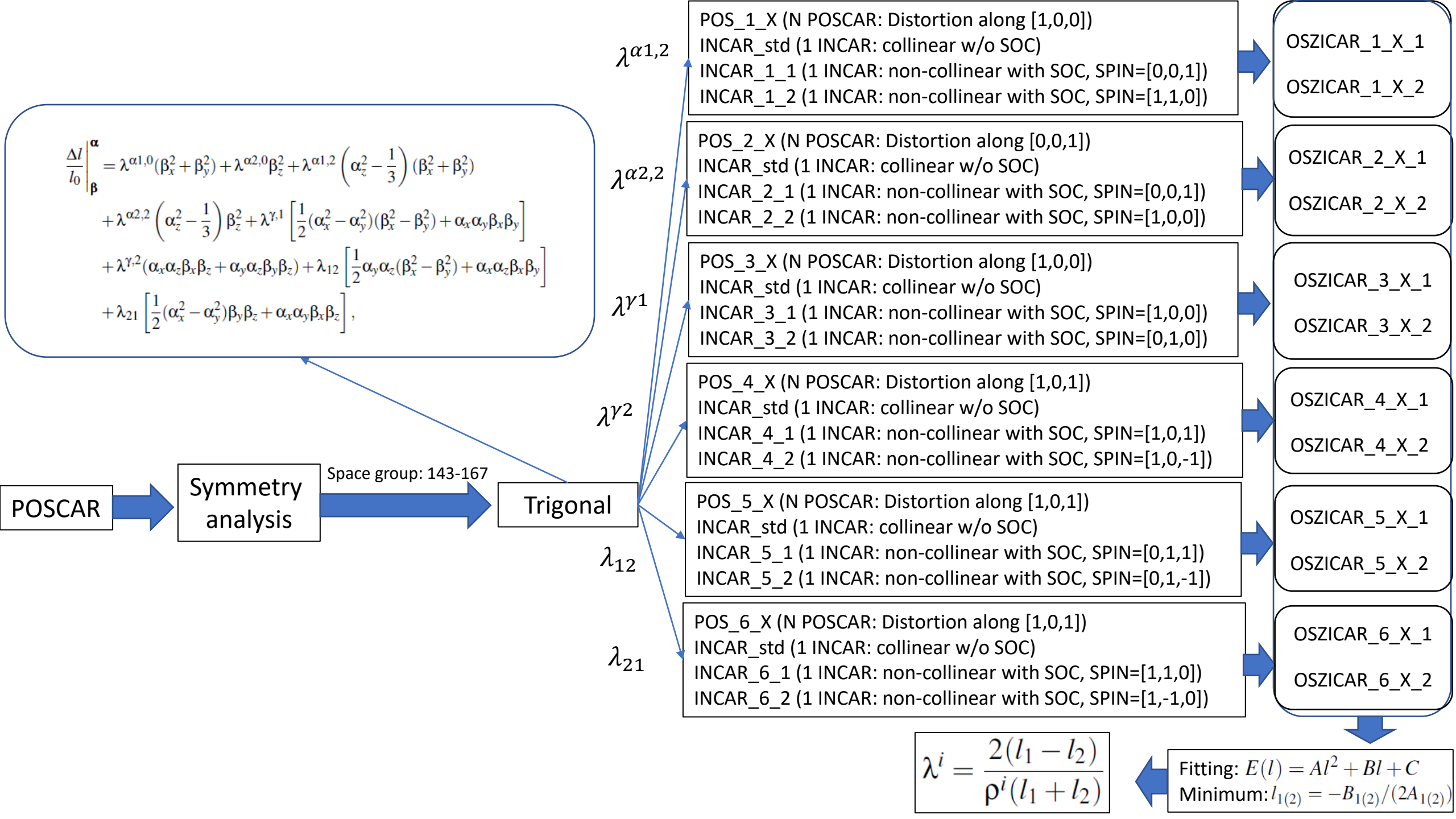
$$\frac{\partial(E_{el} + E_{me})}{\partial\varepsilon_{ij}} = 0$$

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

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

$$\left.\frac{\Delta l}{l_0}\right|_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} = \lambda^{\alpha1,0}(\beta_x^2 + \beta_y^2) + \lambda^{\alpha2,0}\beta_z^2 + \lambda^{\alpha1,2}\left(\alpha_z^2 - \frac{1}{3}\right)(\beta_x^2 + \beta_y^2)$$
$$+ \lambda^{\alpha2,2}\left(\alpha_z^2 - \frac{1}{3}\right)\beta_z^2 + \lambda^{\gamma,1}\left[\frac{1}{2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + \alpha_x\alpha_y\beta_x\beta_y\right]$$
$$+ \lambda^{\gamma,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z) + \lambda_{12}\left[\frac{1}{2}\alpha_y\alpha_z(\beta_x^2 - \beta_y^2) + \alpha_x\alpha_z\beta_x\beta_y\right]$$
$$+ \lambda_{21}\left[\frac{1}{2}(\alpha_x^2 - \alpha_y^2)\beta_y\beta_z + \alpha_x\alpha_y\beta_x\beta_z\right],$$

$$\lambda^{\alpha1,0} = \frac{b_{11}c_{33} + b_{12}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$
$$\lambda^{\alpha2,0} = \frac{2b_{11}c_{13} - b_{12}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$
$$\lambda^{\alpha1,2} = \frac{-b_{21}c_{33} + b_{22}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$
$$\lambda^{\alpha2,2} = \frac{2b_{21}c_{13} - b_{22}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$
$$\lambda^{\gamma,1} = \frac{c_{14}b_{14} - c_{44}b_3}{\frac{1}{2}c_{44}(c_{11} - c_{12}) - c_{14}^2},$$
$$\lambda^{\gamma,2} = \frac{\frac{1}{2}b_4(c_{11} - c_{12}) - b_{34}c_{14}}{\frac{1}{2}c_{44}(c_{11} - c_{12}) - c_{14}^2},$$
$$\lambda_{12} = \frac{c_{14}b_4 - c_{44}b_{34}}{\frac{1}{2}c_{44}(c_{11} - c_{12}) - c_{14}^2},$$
$$\lambda_{21} = \frac{\frac{1}{2}b_{14}(c_{11} - c_{12}) - b_3c_{14}}{\frac{1}{2}c_{44}(c_{11} - c_{12}) - c_{14}^2}.$$


$\frac{\Delta l}{l_0}\Big|_{\beta}^{\alpha} = \lambda^{\alpha1,0}(\beta_x^2+\beta_y^2)+\lambda^{\alpha2,0}\beta_z^2+\lambda^{\alpha1,2}\left(\alpha_z^2-\frac{1}{3}\right)(\beta_x^2+\beta_y^2)$
$+\lambda^{\alpha2,2}\left(\alpha_z^2-\frac{1}{3}\right)\beta_z^2+\lambda^{\gamma,1}\left[\frac{1}{2}(\alpha_x^2-\alpha_y^2)(\beta_x^2-\beta_y^2)+\alpha_x\alpha_y\beta_x\beta_y\right]$
$+\lambda^{\gamma,2}(\alpha_x\alpha_z\beta_x\beta_z+\alpha_y\alpha_z\beta_y\beta_z)+\lambda_{12}\left[\frac{1}{2}\alpha_y\alpha_z(\beta_x^2-\beta_y^2)+\alpha_x\alpha_z\beta_x\beta_y\right]$
$+\lambda_{21}\left[\frac{1}{2}(\alpha_x^2-\alpha_y^2)\beta_y\beta_z+\alpha_x\alpha_y\beta_x\beta_z\right],$
POSCAR
Symmetry analysis
Space group: 143-167
Trigonal
$\lambda^{\alpha1,2}$
$\lambda^{\alpha2,2}$
$\lambda^{\gamma1}$
$\lambda^{\gamma2}$
λ_{12}
λ_{21}
POS_1_X (N POSCAR: Distortion along [1,0,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_1_1 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
INCAR_1_2 (1 INCAR: non-collinear with SOC, SPIN=[1,1,0])
POS_2_X (N POSCAR: Distortion along [0,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_2_1 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])
INCAR_2_2 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
POS_3_X (N POSCAR: Distortion along [1,0,0])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_3_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
INCAR_3_2 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
POS_4_X (N POSCAR: Distortion along [1,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_4_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,1])
INCAR_4_2 (1 INCAR: non-collinear with SOC, SPIN=[1,0,-1])
POS_5_X (N POSCAR: Distortion along [1,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_5_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,1])
INCAR_5_2 (1 INCAR: non-collinear with SOC, SPIN=[0,1,-1])
POS_6_X (N POSCAR: Distortion along [1,0,1])
INCAR_std (1 INCAR: collinear w/o SOC)
INCAR_6_1 (1 INCAR: non-collinear with SOC, SPIN=[1,1,0])
INCAR_6_2 (1 INCAR: non-collinear with SOC, SPIN=[1,-1,0])
OSZICAR_1_X_1
OSZICAR_1_X_2
OSZICAR_2_X_1
OSZICAR_2_X_2
OSZICAR_3_X_1
OSZICAR_3_X_2
OSZICAR_4_X_1
OSZICAR_4_X_2
OSZICAR_5_X_1
OSZICAR_5_X_2
OSZICAR_6_X_1
OSZICAR_6_X_2
$\lambda^i = \frac{2(l_1-l_2)}{\rho^i(l_1+l_2)}$
Fitting: $E(l) = Al^2 + Bl + C$
Minimum: $l_{1(2)} = -B_{1(2)}/(2A_{1(2)})$

Workflow

TETRAGONAL (I)

SG 89-142

Workflow

Tetragonal (I)

Elastic energy

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

Magnetoelastic energy

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

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

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

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

$$\left.\frac{\Delta l}{l_0}\right|_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} = \lambda^{\alpha1,0}(\beta_x^2 + \beta_y^2) + \lambda^{\alpha2,0}\beta_z^2 + \lambda^{\alpha1,2}\left(\alpha_z^2 - \frac{1}{3}\right)(\beta_x^2 + \beta_y^2) + \lambda^{\alpha2,2}\left(\alpha_z^2 - \frac{1}{3}\right)\beta_z^2 + \frac{1}{2}\lambda^{\gamma,2}(\alpha_x^2 - \alpha_y^2)(\beta_x^2 - \beta_y^2) + 2\lambda^{\delta,2}\alpha_x\alpha_y\beta_x\beta_y + 2\lambda^{\varepsilon,2}(\alpha_x\alpha_z\beta_x\beta_z + \alpha_y\alpha_z\beta_y\beta_z),$$

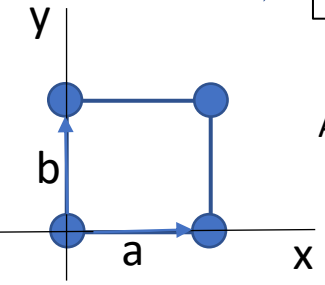
$$\lambda^{\alpha1,0} = \frac{b_{11}c_{33} + b_{12}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$
$$\lambda^{\alpha2,0} = \frac{2b_{11}c_{13} - b_{12}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$
$$\lambda^{\alpha1,2} = \frac{-b_{21}c_{33} + b_{22}c_{13}}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$
$$\lambda^{\alpha2,2} = \frac{2b_{21}c_{13} - b_{22}(c_{11} + c_{12})}{c_{33}(c_{11} + c_{12}) - 2c_{13}^2},$$
$$\lambda^{\gamma,2} = \frac{-b_3}{c_{11} - c_{12}},$$
$$\lambda^{\delta,2} = \frac{-b_3'}{2c_{66}},$$
$$\lambda^{\varepsilon,2} = \frac{-b_4}{2c_{44}}.$$

Workflow

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

same files as the hexagonal case

POSCAR → Symmetry analysis → Space group: 75-142 → Tetragonal



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

$$a1 = b2$$

Tetragonal → $\lambda^{\alpha 1}$, $\lambda^{\alpha 2}$, λ^{γ}, λ^{ε}, $\lambda^{\delta,2}$

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

...
...
...
...

OSZICAR_5_X_1
OSZICAR_5_X_2

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

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

Relation between different notations

Tetragonal (I)

Cullen

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

Mason

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

$$\lambda_{Mason}^{\alpha 1,0} = \lambda^{\alpha 1,0}+\frac{2}{3}\lambda^{\alpha 1,2}$$
$$\lambda_{Mason}^{\alpha 2,0} = \lambda^{\alpha 2,0}+\frac{2}{3}\lambda^{\alpha 2,2}$$
$$\lambda_1 = -\lambda^{\alpha 1,2}+\frac{1}{2}\lambda^{\gamma,2}$$
$$\lambda_2 = \frac{1}{2}\lambda^{\varepsilon,2}-\frac{1}{4}\lambda^{\alpha 2,2}-\frac{1}{4}\lambda^{\alpha 1,2}+\frac{1}{8}\lambda^{\gamma,2}$$
$$\lambda_3 = \frac{1}{2}\lambda^{\delta,2}-\lambda^{\alpha 1,2}$$
$$\lambda_4 = -\lambda^{\alpha 2,2}$$
$$\lambda_5 = -\lambda^{\alpha 1,2}-\frac{1}{2}\lambda^{\gamma,2}.$$

Workflow

ORTHORHOMBIC

SG 16-74

Workflow

Orthorhombic

Elastic energy

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

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

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

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

$$\begin{aligned}\left.\frac{\Delta l}{l_0}\right|_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} &= \lambda^{\alpha1,0}\beta_x^2+\lambda^{\alpha2,0}\beta_y^2+\lambda^{\alpha3,0}\beta_z^2+\lambda_1(\alpha_x^2\beta_x^2-\alpha_x\alpha_y\beta_x\beta_y-\alpha_x\alpha_z\beta_x\beta_z)\\ &+\lambda_2(\alpha_y^2\beta_x^2-\alpha_x\alpha_y\beta_x\beta_y)+\lambda_3(\alpha_x^2\beta_y^2-\alpha_x\alpha_y\beta_x\beta_y)\\ &+\lambda_4(\alpha_y^2\beta_y^2-\alpha_x\alpha_y\beta_x\beta_y-\alpha_y\alpha_z\beta_y\beta_z)+\lambda_5(\alpha_x^2\beta_z^2-\alpha_x\alpha_z\beta_x\beta_z)\\ &+\lambda_6(\alpha_y^2\beta_z^2-\alpha_y\alpha_z\beta_y\beta_z)+4\lambda_7\alpha_x\alpha_y\beta_x\beta_y+4\lambda_8\alpha_x\alpha_z\beta_x\beta_z+4\lambda_9\alpha_y\alpha_z\beta_y\beta_z.\end{aligned}$$

Magnetoelastic energy

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

$$\begin{aligned}b_{01} &= -c_{11}\lambda^{\alpha1,0}-c_{12}\lambda^{\alpha2,0}-c_{13}\lambda^{\alpha3,0}\\ b_{02} &= -c_{12}\lambda^{\alpha1,0}-c_{22}\lambda^{\alpha2,0}-c_{23}\lambda^{\alpha3,0}\\ b_{03} &= -c_{13}\lambda^{\alpha1,0}-c_{23}\lambda^{\alpha2,0}-c_{33}\lambda^{\alpha3,0}\\ b_1 &= -c_{11}\lambda_1-c_{12}\lambda_3-c_{13}\lambda_5\\ b_2 &= -c_{11}\lambda_2-c_{12}\lambda_4-c_{13}\lambda_6\\ b_3 &= -c_{12}\lambda_1-c_{22}\lambda_3-c_{23}\lambda_5\\ b_4 &= -c_{12}\lambda_2-c_{22}\lambda_4-c_{23}\lambda_6\\ b_5 &= -c_{13}\lambda_1-c_{23}\lambda_3-c_{33}\lambda_5\\ b_6 &= -c_{13}\lambda_2-c_{23}\lambda_4-c_{33}\lambda_6\\ b_7 &= c_{66}(\lambda_1+\lambda_2+\lambda_3+\lambda_4-4\lambda_7)\\ b_8 &= c_{55}(\lambda_1+\lambda_5-4\lambda_8)\\ b_9 &= c_{44}(\lambda_4+\lambda_6-4\lambda_9).\end{aligned}$$

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

POSCAR → Symmetry analysis (SG: 16-74) → Orthorhombic

λ_1
- POS_1_X (N POSCAR: Distortion along [1,0,0])
- INCAR_std (1 INCAR: collinear w/o SOC)
- INCAR_1_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
- INCAR_1_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])

→ OSZICAR_1_X_1, OSZICAR_1_X_2

λ_2
- POS_2_X (N POSCAR: Distortion along [1,0,0])
- INCAR_std (1 INCAR: collinear w/o SOC)
- INCAR_2_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
- INCAR_2_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])

→ OSZICAR_2_X_1, OSZICAR_2_X_2

λ_3
- POS_3_X (N POSCAR: Distortion along [0,1,0])
- INCAR_std (1 INCAR: collinear w/o SOC)
- INCAR_3_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
- INCAR_3_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])

→ OSZICAR_3_X_1, OSZICAR_3_X_2

λ_4
- POS_4_X (N POSCAR: Distortion along [0,1,0])
- INCAR_std (1 INCAR: collinear w/o SOC)
- INCAR_4_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
- INCAR_4_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])

→ OSZICAR_4_X_1, OSZICAR_4_X_2

λ_5
- POS_5_X (N POSCAR: Distortion along [0,0,1])
- INCAR_std (1 INCAR: collinear w/o SOC)
- INCAR_5_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,0])
- INCAR_5_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])

→ OSZICAR_5_X_1, OSZICAR_5_X_2

λ_6
- POS_6_X (N POSCAR: Distortion along [0,0,1])
- INCAR_std (1 INCAR: collinear w/o SOC)
- INCAR_6_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,0])
- INCAR_6_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])

→ OSZICAR_6_X_1, OSZICAR_6_X_2

λ_7
- POS_7_X (N POSCAR: Distortion along [1,1,0])
- INCAR_std (1 INCAR: collinear w/o SOC)
- INCAR_7_1 (1 INCAR: non-collinear with SOC, SPIN=[1,1,0])
- INCAR_7_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])

→ OSZICAR_7_X_1, OSZICAR_7_X_2

λ_8
- POS_8_X (N POSCAR: Distortion along [1,0,1])
- INCAR_std (1 INCAR: collinear w/o SOC)
- INCAR_8_1 (1 INCAR: non-collinear with SOC, SPIN=[1,0,1])
- INCAR_8_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])

→ OSZICAR_8_X_1, OSZICAR_8_X_2

λ_9
- POS_9_X (N POSCAR: Distortion along [0,1,1])
- INCAR_std (1 INCAR: collinear w/o SOC)
- INCAR_9_1 (1 INCAR: non-collinear with SOC, SPIN=[0,1,1])
- INCAR_9_2 (1 INCAR: non-collinear with SOC, SPIN=[0,0,1])

→ OSZICAR_9_X_1, OSZICAR_9_X_2

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

Fitting: $E(l) = Al^2 + Bl + C$

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

MAELAS uses the same lattice convention as AELAS code:

c < a < b

BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

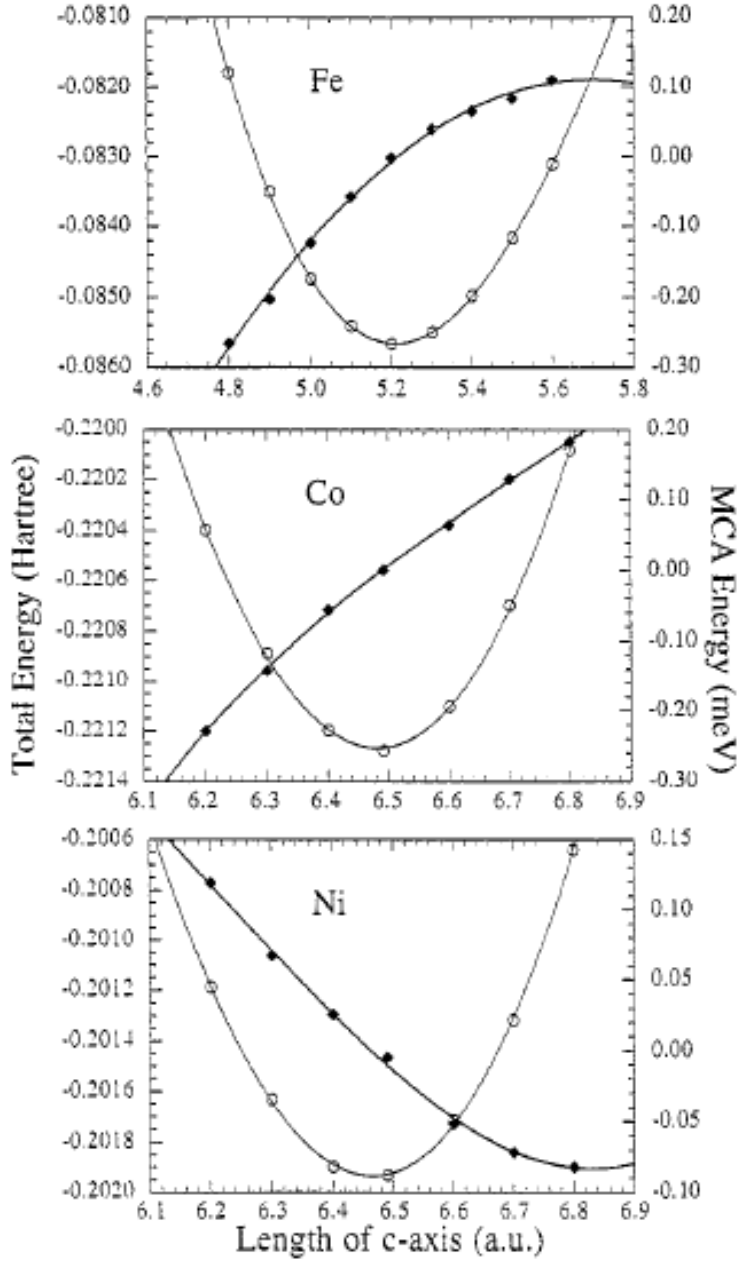
Cubic systems: Itenerant magnets

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

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

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

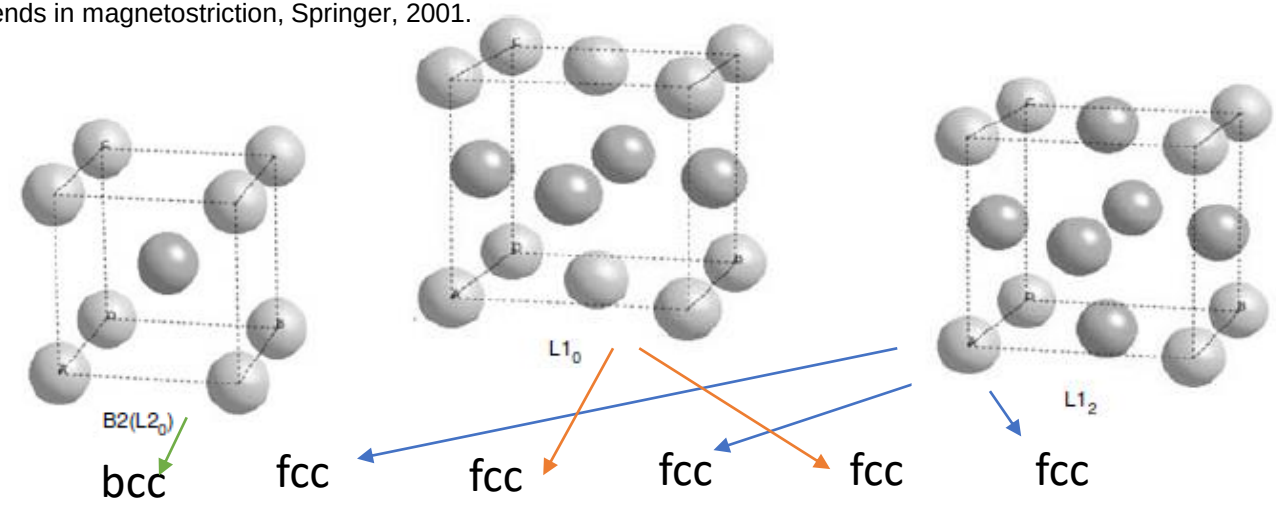
	$T = 4.2$ K		Room Temperature		
	$\lambda_{100}(\lambda^{\gamma,2})$	$\lambda_{111}(\lambda^{\varepsilon,2})$	$\lambda_{100}(\lambda^{\gamma,2})$	$\lambda_{111}(\lambda^{\varepsilon,2})$	Polycrystal λ_s
3d Metals					
BCC-Fe	26	−30	21	−21	−7
HCP-Co[a]	(−150)	(45)	(−140)	(50)	(−62)
FCC-Ni	−60	−35	−46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



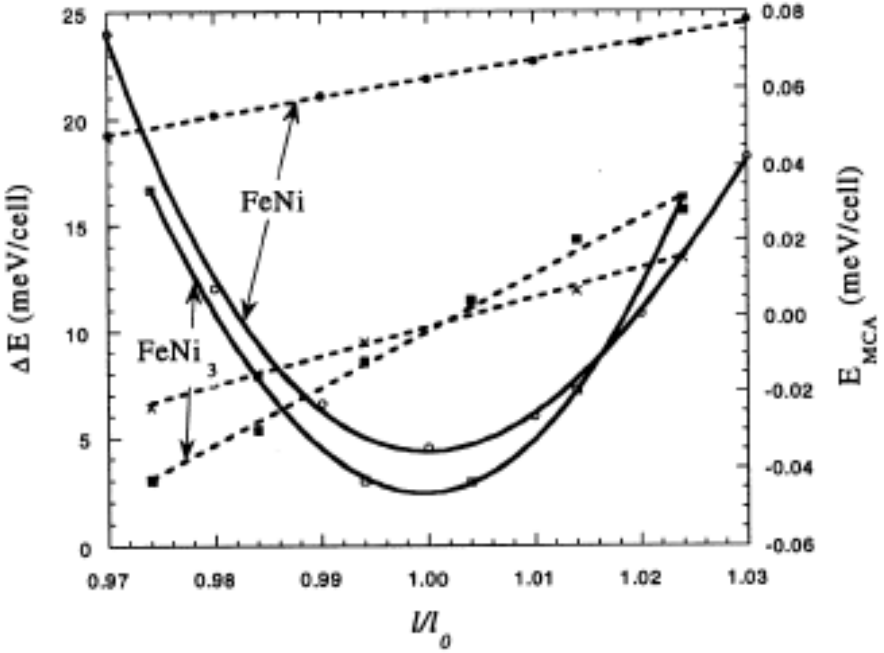
BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

Cubic systems: Itenerant magnets

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)
$E_{MCA}(\mu eV)$	0	0	63	0	143	0
σ	-0.35	-0.36	-0.33	-0.35	-0.34	-0.36
λ_{001} (10^{-6})	83 (125)	-68	10 (12)	27 (13)	42 (42-100)	33



BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

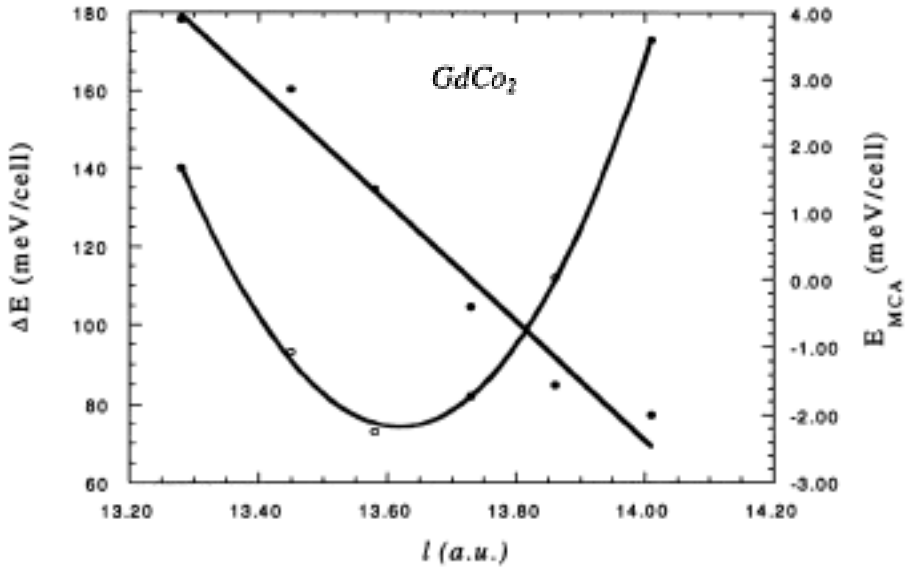
G. Engdahl, Handbook of giant magnetostrictive materials, Academic Press,1999

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



$DyFe_2$

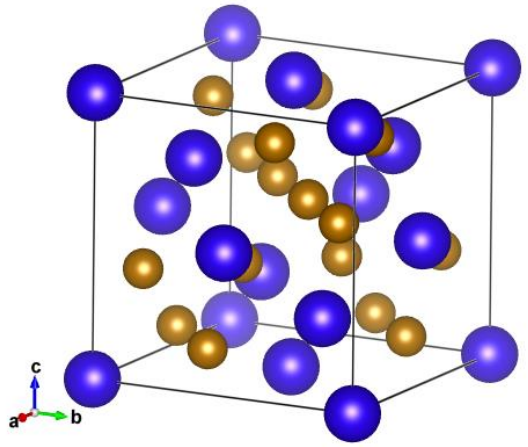


Table 16-10. Low-temperature magnetostriction constants for RCo_2 crystals [from Levitin and Markosyan (1990) unless otherwise noted].

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

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

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

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

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

BRIEF REVIEW OF KNOWN MAGNETOSTRICTIVE MATERIALS

Hexagonal Rare-Earth

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

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

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

Table 14.4. Magnetostriction constants of spinel-type ferrites (mainly after Tsuya[49]).

Composition	λ_{100}	λ_{111}	Temp.	Ref.
$MnFe_2O_4$	-31×10^{-6}	6.5×10^{-6}		38
Fe_3O_4	−20	78	20°C	39
$Co_{0.8}Fe_{2.2}O_4$	−590	120	20°C	40
$NiFe_2O_4$	−42	−14		41
$CuFe_2O_4$	−57.5	4.7		42
$MgFe_2O_4$	−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
$Co_{0.1}Ni_{0.9}Fe_2O_4$	−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	86	80 K	48
$Ti_{0.56}Fe_{2.44}O_4$	170	92	290 K	48
	990	(330)	80 K	48

S Chikazumi - Physics of Ferromagnetism -Oxford University Press, (2009)

Oxide magnets

MAELAS TESTS

Table 3: Anisotropic magnetostrictive coefficients and MAE calculated using the program MAELAS and measured in experiment ($T \approx 0$ K) for a set of magnetic materials. In parenthesis we show the magnetostrictive coefficients with Mason's definitions obtained using the relations given by Eq. A.2. These data correspond to the simulations with the largest number of k-points discussed in the main text.

Material	Crystal system	Method	Magnetostriction coefficient	MAELAS ($\times 10^{-6}$)	Expt. ($\times 10^{-6}$)	MAE	MAELAS (μeV/atom)	Expt. (μeV/atom)
FCC Ni	Cubic (I) SG 225	DFT GGA	λ_{001}	-78.4	-60[a]	$E(110)-E(001)$	0.03	-2.15[b]
			λ_{111}	-46.1	-35[a]	$E(111)-E(001)$	0.34	-2.73[b]
		SD-MD	λ_{001}	-61.9[h]		$E(110)-E(001)$	-2.14[h]	
			λ_{111}	-35.4[h]		$E(111)-E(001)$	-2.86[h]	
BCC Fe	Cubic (I) SG 229	DFT GGA	λ_{001}	25.7	26[a]	$E(110)-E(001)$	0.24	1.0[b]
			λ_{111}	17.2	-30[a]	$E(111)-E(001)$	0.32	1.34[b]
		SD-MD	λ_{001}	25.9[h]		$E(110)-E(001)$	0.99[h]	
			λ_{111}	-30.3[h]		$E(111)-E(001)$	1.33[h]	
HCP Co	Hexagonal (I) SG 194	DFT SCAN	$\lambda^{\alpha 1,2}$ (λ_A)	85 (-78)	95 (-66)[c]	$E(100)-E(001)$	53	61[b]
			$\lambda^{\alpha 2,2}$ (λ_B)	-115 (-92)	-126 (-123)[c]			
			$\lambda^{\gamma,2}$ (λ_C)	15 (115)	57 (126)[c]			
			$\lambda^{\epsilon,2}$ (λ_D)	-19 (-1)	-286 (-128)[c]			
		DFT LSDA+U $J=0.8$eV $U=3$eV	$\lambda^{\alpha 1,2}$ (λ_A)	111 (-109)		$E(100)-E(001)$	58	
			$\lambda^{\alpha 2,2}$ (λ_B)	-251 (-114)				
			$\lambda^{\gamma,2}$ (λ_C)	4 (251)				
			$\lambda^{\epsilon,2}$ (λ_D)	-51 (10)				
YCo_5	Hexagonal (I) SG 191	DFT LSDA+U	$\lambda^{\alpha 1,2}$	-90	$\lvert\lambda^{\alpha 1,2}\rvert < 100$[d]	$E(100)-E(001)$	365	567[e]
			$\lambda^{\alpha 2,2}$	115	$\lvert\lambda^{\alpha 2,2}\rvert < 100$[d]			
			$\lambda^{\gamma,2}$	76				
			$\lambda^{\epsilon,2}$	141				
Fe_2Si	Trigonal (I) SG 164	DFT GGA	$\lambda^{\alpha 1,2}$	-9		$E(100)-E(001)$	-38	
			$\lambda^{\alpha 2,2}$	15				
			$\lambda^{\gamma,1}$	8				
			$\lambda^{\gamma,2}$	28				
			λ_{12}	-3				
			λ_{21}	-13				
$L1_0$ FePd	Tetragonal (I) SG 123	DFT GGA	$\lambda^{\alpha 1,2}$	-21		$E(100)-E(001)$	106	181[f]
			$\lambda^{\alpha 2,2}$	79				
			$\lambda^{\gamma,2}$	31				
			$\lambda^{\epsilon,2}$	28				
			$\lambda^{\delta,2}$	106				
			$\lambda^{\alpha 1,0}-\frac{\lambda^{\alpha 1,2}}{3}+\frac{\lambda^{\gamma,2}}{2}$		100[g]			
YCo	Orthorhombic SG 63	DFT LSDA+U	λ_1	-11		$E(100)-E(001)$	22	
			λ_2	32		$E(010)-E(001)$	-23	
			λ_3	70				
			λ_4	-74				
			λ_5	-30				
			λ_6	7				
			λ_7	36				
			λ_8	-20				
			λ_9	35				

[a]Ref.[40], [b]Ref.[62], [c]Ref.[63], [d]Ref.[7], [e]Ref.[64], [f]Ref.[65], [g]Ref.[66], [h]Ref.[59]

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

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Table 4: Elastic and magnetoelastic constants calculated using the interface between AELAS and MAELAS codes. The third column shows the DFT method used to compute the elastic constants. The experimental elastic constants of FCC Ni and BCC Fe were measured at $T \approx 0$ K, while for HCP Co $T \approx 300$ K. The experimental magnetoelastic constants were estimated using the experimental elastic constants (seventh column) and the experimental magnetostrictive coefficients in Table 3 via the relations given in Section 2. The sixth column presents calculations of the elastic constants available in the Materials Project database [67, 68].

Material	Crystal system	Method	Elastic constant	AELAS (GPa)	Mat.Proj. (GPa)	Expt. (GPa)	Magnetoelastic constant	MAELAS (MPa)	Expt. (MPa)
FCC Ni	Cubic (I) SG 225	DFT GGA	C_{11}	298	276[g]	261[h]	b_1	15.5	9.9
			C_{12}	166	159[g]	151[h]	b_2	19.4	13.9
			C_{44}	140	132[g]	132[h]			
		SD-MD	C_{11}	264[f]			b_1	10.4	
			C_{12}	152[f]			b_2	14.1	
			C_{44}	133[f]					
BCC Fe	Cubic (I) SG 229	DFT GGA	C_{11}	288	247[a]	243[b]	b_1	-5.2	-4.1
			C_{12}	152	150[a]	138[b]	b_2	-5.3	10.9
			C_{44}	104	97[a]	122[b]			
		SD-MD	C_{11}	230[f]			b_1	-3.7	
			C_{12}	134[f]			b_2	10.6	
			C_{44}	116[f]					
HCP Co	Hexagonal (I) SG 194	DFT LSDA+U $J = 0.8$eV $U = 3$eV	C_{11}	327		307[d]	b_{21}	-21.3	-31.9
			C_{12}	157		165[d]	b_{22}	48.3	25.5
			C_{13}	130		103[d]	b_3	-0.7	-8.1
			C_{33}	308		358[d]	b_4	7.1	42.9
			C_{44}	69		75[d]			
		DFT SCAN	C_{11}	648			b_{21}	-51.3	
			C_{12}	212			b_{22}	40.5	
			C_{13}	189			b_3	6.4	
			C_{33}	633			b_4	8.9	
			C_{44}	239					
		DFT GGA	C_{11}		358[c]				
			C_{12}		165[c]				
			C_{13}		114[c]				
			C_{33}		409[c]				
			C_{44}		95[c]				
YCo_5	Hexagonal (I) SG 191	DFT GGA	C_{11}	208	192[e]		b_{21}	14.9	
			C_{12}	103	123[e]		b_{22}	-10.4	
			C_{13}	114	113[e]		b_3	-8.0	
			C_{33}	270	262[e]		b_4	-13.6	
			C_{44}	49	48[e]				
		DFT LSDA+U	C_{11}	-63			b_{21}	13.9	
			C_{12}	363			b_{22}	-7.9	
			C_{13}	115			b_3	32.5	
			C_{33}	249			b_4	-12.4	
			C_{44}	44					

[a]Ref.[69], [b]Ref.[70], [c]Ref.[71], [d]Ref.[72], [e]Ref.[73], [f]Ref.[59], [g]Ref.[74], [h]Ref.[75]

Table 5: Elastic and magnetoelastic constants calculated using the interface between AELAS and MAELAS codes. The third column shows the DFT method used to compute the elastic constants. The experimental elastic constants of $L1_0$ FePd were measured at $T \approx 300$ K. The sixth column presents calculations of the elastic constants available in the Materials Project database [67, 68].

Material	Crystal system	Method	Elastic constant	AELAS (GPa)	Mat.Proj. (GPa)	Expt. (GPa)	Magnetoelastic constant	MAELAS (MPa)	Expt. (MPa)
Fe_2Si	Trigonal (I) SG 164	DFT GGA	C_{11}	428	415[a]		b_{21}	3.1	
			C_{12}	164	169[a]		b_{22}	-4.2	
			C_{13}	133	133[a]		b_3	-0.7	
			C_{14}	-27	-25[a]		b_4	3.3	
			C_{33}	434	428[a]		b_{14}	-1.4	
			C_{44}	118	107[a]		b_{34}	-0.4	
$L1_0$ FePd	Tetragonal (I) SG 123	DFT GGA	C_{11}	324	293[b]	214[c]	b_{21}	-2.4	
			C_{12}	67	62[b]	143[c]	b_{22}	-15.2	
			C_{13}	133	125[b]	143[c]	b_3	-7.9	
			C_{33}	264	254[b]	227[c]	b_3'	-7.9	
			C_{44}	101	99[b]	92[c]	b_4	-5.6	
			C_{66}	37	38[b]	93[c]			
YCo	Orthorhombic SG 63	DFT GGA	C_{11}	76	94[d]		b_1	-0.9	
			C_{12}	45	61[d]		b_2	0.6	
			C_{13}	48	44[d]		b_3	-5.0	
			C_{22}	102	93[d]		b_4	5.7	
			C_{23}	55	56[d]		b_5	0.9	
			C_{33}	141	121[d]		b_6	1.5	
			C_{44}	40	38[d]		b_7	-5.0	
			C_{55}	27	29[d]		b_8	1.1	
			C_{66}	39	41[d]		b_9	-8.2	
		DFT LSDA+U	C_{11}	101			b_1	-1.7	
			C_{12}	65			b_2	1.2	
			C_{13}	58			b_3	-3.8	
			C_{22}	94			b_4	4.3	
			C_{23}	70			b_5	-0.1	
			C_{33}	138			b_6	2.3	
			C_{44}	42			b_7	-4.4	
			C_{55}	29			b_8	1.1	
			C_{66}	35			b_9	-8.7	

[a]Ref.[76], [b]Ref.[77], [c]Ref.[78], [d]Ref.[79]

MAELAS TESTS: FCC Ni

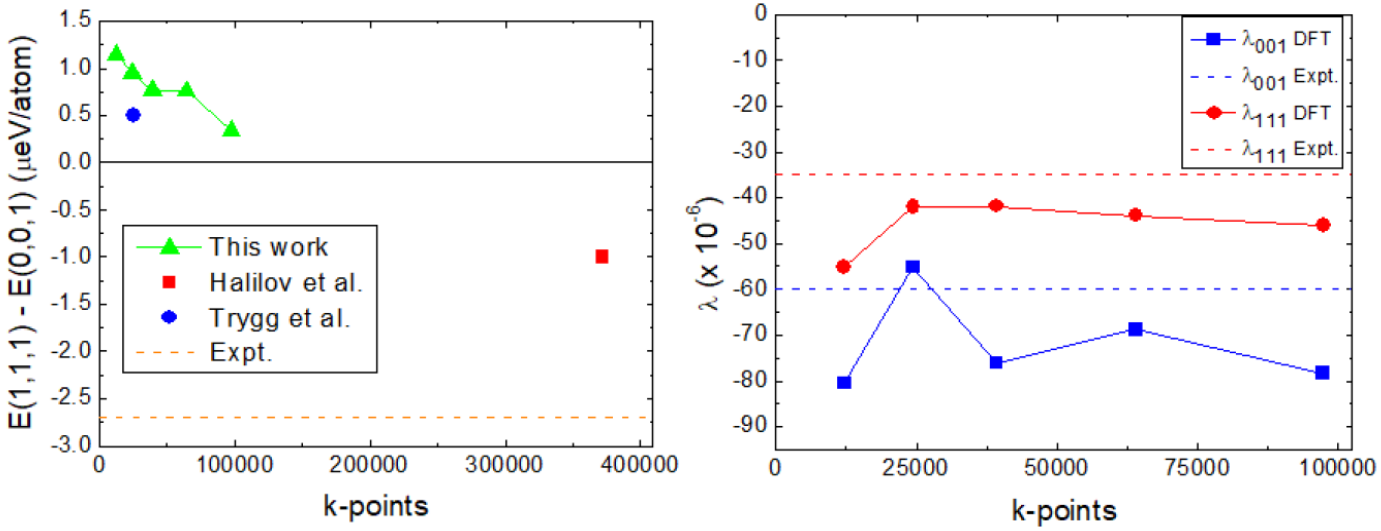


Figure 3: Calculation of (left) MAE of the unstrained unit cell and (right) magnetostrictive coefficients for FCC Ni as a function of k-points.

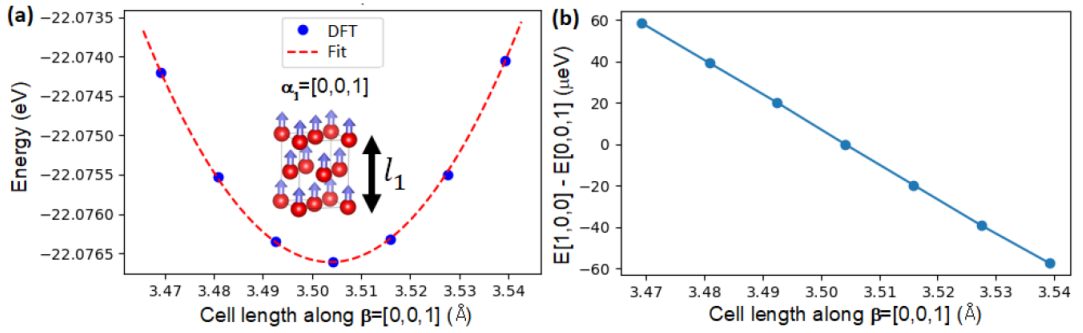


Figure 4: Calculation of λ_{001} for FCC Ni using MAELAS. (Left) Quadratic curve fit to the energy versus cell length along $\boldsymbol{\beta} = (0,0,1)$ with spin direction $\boldsymbol{\alpha}_1 = (0,0,1)$. (Right) Energy difference between states with spin directions $\boldsymbol{\alpha}_2 = (1,0,0)$ and $\boldsymbol{\alpha}_1 = (0,0,1)$ against the cell length along $\boldsymbol{\beta} = (0,0,1)$.

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

MAELAS TESTS: BCC Fe

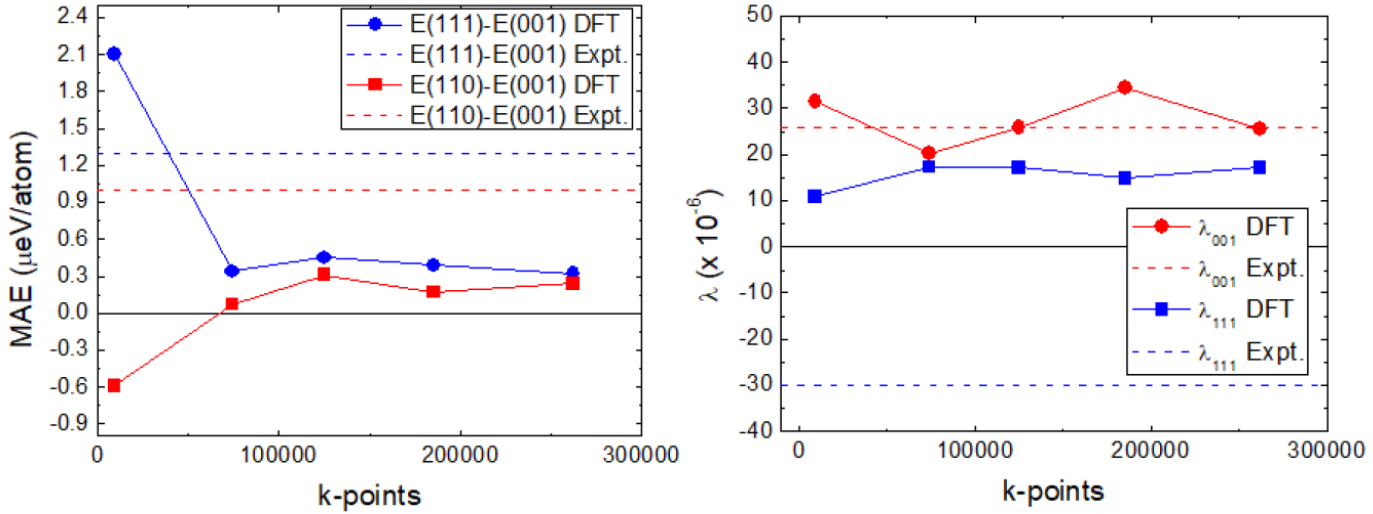


Figure 5: Calculation of (left) MAE of the unstrained unit cell and (right) magnetostrictive coefficients for BCC Fe as a function of k-points.

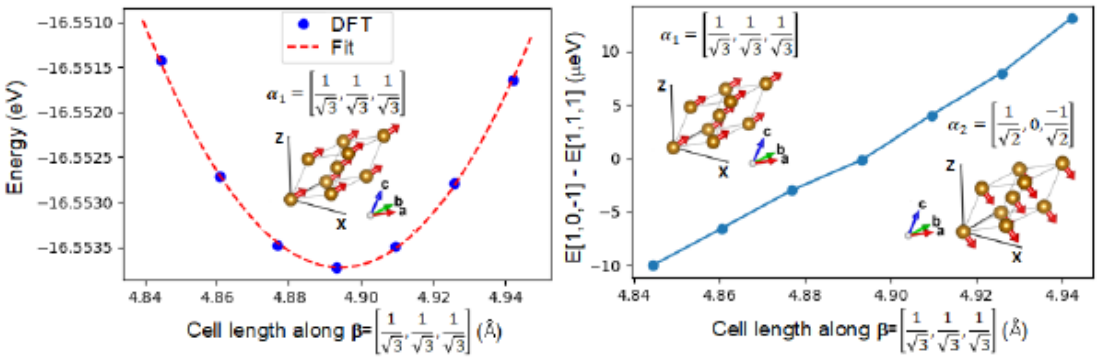


Figure 6: Calculation of λ_{111} for BCC Fe using MAELAS. (Left) Quadratic curve fit to the energy versus cell length along $\boldsymbol{\beta} = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$ with spin direction $\boldsymbol{\alpha}_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$. (Right) Energy difference between states with spin directions $\boldsymbol{\alpha}_2 = \left(\frac{1}{\sqrt{2}}, 0, \frac{-1}{\sqrt{2}}\right)$ and $\boldsymbol{\alpha}_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$ against the cell length along $\boldsymbol{\beta} = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$.

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

MAELAS TESTS: HCP Co

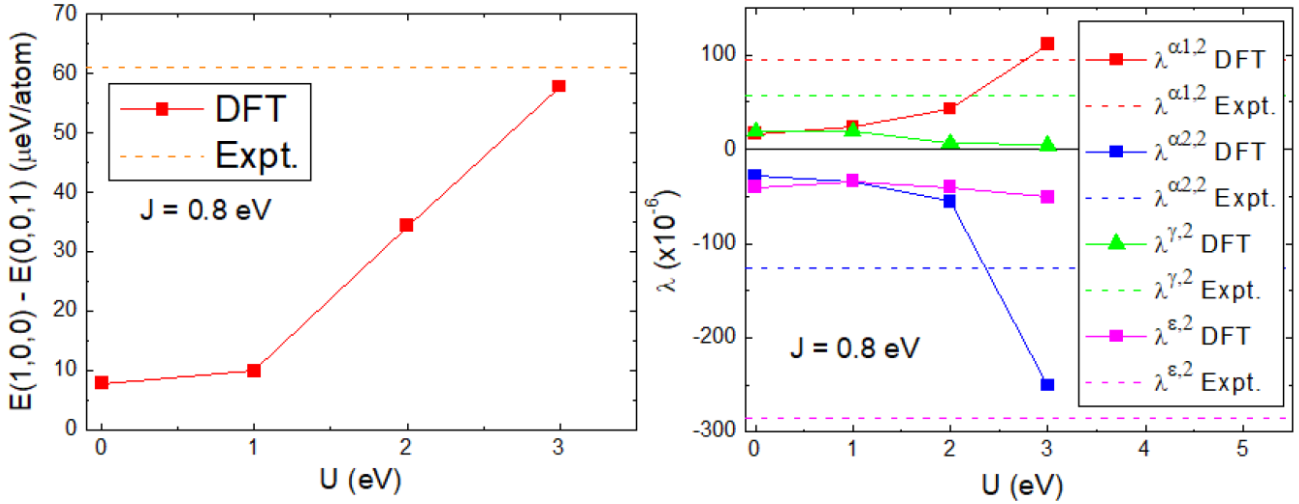


Figure 8: Calculation of (left) MAE of the unstrained unit cell and (right) magnetostrictive coefficients for HCP Co using the LSDA+U approach with different values of parameter U.

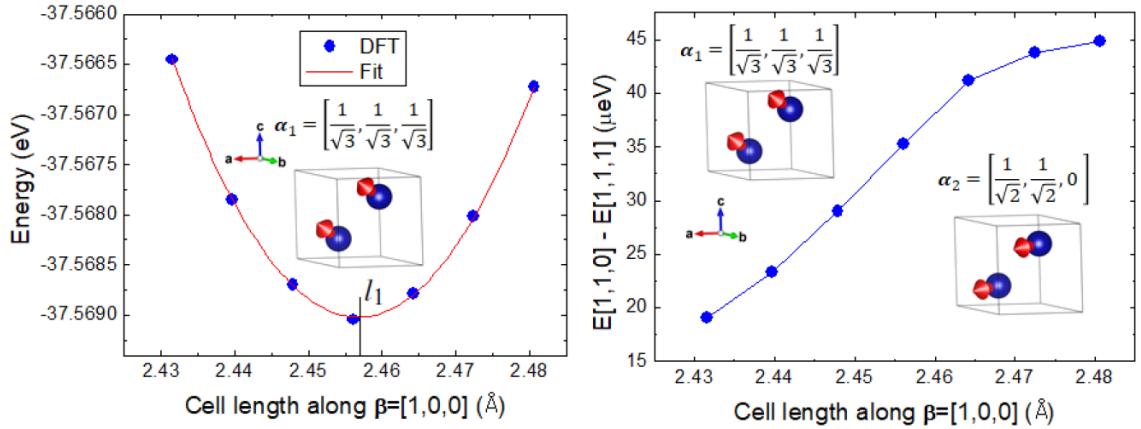


Figure 7: Calculation of $\lambda^{\alpha 1,2}$ for HCP Co using MAELAS with the meta-GGA functional SCAN. (Left) Quadratic curve fit to the energy versus cell length along $\boldsymbol{\beta} = (1,0,0)$ with spin direction $\boldsymbol{\alpha}_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$. (Right) Energy difference between states with spin directions $\boldsymbol{\alpha}_2 = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$ and $\boldsymbol{\alpha}_1 = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$ against the cell length along $\boldsymbol{\beta} = (1,0,0)$.

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

Visualization tool MAELASviewer

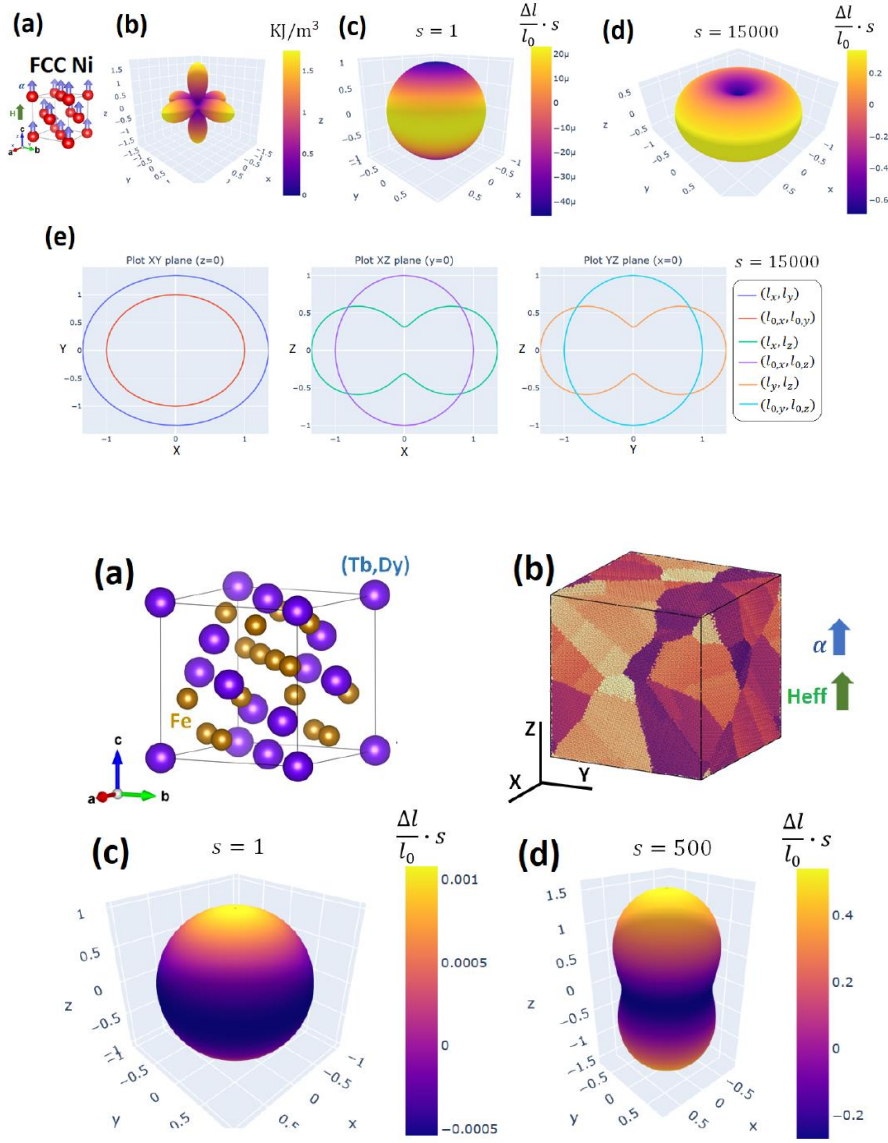
We have also developed an online visualization tool called MAELASviewer that is available at

https://maelasviewer.herokuapp.com

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

More details of this application can be found in:

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



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