

Myelas user manual

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1 How to install Myelas

```
1 | tar -zvxf MyEla.s.tar.gz
2 | cd MyEla
3 | python setup.py install
```

2 Module and Script

2.1 Module introduction

VASP input module (para_vasp.py): Generate KPOINT files and INCAR files .

Read POSCAR module (read_poscar.py): Read the POSCAR-uc file.

Read elastic tensor module (read_elastic.py): Read the elastic tensor from the OUTCAR or elastic.out.

Generate 2D strain POSCAR module (strain_poscar_2D.py): Generate 2D POSCAR of different strains required for calculation.

Generate 3D strain POSCAR module (strain_poscar_3D.py): Generate 3D POSCAR of different strains required for calculation.

Generate 3D third strain POSCAR module (strain_poscar_3rd3D.py): Generate 3D POSCAR of different strains required for the third elastic constants calculation.

Solve the second elastic of 2D module (solve_elastic_2D.py): Used to calculate the second elastic constants and related physical quantities of 2D materials.

Solve the second elastic of 3D module (solve_elastic_3D.py): Used to calculate the second elastic constants and related physical quantities of 3D materials.

Solve the third elastic of 3D module (solve_elastic_3rd3D.py): Used to calculate the third elastic constants and related physical quantities of 3D materials.

Plot the fitting E-V figure (plot_fit_E.py): Plotting the fitting EV figure of each strain matrix.

Plot the 3D figure (plot_project.py plot_project_cubic.py): Visualization of Young's, Bulk, Shear, Poisson ratio, and sound velocity of single-crystal materials.

Calculate elastic constants from phonon spectral data (phonon_to_elas.py): Support the phonon spectral data which generate by TDEP, Alamode and phonopy software.

2.2 Script tool

Some scripts are in the *script_tools* folder.

auto_elas_calculation.sh: Automatic calculation process of elastic constant

```
1 | #!/bin/bash
2 |
3 | # Relax structure
```

```

4  mkdir Relax
5  cd Relax/
6  cp ../POTCAR ./
7  cp ../POSCAR ./
8  Myelas --vasp incar --encut 600.0 --isif 3 --kspace 0.10 -ctype rlx
9  mpirun -np 32 vasp_std >vasp_relax.log
10 cp CONTCAR ../POSCAR-uc
11 cd ..
12
13 # Elastic calculation
14 Myelas -g 3D_2nd -smax 0.018 -snum 13
15 root_path=$(pwd)
16 for i in nelastic_*; do
17   cd ${i}
18   for j in strain_*; do
19
20     cd ${j}
21     cp ${root_path}/POTCAR ./
22
23     # IONIC position relax
24     Myelas --vasp incar --encut 600.0 --isif 2 --kspace 0.10 -ctype rlx
25     time mpirun -np 32 vasp_std >vasp_relax.log
26
27     cp CONTCAR ../POSCAR
28
29     # Static calculation
30     Myelas --vasp incar --encut 600.0 --isif 2 --kspace 0.10 -ctype stc
31
32     # Static calculation for electron temperature
33     #Myelas --vasp incar --encut 600.0 --isif 2 --kspace 0.10 -Te 300.0
34     -ctype stc
35     time mpirun -np 32 vasp_std >vasp_stc.log
36
37     cd ..
38   done
39 done
40
41 # Post-processing
42 Myelas -so 3D_2nd -smax 0.018 -snum 13
43
44 # Visualization
45 Myelas -p3D Youngs -ptype plane          #plot Young's modulus
46 Myelas -p3D Shear -ptype plane -minmax max #plot Max Shear modulus
47 Myelas -p3D Shear -ptype plane -minmax min #plot Min Shear modulus
48 Myelas -p3D Poisson -ptype plane -minmax max #plot Max Shear modulus
49 Myelas -p3D Poisson -ptype plane -minmax min #plot Min Shear modulus
50 Myelas -p3D SV                           #plot single-crystalline sound
      velocity

```

3 Introduction to input and output files

3.1 Input file

POSCAR-uc: The optimized initial stable structure. The primitive cell or the conventional unit cell. Same format as POSCAR.

example:

```
1 strain_poscar
2     1.000000000000000
3         2.3457218738000001    0.0000000000000000    0.0000000000000000
4         -1.1728609369000000   2.0314547329999999    0.0000000000000000
5             0.0000000000000000    0.0000000000000000    3.7183867462000002
6 Fe
7 2
8 Direct
9     0.6666666667000030   0.333333332999970   0.7500000000000000
10    0.333333332999970   0.666666667000030   0.2500000000000000
```

POTCAR: The potential file of VASP.

Phonon.dat: The phonon dispersion data. If we use the “Myelas -rp” command, this file will be needed.

input_direct : If we use the “Myelas -rp” command, this file will be needed.

example: Please set the value according to the actual high symmetry path.

```
1 # Direction Position left(-1)/right(1)
2 Cubic:
3 [100] ***** -1
4 [110] ***** 1
5 [111] ***** 1
6
7 Hexagonal and Trigonal:
8 [100] ***** 1
9 [001] ***** -1
10
11 Tetragonal:
12 [100] ***** -1
13 [001] ***** 1
14 [110] ***** 1
15
16 Orthorhombic:
17 [100] ***** 1
18 [010] ***** -1
19 [001] ***** 1
20
```

OUTCAR or **elastic.out** : The file which include elastic tensor. The OUTCAR is generated by VASP.

example (elastic.out):

```
1 296.036    61.286    26.809    0.000    0.000    0.000
2 61.286    220.654   146.618    0.000    0.000    0.000
3 26.809    146.618   349.260    0.000    0.000    0.000
4 0.000     0.000    0.000    152.599    0.000    0.000
5 0.000     0.000    0.000    0.000    124.848    0.000
6 0.000     0.000    0.000    0.000    0.000    102.399
```

3.2 Output file

RE-POSCAR: The normalized unit cell. Used to generate the strained POSCAR file.

example:

```
1 recell_poscar
2 1.0
3 2.3457218738    0.0000000000    0.0000000000
4 -1.1728609369    2.0314547330    0.0000000000
5 0.0000000000    0.0000000000    3.7183867462
6 Fe
7 2
8 Direct
9 0.6666666667    0.3333333333    0.7500000000
10 0.3333333333   0.6666666667    0.2500000000
```

E_Strain.out: The data used for polynomial fitting and the data regenerated by the parameters obtained by polynomial fitting.

example:

```
1 Space group 227
2 #nelastic 01 strain energy (E-E0)/V0
3 -0.018000  -43.36257630  0.00022698
4 -0.015000  -43.37391881  0.00015762
5 -0.012000  -43.38320566  0.00010083
6 -0.009000  -43.39042023  0.00005671
7 -0.006000  -43.39557190  0.00002521
8 -0.003000  -43.39866221  0.00000631
9 -0.000000  -43.39969451  0.00000000
10 0.003000  -43.39866361  0.00000630
11 0.006000  -43.39557542  0.00002519
12 0.009000  -43.39043256  0.00005664
13 0.012000  -43.38323442  0.00010066
14 0.015000  -43.37398325  0.00015723
15 0.018000  -43.36268100  0.00022634
16
17 #nelastic 02 strain energy (E-E0)/V0
18 -0.018000  -43.32686550  0.00044536
```

```

19 -0.015000 -43.34936909 0.00030774
20 -0.012000 -43.36762455 0.00019611
21 -0.009000 -43.38170239 0.00011002
22 -0.006000 -43.39168722 0.00004897
23 -0.003000 -43.39765857 0.00001245
24 -0.000000 -43.39969451 0.00000000
25 0.003000 -43.39786887 0.00001116
26 0.006000 -43.39226253 0.00004545
27 0.009000 -43.38295199 0.00010238
28 0.012000 -43.37000607 0.00018155
29 0.015000 -43.35349941 0.00028249
30 0.018000 -43.33351492 0.00040469
31
32 #nelastic 03 strain energy (E-E0)/v0
33 -0.018000 -43.25833744 0.00086441
34 -0.015000 -43.30238628 0.00059505
35 -0.012000 -43.33792058 0.00037775
36 -0.009000 -43.36518241 0.00021104
37 -0.006000 -43.38441393 0.00009344
38 -0.003000 -43.39583818 0.00002358
39 -0.000000 -43.39969451 0.00000000
40 0.003000 -43.39619123 0.00002142
41 0.006000 -43.38555478 0.00008647
42 0.009000 -43.36799921 0.00019382
43 0.012000 -43.34373092 0.00034222
44 0.015000 -43.31294881 0.00053046
45 0.018000 -43.27586102 0.00075725
46

```

second_elastic.out: Elastic constants and related properties

example (alpha-Uranium):

```

1 The orthorhombic crystal mechanical properties
2 Orthorhombic crystal (spacegroup No.: 63)
3
4 Elastic tensor C_ij (unit: GPa)
5   296.036   61.286   26.809   0.000   0.000   0.000
6   61.286   220.654   146.618   0.000   0.000   0.000
7   26.809   146.618   349.260   0.000   0.000   0.000
8   0.000   0.000   0.000   152.599   0.000   0.000
9   0.000   0.000   0.000   0.000   124.848   0.000
10  0.000   0.000   0.000   0.000   0.000   102.399
11
12 Compliance tensor S_ij (unit: GPa^-1)
13   0.003594   -0.001130   0.000199   0.000000   0.000000   0.000000
14   -0.001130   0.006641   -0.002701   0.000000   0.000000   0.000000
15   0.000199   -0.002701   0.003982   0.000000   0.000000   0.000000
16   0.000000   0.000000   0.000000   0.006553   0.000000   0.000000
17   0.000000   0.000000   0.000000   0.000000   0.008010   0.000000
18   0.000000   0.000000   0.000000   0.000000   0.000000   0.009766
19
20 mechanical stability: Stable
21

```

```

22 unit cell volume : 80.3273 A^3
23 unit cell density: 19689.2973 kg/m^3
24
25 Polycrystalline modulus
26 (Unit: GPa) Bulk modulus Shear modulus Youngs modulus Possion ratio
27 P-wave modulus
28 Vogit 148.3750 118.0517 279.9180 0.1856
29 305.7772
28 Reuss 143.8584 103.8917 251.2037 0.2090
29 282.3807
29 Hill 146.1167 110.9717 265.5608 0.1973
29 294.0790
30
31 Cauchy Pressure (GPa): -91.3127
32 Pugh's ratio : 0.7595
33 Vickers hardness (GPa): 19.7866
34
35 Anisotropy index:
36 Chung-Buessem anisotropy index: 0.06
37 Universal anisotropy index : 0.71
38 Log-Euclidean anisotropy index: 0.29
39
40 Polycrystalline sound velocity (m/s)
41 Longitudinal sound velocity: 3864.7097
42 Shear sound velocity : 2374.0564
43 Bulk sound velocity : 2724.1738
44 Average sound velocity : 2620.0689
45
46 Pure single-crystal sound velocity (m/s)
47 [100] direction: v1 = 3877.550 vs1 = 2280.517 vs2 = 2518.116
48 [010] direction: v1 = 3347.654 vs1 = 2280.517 vs2 = 2783.944
49 [001] direction: v1 = 4211.716 vs1 = 2518.116 vs2 = 2783.944
50
51 Debye temperature: 287.02 K
52
53 The minimum thermal conductivity:
54 Clark model : 0.597 w/(m K)
55 Chailll model : 0.649 w/(m K)
56

```

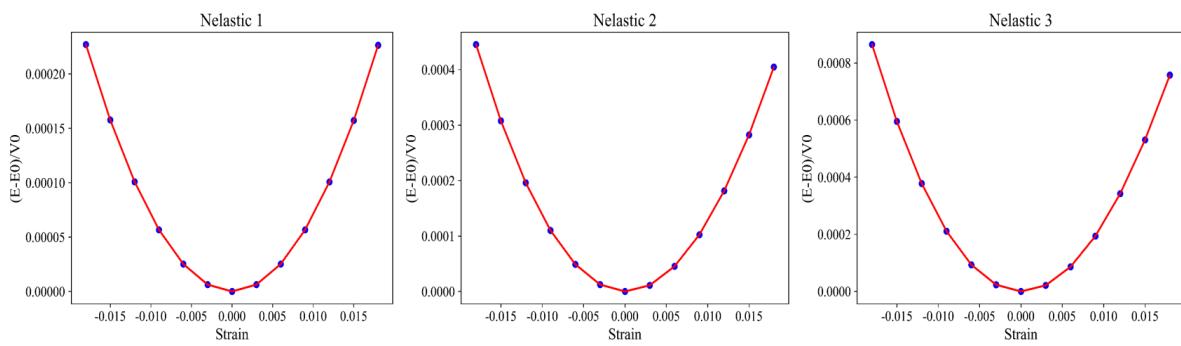
ELADAT_3rd:

```

1 The third elastic constants.
2 Please check the number of elastic constants for your structure.
3
4
5 C111 = -746.5459
6 C112 = -438.7388
7 C123 = -92.4655
8
9
10 C144 = 59.9915
11 C166 = -315.3537
12 C456 = -71.2529
13

```

Nelastic_*.png: the fitting EV figure of each strain matrix.



phonon_elastic.out: The elastic constants which calculated from long wavelength limit.

example (alpha-U):

```

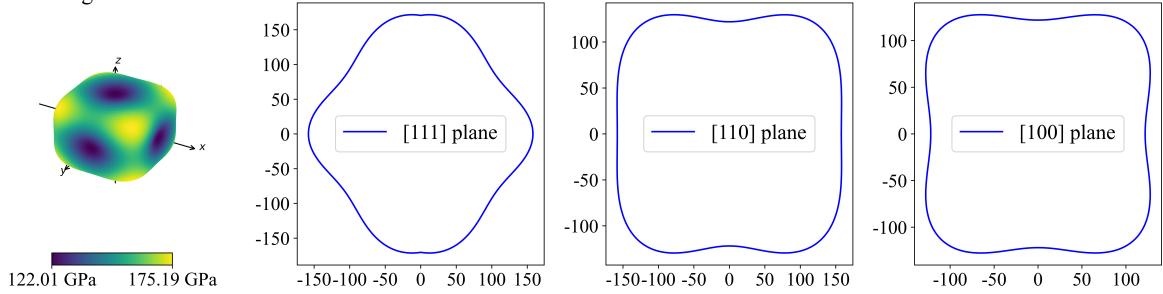
1 orthorhombic crystal:
2
3 C11  C22  C33  C44  C55  C66 (GPa)
4 354.655   257.168   402.203   143.639   120.159   89.186
5
6 Single-crystalline sound velocity (m/s)
7 100  v1 = 4242.888;  vs1 = 2088.201;  vs2 = 2411.127
8 010  v1 = 3612.992;  vs1 = 2166.440;  vs2 = 2665.254
9 001  v1 = 4518.362;  vs1 = 2526.833;  vs2 = 2734.691
10
11 unit cell volume : 80.2805 A^3
12 unit cell density: 19700.7659 kg/m^3
13

```

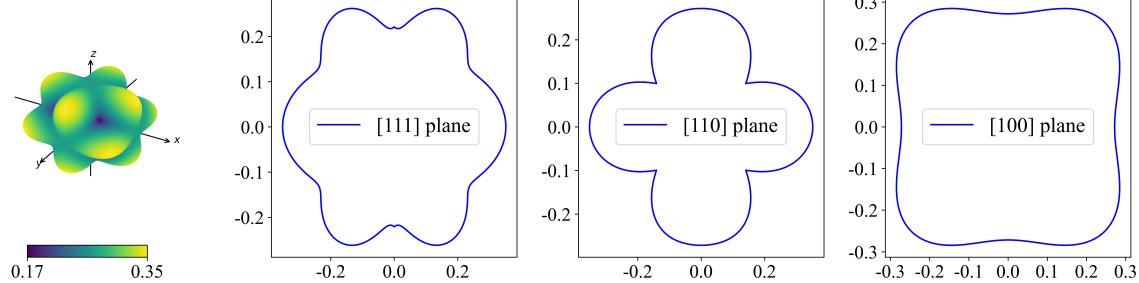
Elastic modulus and sound velocity of single crystal figure:

example:

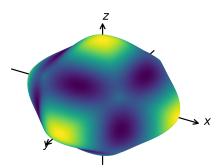
Young's modulus



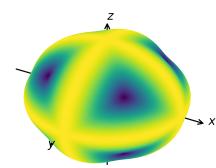
Max poisson ratio



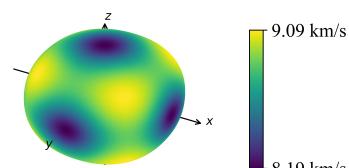
Slow Secondary



Fast Secondary



Primary



4. Command option

```
1 usage: Myelas [-h] [-g 3D_2nd/2D_2nd/3D_3rd] [-so 3D_2nd/2D_2nd/3D_3rd] [-  
2 smax 0.018] [-snum 13]  
3 [-p3D Youngs/Bulk/Shear/Poisson/SV] [-p2D 2D] [-ptype  
3D/plane] [-minmax min/max]  
4 [-vasp incar/kpoints/2D_kpoints] [--encut 600.0] [-Te 300.0]  
5 [-p 1000.0]  
6 [-ismear 0] [-sigma 0.05] [-isif 2]  
7 [-ks 0.10] [-kp 6] [-kt G/M] [-ctype rlc/stc] [-re  
OUTCAR/elastic.out]  
8 [-rp phonopy/alamode/alamode_scph/tdep]  
9 [-pf alamode.bands]  
10  
11 myelas optionn  
12 optional arguments:  
13 -h, --help show this help message and exit  
14 -g 3D_2nd/2D_2nd/3D_3rd, --generate 3D_2nd/2D_2nd/3D_3rd  
15 Generate elastic type which need calculate  
16 -so 3D_2nd/2D_2nd/3D_3rd, --solve 3D_2nd/2D_2nd/3D_3rd  
17 Solve elastic type which need calculate  
18 -smax 0.018, --strainmax 0.018  
19 The strain max number  
20 -snum 13, --strainnum 13  
21 The strain number  
22 -p3D Youngs/Bulk/Shear/Poisson/SV, --plot_3D Youngs/Bulk/Shear/Poisson/SV  
23 plot single crystal modulus  
24 -p2D 2D, --plot_2D 2D  
25 plot 2D materials modulus  
26 -ptype 3D/plane, --plot_3D_type 3D/plane  
27 plot type  
28 -minmax min/max, --minmax min/max  
29 plot maxnum or minnum for shear and poisson ratio  
30 --vasp incar/kpoints/2D_kpoints  
31 Generate the VASP input file  
32 --encut 600.0 The encut energy in INCAR  
33 -Te 300.0, --Temperature 300.0  
34 The electron temperature (K) in INCAR  
35 -p 1000.0, --pressure 1000.0  
36 The pressure in INCAR, unit: GPa, 1GPa=10kB  
37 --ismear 0 The ISMEAR in INCAR  
38 --sigma 0.05 The smearing width in VASP  
39 --isif 2 The ISIF in INCAR  
40 -ks 0.10, --kspace 0.10  
41 The KSPACING value in VASP  
42 -kp 6, --kpoint 6 The kpoint number in KPINTS  
43 -kt G/M, --kpoint_type G/M  
44 The kpoint type  
45 -ctype rlc/stc, --calc_type rlc/stc  
46 The calculation type : relax (rlx) or static (stc)  
47 -re OUTCAR/elastic.out, --read_elastic OUTCAR/elastic.out  
48 Read the elastic tensor from OUTCAR or elastic.out  
file  
-rp phonopy/phonopy_old/alamode/alamode_scph/tdep, --read_phonon_to_calc  
phonopy/alamode/alamode_scph/tdep
```

```
49                                     Read the phonon dispersiaon to calculate elastic  
constants  
50     -pf alamode.bands, --input_phonon_file alamode.bands  
51                         input phonon data file  
52  
53
```

Generate the INCAR or KPOINTS

```
1 # Relax cell  
2 Myelas --vasp incar --encut 600.0 --isif 3 -ctype rlx  
3  
4 # Static calculation  
5 Myelas --vasp incar --encut 600.0 -ctype stc  
6  
7 # Include electron temperature (300 K)  
8 Myelas --vasp incar --encut 600.0 -Te 300.0 -ctype stc  
9  
10 # KPOINTS (Gamma mesh 12 12 12)  
11 Myelas --vasp kpoints -kp 12 -kt G
```

Generate the strain POSCAR

```
1 Myelas -g 3D_2nd -smax 0.018 -snum 13 # The second-order elastic constants of  
3D solid materials  
2 Myelas -g 2D_2nd -smax 0.018 -snum 13 # The second-order elastic constants of  
2D solid materials  
3 Myelas -g 3D_3rd -smax 0.060 -snum 25 # The third-order elastic constants of  
3D solid materials
```

Solve the elastic constants

```
1 Myelas -so 3D_2nd -smax 0.018 -snum 13 # The second-order elastic constants  
of 3D solid materials  
2 Myelas -so 2D_2nd -smax 0.018 -snum 13 # The second-order elastic constants  
of 2D solid materials  
3 Myelas -so 3D_3rd -smax 0.060 -snum 25 # The third-order elastic constants  
of 3D solid materials
```

Calculate the elastic constants from phonon spectral data

```
1 Myelas -rp phonopy -pf band.yaml  
2 Myelas -rp alamode -pf alamode.bands  
3 Myelas -rp alamode_scph -pf alamode.bands  
4 Myelas -rp tdep -pf outfile.dispersion_relations
```

The elastic tensor is read directly from the OUTCAR or elastic.out file to calculate the relevant properties.

```
1 | Myelas -re OUTCAR
2 | Myelas -re elastic.out
```

Visualization

```
1 | # The Youngs modulus in sphere space
2 | Myelas -p3D Youngs -ptype 3D
3 |
4 | # The maxnum Shear modulus in sphere space
5 | Myelas -p3D Shear -ptype 3D -minmax max
6 |
7 | # Distribution of Young's modulus on plane
8 | Myelas -p3D Youngs -ptype plane
9 |
10 | # The single-crystalline sound velocity in sphere space
11 | Myelas -p3D SV
```

5. Example

5.1 Si elastic constants

5.1.1 Elastic constants calculation

Input file:

POSCAR-uc:

```
1 si8
2 1.0000000000000000
3 5.4684663969085214 0.0000000000000000 0.0000000000000000
4 0.0000000000000000 5.4684663969085214 0.0000000000000000
5 0.0000000000000000 0.0000000000000000 5.4684663969085214
6 si
7 8
8 Direct
9 0.0000000000000000 0.0000000000000000 0.0000000000000000
10 0.2500000000000000 0.7500000000000000 0.7500000000000000
11 0.5000000000000000 0.0000000000000000 0.5000000000000000
12 0.0000000000000000 0.5000000000000000 0.5000000000000000
13 0.5000000000000000 0.5000000000000000 0.0000000000000000
14 0.7500000000000000 0.2500000000000000 0.7500000000000000
15 0.7500000000000000 0.7500000000000000 0.2500000000000000
16 0.2500000000000000 0.2500000000000000 0.2500000000000000
17
```

1. Generate the strain POSCAR:

```
1 Myelas -g 3D_2nd -smax 0.018 -snum 13 # Only the second elastic constants
2 Myelas -g 3D_3rd -smax 0.060 -snum 13 # The third elastic constants
```

2. DFT calculation:

Third elastic constants calculation example:

```
1#!/bin/bash
2
3 root_path=$(pwd)
4 for i in nelastic_*; do
5     cd ${i}
6     for j in strain_*; do
7
8         cd ${j}
9         cp ${root_path}/POTCAR ./
10
11         # IONIC position relax
12         Myelas --vasp incar --encut 600.0 --isif 2 --kspace 0.10 -ctype rlx
```

```

13      time mpirun -np 32 vasp_std >vasp_relax.log
14
15      cp CONTCAR POSCAR
16
17      # Static calculation
18      Myelas --vasp incar --encut 600.0 --isif 2 --kspace 0.10 -ctype stc
19      time mpirun -np 32 vasp_std >vasp_stc.log
20
21      cd ..
22      done
23      cd ..
24      done

```

3. Solve elastic constants

```

1 Myelas -so 3D_2nd -smax 0.018 -snum 13 # The second elastic constants
2 calculation
2 Myelas -so 3D_3rd -smax 0.060 -snum 13 # The third elastic constants
3 calculation

```

Results:

`second_elastic.out`:

```

1 The cubic crystal mechanical properties
2 Cubic crystal (spacegroup No.: 227)
3
4 Elastic tensor C_ij (unit: GPa)
5   153.056    57.116    57.116    0.000    0.000    0.000
6   57.116    153.056    57.116    0.000    0.000    0.000
7   57.116    57.116    153.056    0.000    0.000    0.000
8   0.000    0.000    0.000    74.721    0.000    0.000
9   0.000    0.000    0.000    0.000    74.721    0.000
10  0.000    0.000    0.000    0.000    0.000    74.721
11
12 Compliance tensor S_ij (unit: GPa^-1)
13   0.008196   -0.002227   -0.002227   0.000000   0.000000   0.000000
14   -0.002227   0.008196   -0.002227   0.000000   0.000000   0.000000
15   -0.002227   -0.002227   0.008196   0.000000   0.000000   0.000000
16   0.000000   0.000000   0.000000   0.013383   0.000000   0.000000
17   0.000000   0.000000   0.000000   0.000000   0.013383   0.000000
18   0.000000   0.000000   0.000000   0.000000   0.000000   0.013383
19
20 mechanical stability: Stable
21
22 unit cell volume : 163.5297 A^3
23 unit cell density: 2282.2924 kg/m^3
24
25 Polycrystalline modulus
26 (Unit: GPa) Bulk modulus      Shear modulus      Youngs modulus      Possion ratio
          P-wave modulus

```

```

27    vogit      89.0962          64.0205          154.9485          0.2101
28          174.4568
28    Reuss      89.0962          61.0930          149.1814          0.2209
28          170.5536
29    Hill       89.0962          62.5568          152.0649          0.2155
29          172.5052
30
31 Cauchy Pressure (GPa): -17.6046
32 Pugh's ratio : 0.7021
33 Vickers hardness (GPa): 11.8647
34
35 Anisotropy index:
36     Zener anisotropy index : 1.56
37     Chung-Bussem anisotropy index: 0.02
38     Universal anisotropy index : 0.24
39     Log-Euclidean anisotropy index: 0.10
40
41 Polycrystalline sound velocity (m/s)
42     Longitudinal sound velocity: 8693.9170
43     Shear sound velocity : 5235.4196
44     Bulk sound velocity : 6248.0426
45     Average sound velocity : 5789.5759
46
47 Pure single-crystal sound velocity (m/s)
48     [100] direction: v1 = 8189.156 vs1 = 5721.841 vs2 = 5721.841
49     [110] direction: v1 = 8876.011 vs1 = 4584.559 vs2 = 5721.841
50     [111] direction: v1 = 9093.440 vs1 = 4992.522 vs2 = 4992.522
51
52 Debye temperature: 630.48 K
53
54 The minimum thermal conductivity:
55     Clark model : 1.312 W/(m K)
56     Chaill model : 1.427 W/(m K)

```

ELADAT_3rd:

```

1 The third elastic constants.
2 Please check the number of elastic constants for your structure.
3
4
5 C111 = -746.5459
6 C112 = -438.7388
7 C123 = -92.4655
8
9
10 C144 = 59.9915
11 C166 = -315.3537
12 C456 = -71.2529
13

```

5.1.2 Visualization

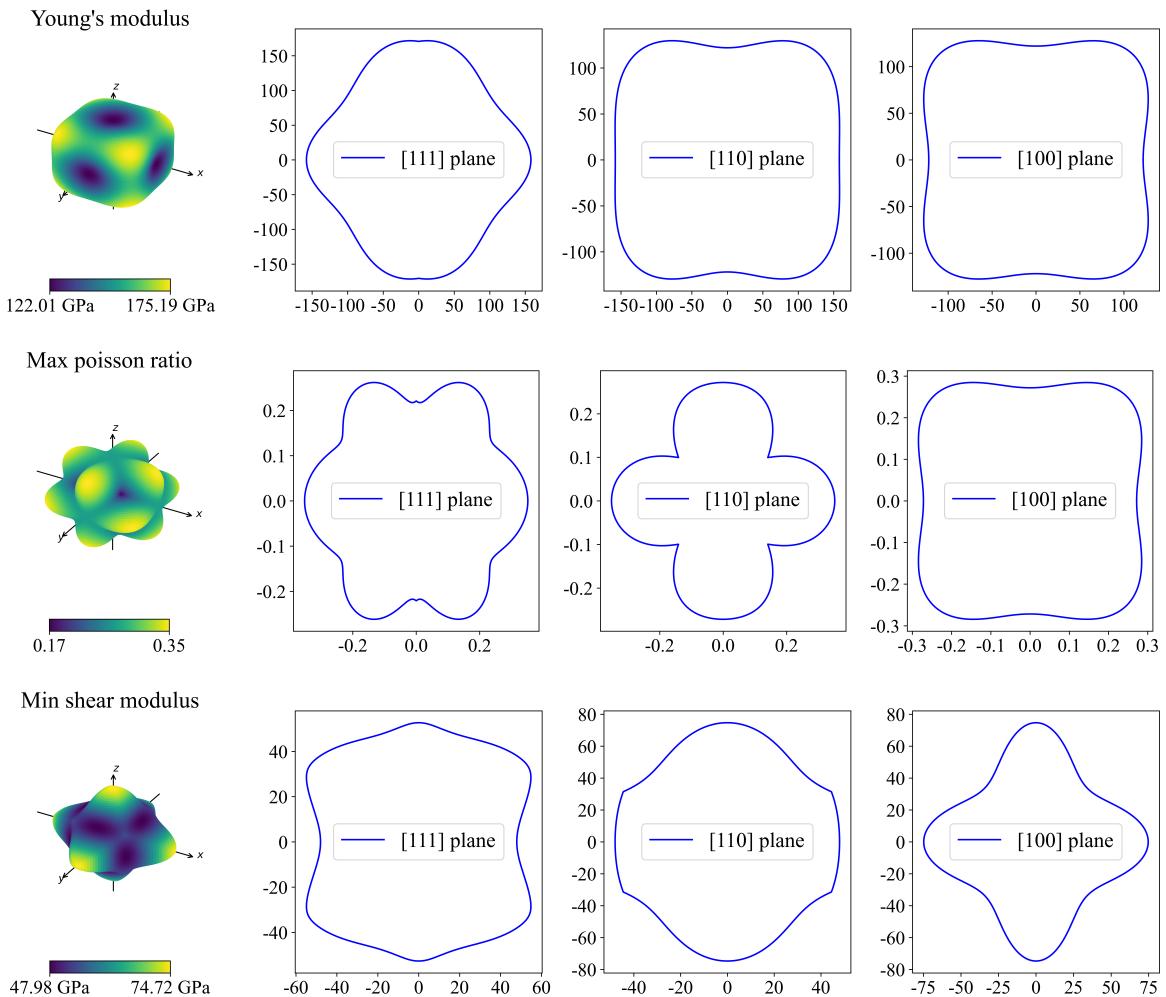
Input file:

```
1 | POSCAR-uc  
2 | POTCAR  
3 | second_elastics.out
```

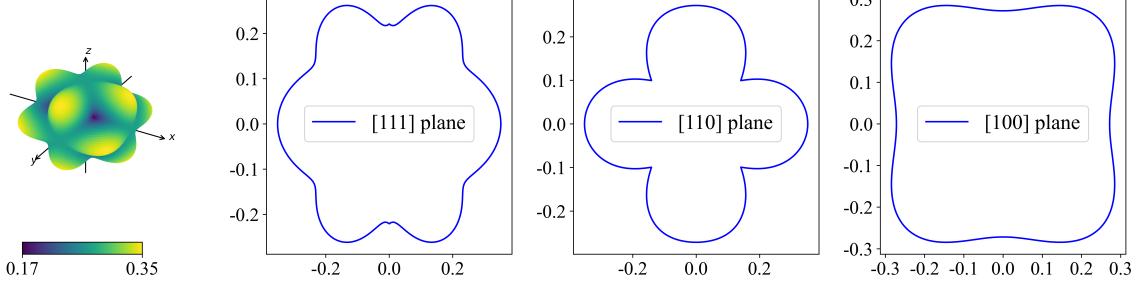
Command:

```
1 | Myelas -p3D Youngs -ptype plane #plot Young's modulus  
2 | Myelas -p3D Shear -ptype plane -minmax max #plot Max Shear modulus  
3 | Myelas -p3D Shear -ptype plane -minmax min #plot Min Shear modulus  
4 | Myelas -p3D Poisson -ptype plane -minmax max #plot Max Poisson ratio  
5 | Myelas -p3D Poisson -ptype plane -minmax min #plot Min Poisson ratio
```

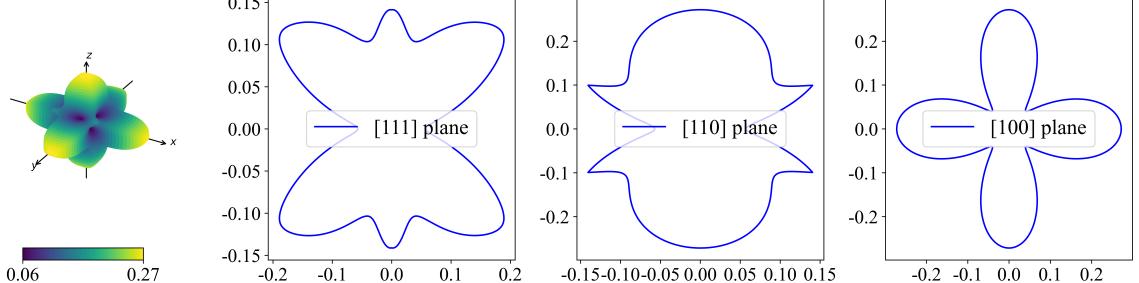
Output file:



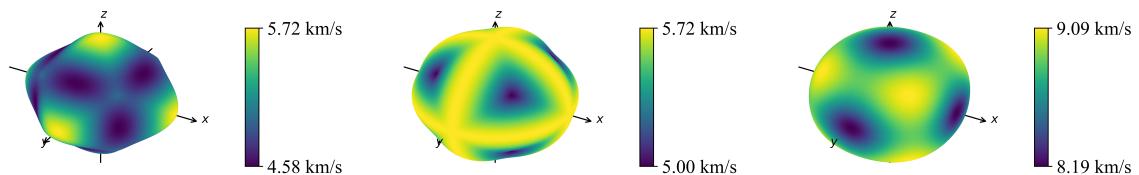
Max poisson ratio



Min poisson ratio



Slow Secondary



5.2 2D-Graphene second elastic constants

5.2.1 Elastic constants calculation

Input file:

POSCAR-uc:

```
1 | c2
2 | 1.000000000000000
3 |     2.4686779615000001    0.0000000000000000    0.0000000000000000
4 |     -1.2343389807000000   2.1379378284000001    0.0000000000000000
5 |     0.0000000000000000   0.0000000000000000   20.0000000000000000
6 | c
7 | 2
8 | Direct
9 |     0.0000000000000000   0.0000000000000000   0.0000000000000000
10 |    0.3333333429999996   0.6666666870000029   0.0000000000000000
11 |
```

1. Generate the strain POSCAR:

```
1 | Myelas -g 2D_2nd -smax 0.018 -snum 13 # only the second elastic constants
```

2. DFT calculation:

Third elastic constants calculation example:

```
1 |#!/bin/bash
2 |
3 |root_path=$(pwd)
4 |for i in 2D_nelastic_*; do
5 |    cd ${i}
6 |    for j in strain_*; do
7 |
8 |        cd ${j}
9 |        cp ${root_path}/POTCAR ./
10 |
11 |        Myelas --vasp 2D_kpoints -kp 12 -kt G
12 |
13 |        # IONIC position relax
14 |        Myelas --vasp incar --encut 600.0 --isif 2 -ctype rlx
15 |        time mpirun -np 32 vasp_std >vasp_relax.log
16 |
17 |        cp CONTCAR POSCAR
18 |
19 |        # Static calculation
20 |        Myelas --vasp incar --encut 600.0 --isif 2 -ctype stc
21 |        time mpirun -np 32 vasp_std >vasp_stc.log
22 |
23 |        cd ..
24 |done
```

```
25 |     cd ..
26 | done
```

3. Solve elastic constants

```
1 | Myelas -so 2D_2nd -smax 0.018 -snum 13 # The second elastic constants
      calculation
```

Results:

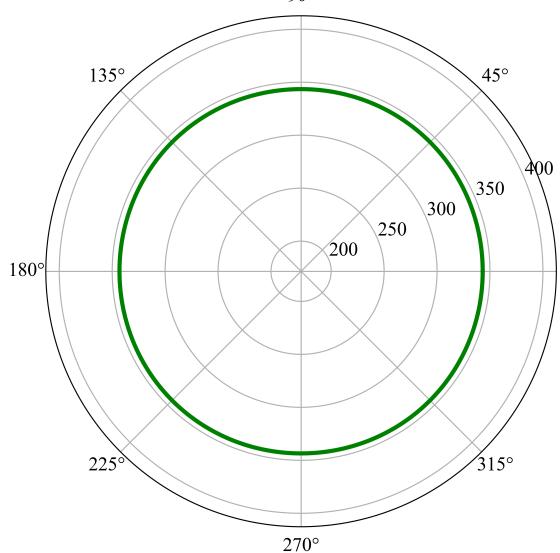
second_elastic.out:

```
1 | 2D elastic constants
2 | Space group: 191
3 |
4 | Elastic tensor C_ij (unit: N/m)
5 |     353.612    60.918    0.000
6 |     60.918    353.975    0.000
7 |     0.000    0.000    146.877
8 |
9 | Compliance tensor S_ij (unit: (N/m)^-1)
10 |    0.002914   -0.000502    0.000000
11 |   -0.000502    0.002911    0.000000
12 |    0.000000    0.000000    0.006808
13 |
14 | 2D area (A^2) : 5.2779
15 |
16 | Young(Ex and Ey) and shear(Gxy) moduli (unit: N/m)
17 | Ex : 343.1280
18 | Ey : 343.4804
19 | Gxy: 146.8774
20 |
21 | Poisson ratios(Muxy and Muyx)
22 | Muxy : 0.1721
23 | Muyx : 0.1723
24 |
25 | mechanical stability: Stable
26 |
27 | Anisotropy index:
28 |     Elastic anisotropy index      : 0.00
29 |     Ranganathan anisotropy index : 0.00
30 |     Kube anisotropy index       : 0.00
31 |
```

5.2.2 Visualization

```
1 | Myelas -p2D 2D
```

Young's modulus (N/m)



Poisson ratio

