ELASTOOL Users Manual

AN AUTOMATED TOOLKIT FOR ELASTIC CONSTANTS CALCULATION

VERSION: 1.1.0

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Table of contents

1 Introduction

ELASTOOL is an automated toolkit for calculating the second-order elastic constants (SOECs) of any crystal systems belonging to two- and three-dimensional. It can utilize three kinds of strain-matrix sets, the high efficiency strain-matrix sets (OHESS) [1], the universal linear-independent coupling strains (ULICS) [2] and the all single-element strain-matrix sets (ASESS) [1] to calculate the SOECs automatically. In an automatic manner, ELASTOOL can deal with both zero- and high-temperature elastic constants.

Presently, ELASTOOL interfaces to VASP package for calculating the accurate stresses of strained cystal. But the interfaces to other DFT packages can also be easily implemented.

2 Installation and run

ELASTOOL is based on Python and its installation is very easy. The necessary libraries can be installed automatically by only one command.

2.1 The third-party libraries

ELASTOOL depends on Python 3 (version 3.5 or later). The following libraries are required:

- NumPy
- Spglib
- ASE
- Pandas

2.2 Installation

In the Python 3 enviroment, the install of ELASTOOL is very easy. One only needs to execute: **python3 setup.py install --prefix=/path/to/install**. Then execute: **export PATH=/path/to/install/bin:$PATH**, or write it in the ~/.bashrc file.

2.3 Run

To run ELASTOOL, one only needs to execute **elastool** in the working directory. ELASTOOL will automatically prepare necessary files for calculating the stresses of crystal under deformation, and then call VASP to optimize initial crystal structure and calculate the stresses for each deformaton defined by OHESS, ASESS, or ULICS. Finally, it analyzes stress-strain relationship according Hooke's law and calculate all the elastic constants.

2.3.1 Interface to VASP

To run ELASTOOL with VASP, one need provide **elastic.in**, **INCARs**, and **POTCAR-XX** files for each kind of atom, where **XX** is the short name of each atom. For example, you can use **POTCAR-Mg**, and **POTCAR-O** for MgO.

2.4 Input files

ELASTOOL needs one main input file for setting the calculation details of elastic constants. The main input file is named **elatool.in**. The crystal structure file is provided either in **POSCAR** or cif format for the structure information of the crystal. For VASP stress tensor calculations, **INCARs**, **KPOINTS-static**, **KPOINTS-dynamic**, and **POTCAR-XX** files are also necessary. In the **INCARs** file, several INCAR files of VASP are collected for optimization, the static calculation, and the molecular dynamics simulations for high-termperature elastic constants. The **KPOINTS-static** file is for the structure optimization and the static calculation of stress tensors. The **KPOINTS-dynamic** file is for the calculation of high-temperature elastic constants using molecular dynamics. **XX** in the **POTCAR** file name is the abbreviated name for an element of the crystal.

3 Input parameters

There are totally 10 controlling parameters for ELASTOOL, as listed in Table.1. The **run_mode** sets the running mode for ElasTool, 1 for automatic run, 2 for pre-processing, and 3 for post-processing. If **run_mode** = 2 or 3, one should ensure the structure has already been optimizated at fixed pressure or volume, *i.e.* both the **CONTCAR** and **OUTCAR** files are in **./OPT** directory. In running mode 2, ELASTOOL will directly prepare all the necessary files for calculating stress tensors. After all the stress tensors calculations are finished, run mode 3 can analyze the output files and extract stress tensors, and then fit the first-order function to the stress-tensor data to obtain elastic constants.

The **dimensional** defines the dimensional of the system, 2D or 3D. If the system is 2D, ELASTOOL supposes the layered sheet in the *xy*-plane.

The **structure_file** specifies the original crystal structure file in POSCAR (.vasp) or cif (.cif) format.

The **if_conventional_cell** determines the usage of primitive cell (no) or conventional cell (yes).

The **method_stress_statistics** chooses the elastic constants calculation method, static or dynamic, **static** for 0 K elastic constants, and **dynamic** for high-temperature. The static method uses the static stresses to compute elastic constants, while the dynamic method deduces elastic constants from the thermal stresses obtained by molecular dynamics simulations.

The **strains_matrix** defines the type of strain-matrix set, OHESS, ASESS, or ULICS.

The **strains_list** gives one or more strains for calculating stresses via the strain-matrix set of OHESS, ASESS, or ULICS.

The **repeat_num** controls how to build a supercell from the primitive or conventional cell defined by **if_conventional_cell** for the dynamic method.

The **num_last_samples** is the number of last MD steps to average thermal stresses

The **parallel_submit_command** is the parallel submitting command of *ab initio* code, e.g. VASP.

Table 1. The controlling parameters and possible values of ELASTOOL

Parameters	Values
run_mode	1/2/3
dimensional	2D/3D
structure_file	file name ended with .vasp or .cif
if_conventional_cell	yes/no
method_stress_statistics	static/dynamic
strains_matrix	ohess/asess/ulics
strains_list	one or more numbers
repeat_num	3 integers
num_last_samples	1 integer
parallel_submit_command	DFT parallel run command

4 Example

ELASTOOL can calculate zero-temperature and high-temperature elastic constants. The zero-temperature calculations can be conducted by the static stress computation. The high-temperature elastic constants can be derived by molecular dynamics simulations.

4.1 Zero-temperature elastic constants

We take the 0 K elastic constants calculation of diamond as the static example. The content of the input file **elastool.in** is as follows.

```
run_mode = 1

dimensional = 3D

structure_file = diamond.cif

if_conventional_cell = no

method_stress_statistics = static

strains_matrix = ohess

strains_list = -0.06 -0.03 0.03 0.06

#repeat_num = 1 1 1

#num_last_samples = 1

parallel_submit_command = mpirun -np 28 vasp544
```

4.2 High-temperataure elastic constants

4.2.1 3D case

The high temperature elastic constants calculation of metal copper is the high-temperature example. We build a 3×3×3 supercell from the conventional cell of face-centered-cubic of Cu and then perform long-time MD simulations defined in the INCAR-dynamic file. Because MD is very time consuming, there is only one strain of -0.06 is used. The last 500 MD steps are used to average thermal stresses.

run_mode = 1

dimensional = 3D

structure_file = CONTCAR.vasp

if_conventional_cell = yes

method_stress_statistics = dynamic

strains_matrix = ohess

strains_list = -0.06

repeat_num = 3 3 3

num_last_samples = 500

parallel_submit_command = mpirun -np 28 vasp544

4.2.2 2D case

run_mode = 1

dimensional = 2D

structure_file = CONTCAR.vasp

if_conventional_cell = no

method_stress_statistics = dynamic

strains_matrix = ohess

strains_list = -0.06

repeat_num = 4 4 1

num_last_samples = 500

parallel_submit_command = mpirun -np 28 vasp544

4.3 Output files

The elastool.out file is the unique output file of ELASTOOL. It includes the calculated elastic constants data, the elastic muduli, the sound velocity, the Debye temparture, the elastic anisotropy, and the stability analysis results of the crystal structure based on Born elastic creteria. The printed information on screen of the diamond example is as follows.

Reading controlling parameters from elastool.in...

Calculating stresses using the OHESS strain matrices...

strain = -0.060

strain = -0.030

strain = 0.030

strain = 0.060

Fitting the first-order function to the collected

stress-strain data according to Hooke's law...

The finnal results are as follows:

+==========+

|This is a 3D Cubic lattice. |

|———————————|

|Mean Pressure = -0.08 GPa |

|———————————|

|Elastic constants: |

|C11 = 1055.04 GPa |

|C12 = 136.56 GPa |

|C44 = 567.76 GPa |

|———————————|

|Elastic moduli: |

|B_V = 442.72 GPa |

|B_R = 442.72 GPa |

|G_V = 524.36 GPa |

|G_R = 518.73 GPa |

|B_VRH = 442.72 GPa |

|G_VRH = 521.54 GPa |

|Young's modulus (E) = 1123.47 GPa |

|Possion's ratio (V) = 0.0771 |

|———————————|

|Sound velocity: |

|V_S = 12.20 Km/s |

|V_B = 11.24 Km/s |

|V_P = 18.03 Km/s |

|V_M = 13.31 Km/s |

|———————————|

|Debye temperature: |

```
|T_D = 1761.03 K                    |
|-----------------------------------|
|Elastic anisotropy:                |
|A_U = 0.0542                       |
|A_C = 0.0054                       |
|-----------------------------------|
|Structure stability analysis...    |
|This structure is mechanically STABLE.|
+===================================+
Results are also saved in the elastool.out file.
Well done! GOOD LUCK!
```

5 How to cite

Please cite the following article when you use ELASTOOL:

Z. L. Liu. ELASTOOL: An automated toolkit for elastic constants calculation (arxiv:2002.06535). 2020.

Z. L. Liu. High-efficiency calculation of elastic constants enhanced by the optimized strain-matrix sets (arxiv:2002.00005). 2020.

6 Acknowledgment

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Bibliography

[1] Z. L. Liu. High-efficiency calculation of elastic constants enhanced by the optimized strain-matrix sets (arxiv:2002.00005). 2020.

[2] R. Yu, J. Zhu, and H. Q. Ye. Calculations of single-crystal elastic constants made simple. *Comput. Phys. Commun.*, 181:671, 2010.