

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

User's guide, Elastic Cubic_11.1(Release 22.03.2011)
Morteza Jamal

Ghods city – Tehran-Iran

If you want to use cubic-elastic package Please follow the following steps.
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.

```
tar -zxvf cubic-elastic.tar.gz  
cd cubic-elastic
```

2_Edit "Makefile" and select your Fortran compiler (FC) and Fortran compiler options (FOPT) and the path of MKL library (LDFLAGS) and then save it (you can type options that used for compiling Wien2k Package). Now type in Terminal environment:

```
make  
make clean
```

3_Run “**addbash_lapw**” program (type **addbash_lapw** in terminal). This program define Environment Variable **ELASTC_PATH** and add it at the end of **.bashrc** file. Therefore you will able to call cubic-elastic's programs in each Directory.

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_elastic_lapw" in Terminal.

Optionally you can specify more cases by rerunning “**setup_elast_lapw**”. 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

init_elastic_lapw : makes "elastic" 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_elastic_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.

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

calljob_lapw : calls job files for running.

ana_elastic_lapw : calls ana_elasteos_lapw, ana_elasttetra_lapw, and ana_elastrhomb_lapw programs for calculations elastic constants and makes an output file in elastic 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 : In this calculations, I use the highest polynomial for the final results. Usually this is VERY BAD !!! It follows all your numerical noise and although such a fit may go through all points (leading to the smallest RMS), it may strongly oscillate between the points and give wrong results. **SO, WE HIGHLY RECOMMEND TO CHECK THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT by using ana_elastorder_lapw program and then select suitable values for Elastic Constants (This program saves these data in the output-order file in the elastic directory.)**. You can run it in the elastic directory. Moreover ana_elastic_lapw calls ana_elastorder_lapw at the end of calculations.

command_init_lapw : gets informations for making "auto_init_lapw".

Suppose we only want to calculate $(c_{11}+2c_{12})/3$ or $(c_{11}-c_{12})$ or $(c_{11}+2c_{12})+4c_{44}$.

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 $(c_{11}-c_{12})$ or $(c_{11}+2c_{12})+4c_{44}$. 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 add some points to EOS calculations.

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".

Converged check

Since our results will be quite sensitive to the choice of strains and there is not a main rule for finding the best values of elastic constants, here I obtain some note that will be useful.

Since this package computes elastic constants by using second-order derivative ($E''(\epsilon)$) of Polynomial fit ($E=E(\epsilon)$) of Energy vs. Strains (ϵ) at zero strain ($\epsilon=0$). 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 we expect the behavior of elastic constants (second-order derivative of Energy vs. strain) vs. strains around zero strain (for example $[-0.005, +0.005]$) to be plateau and you can find these data in unit of GPa vs. strain in rhomb and tetra directory with name *rhombdiv2.fit* and *tetradiv2.fit* respectively. I recommend to plot them and check

this behavior for different data. 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.

EXAMPLE

Calculation 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(2010) by Morteza Jamal #
# using ana_elasteos_lapw, #
# ana_elasttetra_lapw #
# ana_elastrhomb_lapw #
#####
```

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

```
#####
# ana_elasteos_lapw analyses Elastic #
# constant #
# C(2010) by Morteza Jamal #
# 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 equilibrium volume. Make sure there is a `` in the number. (Fill out `0` if you are interested the (Birch-)Murnaghan equation of state only.) :

```
0.002u 0.005s 0:02.91 0.0% 0+0k 0+0io 0pf+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
 $E = E_0 + 9/16*(B/14703.6)*V_0*[(\eta^{**2-1})^{**3*BP} + (\eta^{**2-1})^{**2*(6-4*\eta^{**2})}]$

--> $\eta = (V_0/V)^{**}(1/3)$
 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

 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(2010) by Morteza Jamal           #
#   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 0.537365E-11 was achieved using a polynome of degree : 10

At volume= 106.3885 bohr^3
C11-C12 is: 0.007306 a.u or 107.4818 GPa

Analyze done.....
Press <enter> to continue
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(2010) by Morteza Jamal #
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 0.542318E-11 was achieved using a polynome of degree : 8
```

```
At volume= 106.3885 bohr^3  
C11+2C12+4C44 is: 0.077378 a.u or 1138.2665 GPa  
*****
```

```
Analyze done.....  
Press <enter> to continue
```

```
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) = 107.4818 (GPa)  
-----
```

```
At volume = 106.3885 (bohr^3)  
(c11+2c12)+4c44 = 1138.2665 (GPa)  
-----
```

```
c11 = 327.3820 (GPa)
```

```
c12 = 219.9002 (GPa)
```

```
C44 = 92.7710 (GPa)
```

```
#####
```

```
#####  
# ana_elastorder_lapw analyses Elastic #  
# constant #  
# C(2011) by Morteza Jamal #  
# using rhomborder.fit, #  
# tetraorder.fit #  
# and eos.outputeos files #  
#####
```

IN THIS CALCULATIONS, WE USE the highest polynomial for the final results.
Usually this is VERY BAD. It follows all your numerical noise and although such a fit may go through all points (leading to the smallest RMS),
it may strongly oscillate between the points and give wrong results.

SO, WE HIGHLY RECOMMEND TO 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

After checking the sensitivity of our results to the order of fit, I prefer to select:

```

c11 = 332.5339 (GPa)
c12 = 217.3242 (GPa)
C44 = 107.3335 (GPa)

```

	Our calculations	Exp¹
C11 (GPa)	332	347
C12 (GPa)	217	251
C44 (GPa)	107	76

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

Morteza Jamal
Email: m_jamal57@yahoo.com
