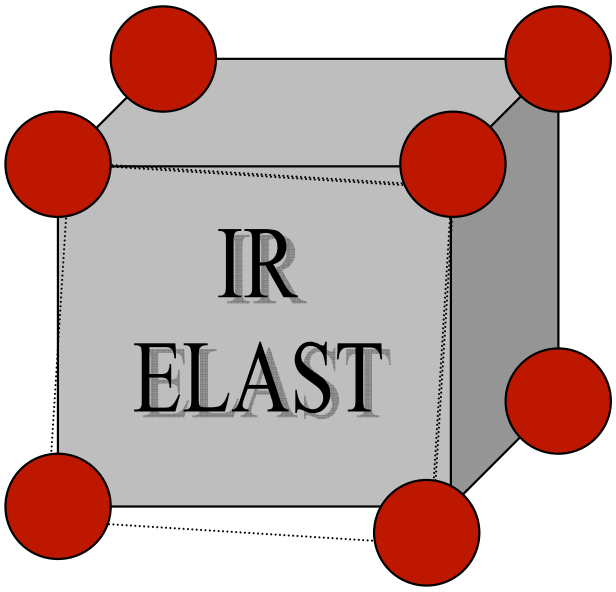

IR ELAST

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WIEN2k

A Package for calculating elastic tensors of tetragonal Phases *by using second-order derivative* with Wien2k Package

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User's guide, Elastic Tetragonal_12.1 (Release 11.09.2012)
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and special thanks
B. Z. Yanchitsky
for fruitful discussions.

Installation guide

1_ Copy **“tetra-elastic.tar.gz”** file in each Directory then do:
tar –zxvf tetra-elastic.tar.gz
cd tetra-elastic

2_ Run **buildTIRelast_lapw**

This program helps you to provide "Makefile" and then compile tetra-elastic. Then define Environment Variable ELASTT_PATH and add it at the end of **.bashrc** file. Therefore you will be able to call tetra-elastic’s programs from each Directory.

Call Package

1_ Make struct file and we recommend then run "sgroupcheck_lapw".

2_ Do initialization (run "instgen_lapw" and "init_lapw" in Terminal).
It is not necessary to do step 2. This program can do that.

3_ If you want to do Spin-Orbit calculations run "command_initso_lapw" in Terminal.

4_ If you want to do LDA+U calculations run "command_initu_lapw" and then "auto_initu_lapw" in Terminal.

NOTE ABOUT STEPS 3 AND 4

After using distortion for calculation C11-C12 , C44, and C66, the symmetry of tetragonal compounds changes and maybe Number of atoms change. So when you run "command_initso_lapw" or "command_initu_lapw" ,in section name of atom, type "all name of atom" (e.g. all Mn). With this command, you use SO or LDA+U calculations for example for all Mn atoms.

5_ Run "T_set_elast_lapw" in Terminal.

6_Now you must modify job files according to your needs (you can run "T_modifyjob_lapw" in Terminal).
It is not necessary to do step 6 if you define COMMANDS RUN in step 5.

7_ Now you must run job files (you can run "T_calljob_lapw" in Terminal). It will take time.

Note 1: When you want to rerun **job** files with modifications in (RKmax, k-mesh, XC-potentials) **call “command_init_lapw”** and after that choose "answscf=no" in **“TETRA.job”** files and a new "savename" (eg. "_use_pbe_rk8").

8_ Run "T_ana_elast_lapw" in Terminal.

Optionally you can specify more cases by rerunning "**T_setupcXX" (XX=1112,44,33,.. see Suppose section)**. Specify also your **''old'' cases**. The old results will then be taken automatically into account without recalculation (unless you modify **job** files i.e: set answscf=no).

NOTE ABOUT PROGRAMS

T_set_elast_lapw : makes elast-constant directory in present work directory (PWD) and c11+c12, c11-c12, c33, c44, c66, and czz directories in elast-constant directory. Moreover T_set_elast_lapw program copies information of "PWD" in c11+c12, c11-c12, c33, c44, c66, and czz directories and calls "command_init_lapw", T_command_run_lapw, T_setupc1112, T_setupc11m12, T_setupc33, T_setupc44, T_setupc66, and T_setupczz programs.

T_command_run_lapw : gets commands run for making "TETRA.job".

T_modifyjob_lapw : Edits job files for modifying them according to your needs.

T_calljob_lapw : calls job files for running.

T_ana_elast_lapw : calls T_ana_elastc_lapw programs for calculation elastic constants and then calculates **Voigt, Reuss, and Hill bulk, shear, and Young modulus as well as Poisson ratio and makes an output file in elast-constant directory with name case.output_elastic.**

Moreover T_ana_elastc_lapw. makes an output with name ELC.output with in present work directory.

T_ana_elastorder_lapw : THIS PROGRAM CHECK THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT (This program saves these data in the **output-order** file in the elast-constant directory.). You can run it in the elast-constant directory. Moreover T_ana_elast_lapw calls T_ana_elastorder_lapw at the end of calculations.

TO AVOID THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT, WE HIGHLY RECOMMEND TO USE VERY SMALL STRAINS.

command_init_lapw : gets informations for making "auto_init_lapw".

sgroupcheck_lapw : finds best value of tol in sgroup program and copies case.struct_sgroup as case.struct.

Suppose

Suppose we only want to calculate c33.

We do these stages as following:

1) Make a directory for example c33.
2) Make "case" directory in c33 directory.
3) Make "case.struct" file in "case" directory and copy it as "init.struct".
Moreover make "pwdname" file and write in it "**case.**" and save it.
4) Run command_init_lapw
5) chmod +x auto_init_lapw
6) For SO calculations, run command_initso_lapw.
7) For LDA+U calculations, run command_initu_lapw and auto_initu_lapw.

7-1) To avoid step 10, you can run "T_command_run_lapw" for getting COMMANDS RUN for making "TETRA.job" .

8) Run T_setupc33 program.
9) chmod +x TETRA.job file.
10) Modify TETRA.job file.
11) Call TETRA.job
12) Call T_ana_elastc_lapw

Suppose we want to rerun czz with more data points.

We do these stages as following:

1) cd "elast-constant" directory.
2) cd "czz" directory.
3) cd "case" directory.

3-1) To avoid step 6, you can run "T_command_run_lapw" for getting COMMANDS RUN for making "TETRA.job" .

4) Run T_setupczz program.
5) If you want to rerun **job** files with modifications in (RKmax, k-mesh, XC-potentials) **call "command_init_lapw"** and after that choose "answscf=no" in **"TETRA.job"** files and a new "savename" (eg. "_use_pbe_rk8").
6) Modify TETRA.job file.
7) Call TETRA.job
8) Call T_ana_elastc_lapw

IMPORTANT NOTE

For calculation best values of elastic constants, please find EOS and then copy case.outputeos in "case" directory within c11+c12, c11-c12, c33, c44, c66, and czz directories. **Otherwise this program set an arbitrary number for optimized volume (Vopt=999).**

Converged check

Since this package computes elastic constants by using second-order derivative (E”(ϵ)) of Polynomial fit (E=E(ϵ)) of Energy vs. Strains (ϵ) at zero strain (ϵ=0). So, you must use values of strain around zero and **from the viewpoint of fit convergence,** we usually expect to see a minimum when we plot Energy vs. strain (this Package plots it). Moreover I recommend to check the sensitivity of the results to the order of fit. This program shows them. You can see in the example.

We recommend to use more data-points, more k-points and larger RKmax for all calculations to reduce numerical noise.

TO AVOID THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT, WE HIGHLY RECOMMEND TO USE VERY SMALL STRAINS.

EXAMPLE

Calculation elastic-constants for α-Pt2Si

```
alpha Pt2Si
B   LATTICE,NONEQUIV.ATOMS:  2139_I4/mmm
MODE OF CALC=RELA unit=bohr
  7.461000  7.461000 11.268000 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.50000000 Z=0.25000000
          MULT= 2          ISPLIT=-2
      -1: X=0.00000000 Y=0.50000000 Z=0.75000000
Pt         NPT=  781  R0=0.00000500 RMT=    2.4600   Z: 78.0
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=-2
```

```
Si         NPT=  781  R0=0.00010000 RMT=    2.1800   Z: 14.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  16      NUMBER OF SYMMETRY OPERATIONS
```

Select Xc = PBE-GGA, R_Kmax = 7, L_max = 8, and nkpoint = 5000

In the following examples you can find which percents I used for Strains.

```
########################################
#  T_ana_elast_lapw analyses Elastic  #
#            constant                #
#     C(2012) by Morteza Jamal       #
########################################

##########################################
# T_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#                TETRA.job               #
##########################################
-0.020000   -74367.072429
-0.010000   -74367.078761
 0.000000   -74367.082546
 0.010000   -74367.083740
 0.020000   -74367.082833
 0.030000   -74367.080021
 ============================================================
Order of fit:  2 C11+C12 is:    540.1454 GPa, RMS: 0.145268E-03
Order of fit:  3 C11+C12 is:    570.6507 GPa, RMS: 0.282807E-04
Order of fit:  4 C11+C12 is:    583.0759 GPa, RMS: 0.213386E-04
Order of fit:  5 C11+C12 is:    618.2109 GPa, RMS: 0.168031E-10
 ****************************************
 Polynomial fit for C11+C12 done
A RMS of 0.145268E-03 was achieved using a polynome of degree :  2

At volume=  313.6252 bohr^3
 C11+C12 is:   0.036718 a.u or    540.1454 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************
```

```
##########################################
# T_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#               TETRA.job                #
##########################################
-0.020000   -74367.078725
-0.010000   -74367.080982
 0.000000   -74367.082546
 0.010000   -74367.083363
 0.020000   -74367.083711
 0.030000   -74367.083443
 0.040000   -74367.082684
 ============================================================
Order of fit:  2 C33 is:    281.2080 GPa, RMS: 0.554340E-04
Order of fit:  3 C33 is:    307.2910 GPa, RMS: 0.205522E-04
Order of fit:  4 C33 is:    303.3959 GPa, RMS: 0.183031E-04
Order of fit:  5 C33 is:    309.5179 GPa, RMS: 0.181199E-04
Order of fit:  6 C33 is:    356.2948 GPa, RMS: 0.110002E-10
 ****************************************
 Polynomial fit for C33 done
A RMS of 0.554340E-04 was achieved using a polynome of degree :  2

At volume=  313.6252 bohr^3
 C33 is:   0.019116 a.u or    281.2080 GPa
 ****************************************


 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************

##########################################
# T_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#               TETRA.job                #
##########################################
-0.020000   -74367.078654
-0.010000   -74367.081520
 0.000000   -74367.082546
 0.010000   -74367.081565
 0.020000   -74367.079876
 ============================================================
Order of fit:  2 Czz is:    372.4329 GPa, RMS: 0.178388E-03
Order of fit:  3 Czz is:    372.4329 GPa, RMS: 0.785657E-04
Order of fit:  4 Czz is:    499.6474 GPa, RMS: 0.920344E-11
 ****************************************
 Polynomial fit for Czz done
A RMS of 0.178388E-03 was achieved using a polynome of degree :  2
```

```
At volume=  313.6252 bohr^3
 Czz is:   0.025317 a.u or    372.4329 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************

##########################################
# T_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#               TETRA.job                #
##########################################
-0.020000   -74367.081538
-0.010000   -74367.081149
 0.000000   -74367.082411
 0.010000   -74367.081149
 0.020000   -74367.081538
 ================================================================
Order of fit:  2 C11-C12 is:     32.3723 GPa, RMS: 0.446171E-03
Order of fit:  3 C11-C12 is:     32.3723 GPa, RMS: 0.446171E-03
Order of fit:  4 C11-C12 is:    754.8177 GPa, RMS: 0.000000E+00
 ****************************************
 Polynomial fit for C11-C12 done
A RMS of 0.446171E-03 was achieved using a polynome of degree :  2

At volume=  313.6252 bohr^3
 C11-C12 is:   0.002201 a.u or     32.3723 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************

##########################################
# T_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#               TETRA.job                #
##########################################
-0.020000   -74367.080087
-0.010000   -74367.081857
 0.000000   -74367.082548
 0.010000   -74367.081856
 0.020000   -74367.080079
```

```
 ================================================================
Order of fit:  2 C44 is:     71.0193 GPa, RMS: 0.321798E-04
Order of fit:  3 C44 is:     71.0193 GPa, RMS: 0.321606E-04
Order of fit:  4 C44 is:     84.0381 GPa, RMS: 0.184069E-10
 ****************************************
 Polynomial fit for C44 done
A RMS of 0.321798E-04 was achieved using a polynome of degree :  2

At volume=  313.6252 bohr^3
 C44 is:   0.004828 a.u or     71.0193 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************

##########################################
# T_ana_elastc_lapw analyses Elastic     #
#              constant                  #
#       C(2012) by Morteza Jamal         #
#     using case.outputeos               #
#                          VstVene       #
#    which have been created by          #
#               TETRA.job                #
##########################################
-0.020000   -74367.079616
-0.010000   -74367.081826
 0.000000   -74367.082546
 0.010000   -74367.081826
 0.020000   -74367.079616
 ================================================================
Order of fit:  2 C66 is:    172.2018 GPa, RMS: 0.506683E-05
Order of fit:  3 C66 is:    172.2018 GPa, RMS: 0.506674E-05
Order of fit:  4 C66 is:    168.0998 GPa, RMS: 0.130156E-10
 ****************************************
 Polynomial fit for C66 done
A RMS of 0.506683E-05 was achieved using a polynome of degree :  2

At volume=  313.6252 bohr^3
 C66 is:   0.011706 a.u or    172.2018 GPa
 ****************************************

 Analyze done.....
Do you want a hardcopy? (y/N)
************************************
You can find data in ELC.output file.
************************************

Printing final Elastic constant At voulme= 313.6252 bohr^3 .

=========================================================================

C11+C12 = 540.1454 GPa      C11-C12 = 32.3723 GPa
C33 = 281.2080 GPa            C44 = 71.0193 GPa
Czz = C11+C12+2C33-4C13 = 372.4329 GPa
```

```
        C66 = 172.2018 GPa
        ========================================================================

        C11 = 286.2588 GPa                              C12 = 253.8865 GPa
                             C13 = 182.5321 GPa
        C33 = 281.2080 GPa                              C44 = 71.0193 GPa
                             C66 = 172.2018 GPa

Prediction VOIGT Bulk modulus by using elastic constant values  = 232.403 (GPa)
Prediction REUSS Bulk modulus by using elastic constant values  = 228.919 (GPa)
Prediction HILL  Bulk modulus by using elastic constant values  = 230.661 (GPa)


Prediction VOIGT Shear modulus by using elastic constant values = 78.499  (GPa)
Prediction REUSS Shear modulus by using elastic constant values = 44.776  (GPa)
Prediction HILL  Shear modulus by using elastic constant values = 61.637  (GPa)

Prediction VOIGT Young modulus by using elastic constant values = 211.665 (GPa)
Prediction REUSS Young modulus by using elastic constant values = 126.105 (GPa)
Prediction HILL  Young modulus by using elastic constant values = 169.787 (GPa)

Prediction VOIGT Poisson's coefficient by using elastic constant values = .348
Prediction REUSS Poisson's coefficient by using elastic constant values = .408
Prediction HILL  Poisson's coefficient by using elastic constant values = .377
        ========================================================================

         Press enter key to continue....

        ################################################
        # T_ana_elastorder_lapw checks the sensitivity #
        #   of elastic constants to the order of fit   #
        #       by using   ELCorder.fit file           #
        #         C(2012) by Morteza Jamal             #
        #                                              #
        ################################################

        CHECK THE SENSITIVITY
              OF YOUR RESULT TO THE ORDER OF FIT

         Press enter key to continue....
         Order of fit for calculations were 4,6,4,5, 4 , and 4
         We select minimum value for ORDER OF FIT i.e. 4

         Press enter key to continue....

        ######## ORDER OF FIT IS :  2 , At volume = 313.62518 (bohr^3) ########
        (c11-c12) = 32.372 (GPa)
        (c11+c12) = 540.145 (GPa)
        (c33) = 281.208 (GPa)
        (c44) = 71.019 (GPa)
        (czz=c11+c12+2c33-4c13) = 372.433 (GPa)
        (c66= 172.202 (GPa)
        ____________________________________________
        c11 = 286.258 (GPa)
        c12 = 253.886 (GPa)
        c13 = 182.532 (GPa)
        c33 = 281.208 (GPa)
```

```
        c44 = 71.019 (GPa)
        c66 = 172.202 (GPa)
        ========================================================================
Prediction VOIGT Bulk modulus by using elastic constant values  = 232.402 (GPa)
Prediction REUSS Bulk modulus by using elastic constant values  = 228.919 (GPa)
Prediction HILL  Bulk modulus by using elastic constant values  = 230.660 (GPa)


Prediction VOIGT Shear modulus by using elastic constant values = 78.499  (GPa)
Prediction REUSS Shear modulus by using elastic constant values = 44.776  (GPa)
Prediction HILL  Shear modulus by using elastic constant values = 61.637  (GPa)


Prediction VOIGT Young modulus by using elastic constant values = 211.665 (GPa)
Prediction REUSS Young modulus by using elastic constant values = 126.105 (GPa)
Prediction HILL  Young modulus by using elastic constant values = 169.787 (GPa)

Prediction VOIGT Poisson's coefficient by using elastic constant values = .348
Prediction REUSS Poisson's coefficient by using elastic constant values = .408
Prediction HILL  Poisson's coefficient by using elastic constant values = .377
        ========================================================================
        ######## ORDER OF FIT IS :  3 , At volume = 313.62518 (bohr^3) ########
        (c11-c12) = 32.372 (GPa)
        (c11+c12) = 570.651 (GPa)
        (c33) = 307.291 (GPa)
        (c44) = 71.019 (GPa)
        (czz=c11+c12+2c33-4c13) = 372.433 (GPa)
        (c66= 172.202 (GPa)
        _____________________________________
        c11 = 301.511 (GPa)
        c12 = 269.139 (GPa)
        c13 = 203.200 (GPa)
        c33 = 307.291 (GPa)
        c44 = 71.019 (GPa)
        c66 = 172.202 (GPa)
        ========================================================================
Prediction VOIGT Bulk modulus by using elastic constant values  = 251.265 (GPa)
Prediction REUSS Bulk modulus by using elastic constant values  = 249.106 (GPa)
Prediction HILL  Bulk modulus by using elastic constant values  = 250.185 (GPa)

Prediction VOIGT Shear modulus by using elastic constant values = 78.499  (GPa)
Prediction REUSS Shear modulus by using elastic constant values = 44.910  (GPa)
Prediction HILL  Shear modulus by using elastic constant values = 61.704  (GPa)

Prediction VOIGT Young modulus by using elastic constant values = 213.285 (GPa)
Prediction REUSS Young modulus by using elastic constant values = 127.092 (GPa)
Prediction HILL  Young modulus by using elastic constant values = 171.049 (GPa)

Prediction VOIGT Poisson's coefficient by using elastic constant values = .358
Prediction REUSS Poisson's coefficient by using elastic constant values = .414
Prediction HILL  Poisson's coefficient by using elastic constant values = .386
        ========================================================================
        ######## ORDER OF FIT IS :  4 , At volume = 313.62518 (bohr^3) ########
        (c11-c12) = 754.818 (GPa)
        (c11+c12) = 583.076 (GPa)
        (c33) = 303.396 (GPa)
        (c44) = 84.038 (GPa)
```

```
        (czz=c11+c12+2c33-4c13) = 499.647 (GPa)
        (c66= 168.100 (GPa)
        _____________________________________
        c11 = 668.947 (GPa)
        c12 = -85.871 (GPa)
        c13 = 172.555 (GPa)
        c33 = 303.396 (GPa)
        c44 = 84.038 (GPa)
        c66 = 168.100 (GPa)
        ========================================================================
Prediction VOIGT Bulk modulus by using elastic constant values  = 239.974 (GPa)
Prediction REUSS Bulk modulus by using elastic constant values  = 234.870 (GPa)
Prediction HILL  Bulk modulus by using elastic constant values  = 237.422 (GPa)

Prediction VOIGT Shear modulus by using elastic constant values = 159.371 (GPa)
Prediction REUSS Shear modulus by using elastic constant values = 114.503 (GPa)
Prediction HILL  Shear modulus by using elastic constant values = 136.937 (GPa)

Prediction VOIGT Young modulus by using elastic constant values = 391.455 (GPa)
Prediction REUSS Young modulus by using elastic constant values = 295.490 (GPa)
Prediction HILL  Young modulus by using elastic constant values = 344.566 (GPa)

Prediction VOIGT Poisson's coefficient by using elastic constant values = .228
Prediction REUSS Poisson's coefficient by using elastic constant values = .290
Prediction HILL  Poisson's coefficient by using elastic constant values = .258
        ========================================================================

         You can find these data in the output-order file.
```

C11 = 286.3 GPa
C12 = 253.9 GPa
C13 = 182.5 GPa
C33 = 281.2 GPa
C44 = 71.0 GPa
C66 = 172.2 GPa

	α-Pt_2Si [1] **(others)**	**α-Pt_2Si (our Cal)**
Method	FPLMTO	**FPLAPW**
Exchange	LDA	**PBE**
a (Å)	3.9196	3.9482
c (Å)	5.9485	5.9628
C11	332.4	**286.3**
C12	239.6	**253.9**
C13	169.4	**182.5**
C33	298.0	**281.2**
C44	62.7	**71.0**
C66	169.3	**172.2**

1) O. Beckstein, J. E. Klepeis, G. L. W. Hart, and O. Pankratov , cond-mat/0008200v2 (2001).

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