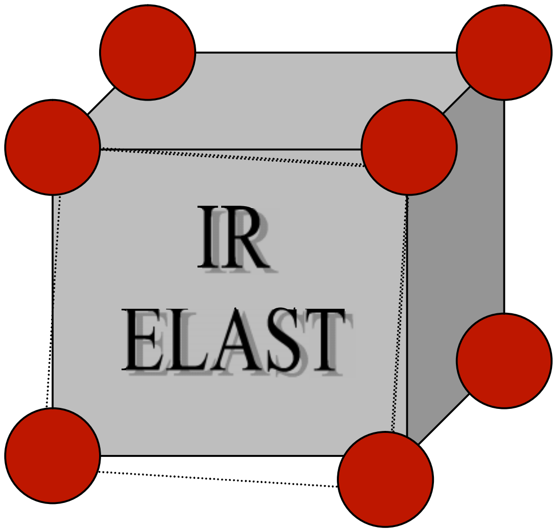


# IR ELAST

# +

# WIEN2k

**A Package for calculating elastic tensors of cubic structure**
***by using second-order derivative*** **with Wien2k package**
**This Package has been modified by using Thomas Charpin Package**

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**User's guide, Elastic Cubic_12.1(Release 26.01.2012)**

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For using the cubic-elastic package please follow the steps below;
You can install cubic-elastic package in each directory that you would like.

## Installation guide

1_ Copy **“cubic-elastic.tar.gz”** file in your computer. Then do the following;
tar –zxvf cubic-elastic.tar.gz
cd cubic-elastic

2_ Run **buildCIRelast_lapw**

This program helps you to provide "Makefile" and then compile cubic-elastic. Then define Environment Variable ELASTC_PATH and add it at the end of **.bashrc** file.
.

## Call Package

1_ Make struct file and run "init_elastc_lapw" and then change to "elast" directory.
2_ Run "setup_elast_lapw".
3_ Now you must modify job files according to your needs ( you can run "modifyjobc_lapw" in Terminal ).
5_ Now you must run job files ( you can run "calljobc_lapw" in Terminal ). It will take time.

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

6_ Run "ana_elastc_lapw" in Terminal.

Optionally you can specify more cases by rerunning “**setupeos, setuptetra,….” (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
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**init_elastc_lapw** : makes "elast" and with in "eos", "tetra", "rhomb", and "result" directories and calls "command_init_lapw" if you decide to run "init_lapw" as automatically. Moreover "init_elastc_lapw" program copies "case.struct" file as "init.struct" and "eos.templ" and produces "tetra.templ" and "rhomb.templ" by calling "genetemplc" program and then copies them in "eos", "tetra", and "rhomb" directories and then runs "auto_init_lapw" or "init_lapw" within them.
In “result” directory , you can find all struct , scf, and clm* files.

**setup_elast_lapw** : Produces structs file that will be necessary for calculations by using "setupeos", "setuptetra" and "setuprhomb" programs.

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

**calljobc_lapw** : calls job files for running.

**ana_elastc_lapw** : calls ana_elasteos_lapw, ana_elasttetra_lapw, and ana_elastrhomb_lapw programs for calculations elastic constants and makes an output file in elast directory with name "outputs".

Moreover ana_elasteos_lapw, ana_elasttetra_lapw, and ana_elastrhomb_lapw programs produce eos.output, tetra.output, and rhomb.output in "eos", "tetra", and "rhomb" directories, respectively.

**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 directory.). You can run it in the elast directory. Moreover ana_elastc_lapw calls 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".

## Suppose

Suppose we only want to calculate (c11+2c12)/3 or (c11-c12) or (c11+2c12)+4c44.

We do these stages as following:

1) Make a directory with name "elast" and within "eos" or "tetra" or "rhomb" directory.
2) copy "case.struct" file as "init.struct" and "eos.templ" and then copy them within "eos" or "tetra" or "rhomb" directory.
3) Within "tetra" or "rhomb" directory run "genetemplc" program (only for (c11-c12) or (c11+2c12)+4c44. calculations).
4) copy "eos.templ" as "eos.struct" within "eos" directory or copy "tetra.templ" as "tetra.struct" within "tetra" directory or copy "rhomb.templ" as "rhomb.struct" within "rhomb" directory
4) Run instgen_lapw and init_lapw within "eos" or "tetra" or "rhomb" directory.
5) Run "setupeos" or "setuptetra" or setuprhomb" within "eos" or "tetra" or "rhomb" directory, respectively.
6) Modify "eos.job" or "tetra.job" or "rhomb.job" file according your needs within "eos" or "tetra" or "rhomb" directory.

7) “chmod +x eos.job” or “chmod +x tetra.job” or “chmod +x rhomb.job”
8) Run job file within “eos” or “tetra” or “rhomb” directory.
9) Within elast directory, run “ana_elasteos_lapw” or “ana_elasttetra_lapw” or ana_elastrhomb_lapw”.

**Suppose we only want to to rerun EOS with more data points.**

In present work directory, we go to “elast” directory and then within “eos” directory. Now run “setupeos” and select more cases. After that we modify “eos.job” file according to our needs and then run “eos.job” file ( do not forget to do “chmod +x eos.job” before running). Now in “elast” directory, we run “ana_elastc_lapw”.

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 **“job”** files and a new "savename" (eg. "_use_pbe_rk8").

## 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 will plot it). Moreover we 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 using 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
--------------

***Calculating elastic-constant for Pt***

```
Pt
F   LATTICE,NONEQUIV.ATOMS:  1
MODE OF CALC=RELA unit=bohr
  7.407729  7.407729  7.407729 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Pt1        NPT=  781  R0=0.00000500 RMT=    2.5000   Z: 78.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48      NUMBER OF SYMMETRY OPERATIONS
```

**Select Xc = PBE-GGA , R_Kmax = 11 , L_max = 12 and nkpoint = 9000**

**I used -5%, 0%, 5%, 10%, 15% for EOS calculations and -6%, -4%, -2%, 0%, 2%, 4%, 6%, 8%, 10% for Rhombohedral calculations and -10%, -8%, -6%, -4%, -2%, 0%, 2%, 4%, 6%, 8%, 10% for Tetragonal calculations.**

```
########################################
# ana_elast_lapw analyses Elastic      #
#            constant                  #
#     C(2012) by Morteza Jamal         #
#          Ali H. Reshak               #
#   using ana_elasteos_lapw,           #
#  ana_elasttetra_lapw                 #
# ana_elastrhomb_lapw                  #
########################################

********************
I am in eos directory
********************

######################################
# ana_elasteos_lapw analyses Elastic #
#            constant                #
#     C(2012) by Morteza Jamal       #
#          Ali H. Reshak             #
#   using eos.vol                    #
#  which has been created by         #
#             eos.job                #
######################################

 Enter V0-exp. for an estimate of B and BP using EOS2 and the
experimental
 equillibrium volume. Make sure there is a `.` in the number. (Fill out
`0` if
 you are interested the (Birch-)Murnaghan equation of state only.) :
0.005u 0.004s 0:31.02 0.0%    0+0k 0+0io 9pf+0w
       "display Birch-Murnaghan fit:"
You may want to print eos.outputeos
 Equation of state: EOS2 (PRB52,8064)        info          2
 a,b,c,d    -36899.512970       125.816150      -783.275885
1532.670757
 V0,B(GPa),BP,E0       106.3782       256.0131         4.7286
cubic lattice parameter:    7.5215 bohr =     3.9802 Ang

 Equation of state: Murnaghan                info          2
 E=E0+[B*V/BP*(1/(BP-1)*(V0/V)**BP +1)-B*V0/(BP-1)]/14703.6
 Pressure=B/BP*((V0/V)**BP -1)
 V0,B(GPa),BP,E0       106.4111       254.7922         4.4869     -
36893.440183
cubic lattice parameter:    7.5223 bohr =     3.9806 Ang
         vol       energy         de(EOS2)      de(Murnaghan)
Pressure(GPa)
      91.4614   -36893.416008     0.000044     0.000042         55.222
```

```
      96.5426   -36893.430507    -0.000163    -0.000167         31.095
     101.6238   -36893.438351     0.000184     0.000199         13.028
     106.7050   -36893.440170    -0.000007    -0.000006         -0.698
     111.7861   -36893.437906    -0.000103    -0.000126        -11.264
     116.8673   -36893.432717     0.000046     0.000058        -19.496
                   Sigma:         0.000112     0.000122

 Equation of state: Birch-Murnaghan                info           2
 E = E0 + 9/16*(B/14703.6)*V0*[(eta**2-1)**3*BP + (eta**2-1)**2*(6-
4*eta**2)]
        --> eta = (V0/V)**(1/3)
 Pressure = 3/2*B*(eta**7 - eta**5)*(1 + 3/4*(BP-4)*[eta**2 - 1])
 V0,B(GPa),BP,E0       106.3885       255.7275         4.6555     -
36893.440186
cubic lattice parameter:    7.5217 bohr =     3.9803 Ang
         vol       energy         de(Birch-Murnaghan)  Pressure(GPa)
      91.4614   -36893.416008     0.000042             55.060
      96.5426   -36893.430507    -0.000163             31.155
     101.6238   -36893.438351     0.000188             13.038
     106.7050   -36893.440170    -0.000008             -0.754
     111.7861   -36893.437906    -0.000111            -11.281
     116.8673   -36893.432717     0.000051            -19.318
                   Sigma:         0.000114

 Murnaghan-data are in eos.eosfit
 Birch-Murnaghan-data are in eos.eosfitb
press RETURN to continue

Do you want a hardcopy? (y/N)
 ************************************
Equation of state:Birch-Murnaghan

At volume= 106.3885 (bohr^3)
Bulk modulus is: 255.7275 (GPa) = (C11+2C12)/3
 ************************************

*************************************************
You can find eos.output file in eos directory.
*************************************************

*********************
I am in tetra directory
*********************

########################################
# ana_elasttetra_lapw analyses Elastic #
#           constant                   #
#     C(2012) by Morteza Jamal         #
#          Ali H. Reshak               #
#   using eos.outputeos                #
#         tetra.strain                 #
#  which has been created by           #
#            tetra.job                 #
########################################
 0.035744   -36893.436126
 0.028184   -36893.436831
 0.020839   -36893.437487
```

```
 0.013700   -36893.437941
 0.006757   -36893.438228
 0.000000   -36893.438333
-0.006579   -36893.438230
-0.012988   -36893.437878
-0.019236   -36893.437229
-0.025327   -36893.436312
-0.031271   -36893.435104
 ===============================================================
Order of fit:  2, C11-C12 is:    112.0249 GPa, RMS: 0.163830E-03
Order of fit:  3, C11-C12 is:    118.7834 GPa, RMS: 0.141969E-04
Order of fit:  4, C11-C12 is:    115.2097 GPa, RMS: 0.112040E-04
Order of fit:  5, C11-C12 is:    115.2084 GPa, RMS: 0.112040E-04
Order of fit:  6, C11-C12 is:    106.0468 GPa, RMS: 0.588000E-05
Order of fit:  7, C11-C12 is:    108.9075 GPa, RMS: 0.225592E-05
Order of fit:  8, C11-C12 is:    108.2282 GPa, RMS: 0.223224E-05
Order of fit:  9, C11-C12 is:    105.7094 GPa, RMS: 0.301853E-06
Order of fit: 10, C11-C12 is:    107.4818 GPa, RMS: 0.537365E-11
 ******************************************
Polynomial fit or tetragonal strain done
A RMS of 0.163830E-03 was achieved using a polynome of degree :  2

At volume=  106.3885 bohr^3
C11-C12 is:   0.007615 a.u or    112.0249 GPa
 ******************************************

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

*********************
I am in rhomb directory
*********************


########################################
# ana_elastrhomb_lapw analyses Elastic #
#            constant                  #
#     C(2012) by Morteza Jamal         #
#          Ali H. Reshak               #
#   using eos.outputeos                #
#         rhomb.strain                 #
#  which has been created by           #
#             rhomb.job                #
########################################
-0.060000   -36893.419398
-0.040000   -36893.424972
-0.020000   -36893.428594
 0.000000   -36893.430826
 0.020000   -36893.431940
 0.040000   -36893.431965
 0.060000   -36893.431126
 0.080000   -36893.429657
 0.100000   -36893.427646
 ===============================================================
```

```
Order of fit:  2, C11+2C12+4C44 is:   1087.2245 GPa, RMS: 0.422059E-03
Order of fit:  3, C11+2C12+4C44 is:   1294.1765 GPa, RMS: 0.539048E-04
Order of fit:  4, C11+2C12+4C44 is:   1259.6826 GPa, RMS: 0.352587E-04
Order of fit:  5, C11+2C12+4C44 is:   1196.5166 GPa, RMS: 0.209803E-04
Order of fit:  6, C11+2C12+4C44 is:   1200.6698 GPa, RMS: 0.626464E-05
Order of fit:  7, C11+2C12+4C44 is:   1176.0580 GPa, RMS: 0.481192E-05
Order of fit:  8, C11+2C12+4C44 is:   1138.2665 GPa, RMS: 0.542318E-11
 ******************************************
Polynomial fit or rhombohedral strain done
A RMS of 0.422059E-03 was achieved using a polynome of degree :  2

At volume=  106.3885 bohr^3
C11+2C12+4C44 is:   0.073908 a.u or   1087.2245 GPa
 ******************************************

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

#################################################
Final elastic constant tensor for Cubic structure
-------------------------------------------------


#############################
At volume = 106.3885 (bohr^3)
(c11+2c12)/3 = 255.7275 (GPa)
-----------------------------
At volume = 106.3885 (bohr^3)
(c11-c12) = 112.0249 (GPa)
-----------------------------
At volume = 106.3885 (bohr^3)
(c11+2c12)+4c44 = 1087.2245 (GPa)
-----------------------------
c11 = 330.4107 (GPa)

c12 = 218.3858 (GPa)

C44 = 80.0105 (GPa)
#############################

 Press enter key to continue....

#############################################
# ana_elastorder_lapw analyses Elastic      #
#              constant                     #
#        C(2012) by Morteza Jamal           #
#             Ali H. Reshak                 #
#   using rhomborder.fit,                   #
#  tetraorder.fit                           #
#     and eos.outputeos files               #
#############################################

 CHECK THE SENSITIVITY
       OF YOUR RESULT TO THE ORDER OF FIT
```

```
 Press enter key to continue....
 Order of fit for TETRAGONAL and RHOMBOHEDRAL calculations were 10 and
8
 We select minimum value for ORDER OF FIT i.e. 8

 Press enter key to continue....
######## ORDER OF FIT IS :  2 , At volume = 106.3885 (bohr^3) ########
(c11+2c12)/3 = 255.7275 (GPa)
(c11-c12) = 112.0249 (GPa)
(c11+2c12)+4c44 = 1087.2245 (GPa)
c11 = 330.4107 (GPa)
c12 = 218.3858 (GPa)
C44 = 80.0105 (GPa)
######## ORDER OF FIT IS :  3 , At volume = 106.3885 (bohr^3) ########
(c11+2c12)/3 = 255.7275 (GPa)
(c11-c12) = 118.7834 (GPa)
(c11+2c12)+4c44 = 1294.1765 (GPa)
c11 = 334.9164 (GPa)
c12 = 216.1330 (GPa)
C44 = 131.7485 (GPa)
######## ORDER OF FIT IS :  4 , At volume = 106.3885 (bohr^3) ########
(c11+2c12)/3 = 255.7275 (GPa)
(c11-c12) = 115.2097 (GPa)
(c11+2c12)+4c44 = 1259.6826 (GPa)
c11 = 332.5339 (GPa)
c12 = 217.3242 (GPa)
C44 = 123.1250 (GPa)
######## ORDER OF FIT IS :  5 , At volume = 106.3885 (bohr^3) ########
(c11+2c12)/3 = 255.7275 (GPa)
(c11-c12) = 115.2084 (GPa)
(c11+2c12)+4c44 = 1196.5166 (GPa)
c11 = 332.5331 (GPa)
c12 = 217.3247 (GPa)
C44 = 107.3335 (GPa)
######## ORDER OF FIT IS :  6 , At volume = 106.3885 (bohr^3) ########
(c11+2c12)/3 = 255.7275 (GPa)
(c11-c12) = 106.0468 (GPa)
(c11+2c12)+4c44 = 1200.6698 (GPa)
c11 = 326.4253 (GPa)
c12 = 220.3785 (GPa)
C44 = 108.3718 (GPa)
######## ORDER OF FIT IS :  7 , At volume = 106.3885 (bohr^3) ########
(c11+2c12)/3 = 255.7275 (GPa)
(c11-c12) = 108.9075 (GPa)
(c11+2c12)+4c44 = 1176.0580 (GPa)
c11 = 328.3325 (GPa)
c12 = 219.4250 (GPa)
C44 = 102.2188 (GPa)
######## ORDER OF FIT IS :  8 , At volume = 106.3885 (bohr^3) ########
(c11+2c12)/3 = 255.7275 (GPa)
(c11-c12) = 108.2282 (GPa)
(c11+2c12)+4c44 = 1138.2665 (GPa)
c11 = 327.8796 (GPa)
c12 = 219.6514 (GPa)
C44 = 92.7710 (GPa)
=======================================================================
```

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


Have a good day...
Thomas Charpin and Morteza Jamal
```

**c11 = 330.4107 (GPa)**
**c12 = 218.3858 (GPa)**
**C44 = 80.0105  (GPa)**

| | **Our calculations** | **Exp[1]** |
|---|---|---|
| C11 (GPa) | **330** | 347 |
| C12 (GPa) | **218** | 251 |
| C44 (GPa) | **80** | 76 |

**1) Michael J. Mehl and Dimitrios A. Papaconstantopoulos, PRB, 54, 1996**

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