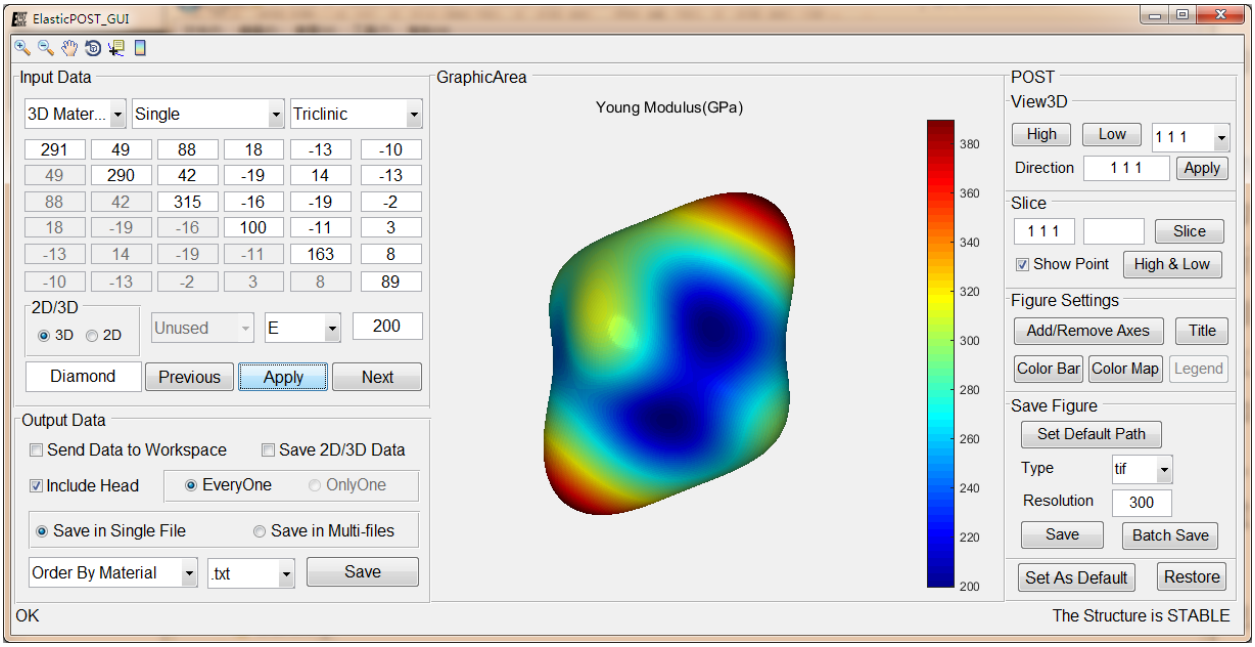
ElasticPOST Documentation

Release 1.0

ElasticPOST Developers

Apr 14, 2020

Contents


ElasticPOST_GUI
Input Data
3D Mater...
Single
Triclinic
291 49 88 18 -13 -10
49 290 42 -19 14 -13
88 42 315 -16 -19 -2
18 -19 -16 100 -11 3
-13 14 -19 -11 163 8
-10 -13 -2 3 8 89
2D/3D
3D
2D
Unused
E
200
Diamond
Previous
Apply
Next
Output Data
Send Data to Workspace
Save 2D/3D Data
Include Head
EveryOne
OnlyOne
Save in Single File
Save in Multi-files
Order By Material
.txt
Save
GraphicArea
Young Modulus(GPa)
380
360
340
320
300
280
260
240
220
200
POST
View3D
High
Low
1 1 1
Direction
1 1 1
Apply
Slice
1 1 1
Slice
Show Point
High & Low
Figure Settings
Add/Remove Axes
Title
Color Bar
Color Map
Legend
Save Figure
Set Default Path
Type
tif
Resolution
300
Save
Batch Save
Set As Default
Restore
OK
The Structure is STABLE

Contents:

CHAPTER 1

Introduction

This is an open source code to calculate the higher order elastic constants(HOECs) from first principles.

1.1 Features

The software is design for post processing the elastic stiffness matrix, it has several feathers, which are listed as follows:

- a. For 3D materials in any symmetry, supporting the elastic anisotropy of bulk modulus, Young's modulus, shear modulus, Poisson's ratio and hardness in 3D;
- b. For 2D materials in any symmetry, supporting the elastic anisotropy of Young's modulus, shear modulus and Poisson's ratio;
- c. Supporting *.xlsx, *.xls, *.txt, *.dat and *.mat data format;
- d. Supporting Voigt-Reuss-Hill approximation to average the elastic modulus;
- e. Supply some useful tools for 3D figures, such as slice and view point;
- f. Supporting *.tif, *.jpg, *.emf, *.eps, *pdf, *.fig figure format;
- g. Supporting Windows and Linux system;
- h. It will give some tips for errors(Marked in red in the bottom of the GUI).

1.2 Release

TODO

CHAPTER 2

Get Started

2.1 Install

To use this code, you can or set the folder containing the whole scripts as current path or install it.

To install the package, there are two different ways.

- a. By add the folder to matlabpath by hand

This first way is copying the package to the destination folder you want to install, and then adding the folder to the variable of matlabpath.

How to add the folder, please ref https://www.mathworks.com/help/matlab/matlab_env/add-folders-to-matlab-search-path-at-startup.html

- b. By the install script

The other way is just running following script, and in this way, you need to run the MATLAB as administrator.

EPOST_INSTALL

EPOST_INSTALL('destination folder')

To uninstall the software, you just need to type EPOST_UNINSTALL in the MATLAB commend window.

After installation of the package, you can type ElasticPOST_GUI to run the software.

2.2 Get Started

TODO

CHAPTER 3

Theory Background

3.1 Crystal type and independent elastic constants

- 3D crystal

The different crystal symmetry of 3D materials are illustrated in Fig. 1, and the corresponding independent elastic constants are shown in Fig. 2.

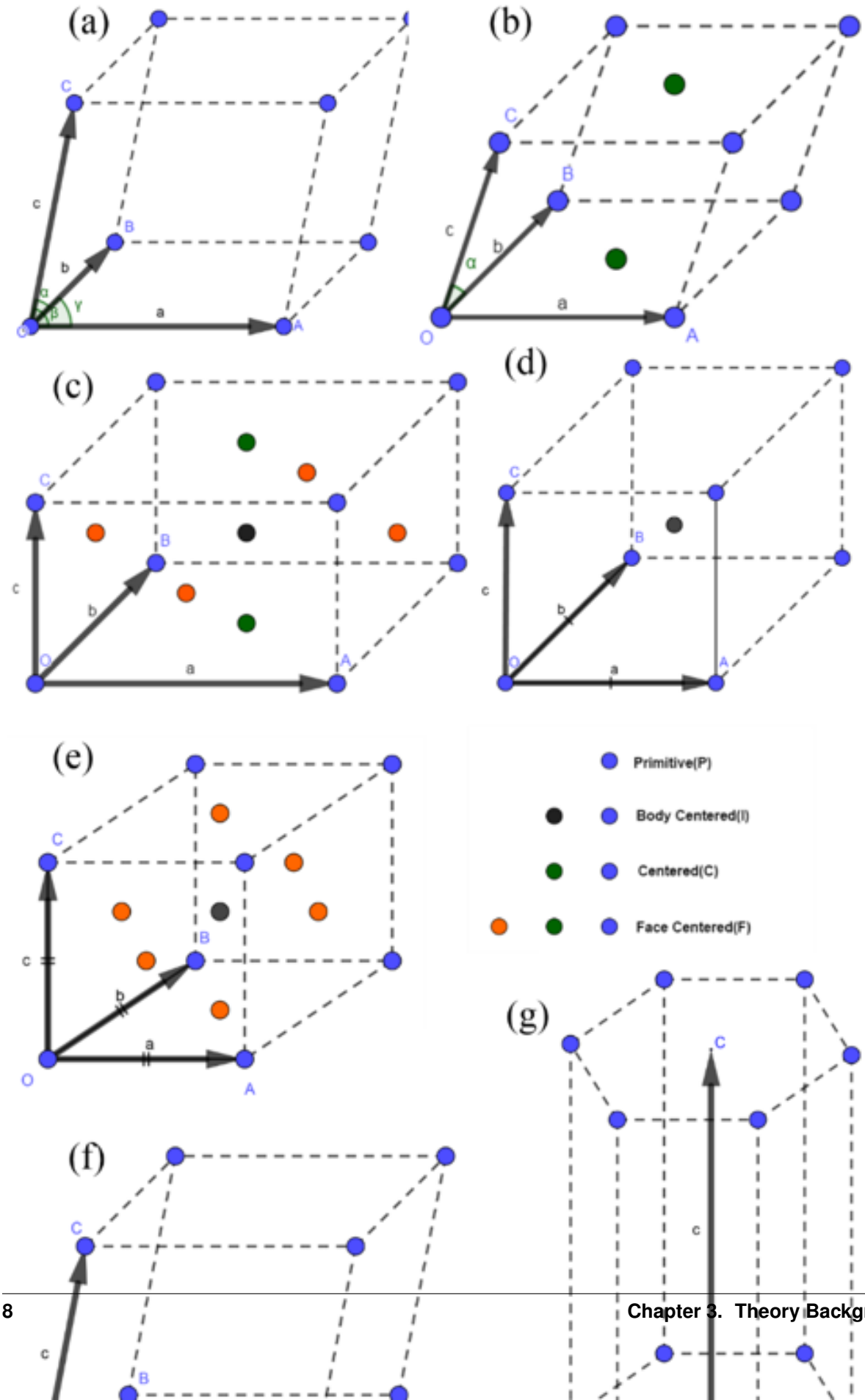
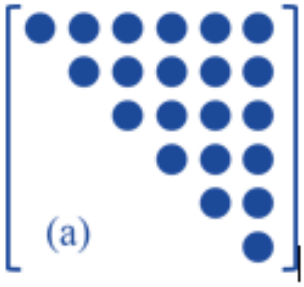

(a)
(b)
(c)
(d)
(e)
(f)
(g)
Primitive(P)
Body Centered(I)
Centered(C)
Face Centered(F)

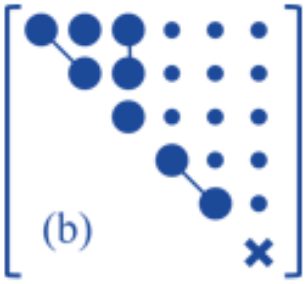
Fig. 1 Symmetry in 3D crystal

(a)Triclinic; (b)Monoclinic; (c)Orthorhombic; (d)Tetragonal; (e)Cubic; (f)Trigonal; (g)Hexagonal

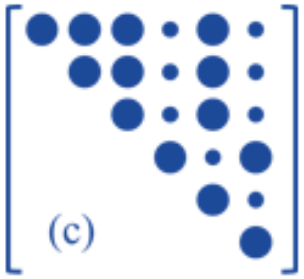
Triclinic



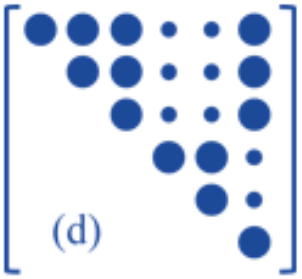
Hexagonal



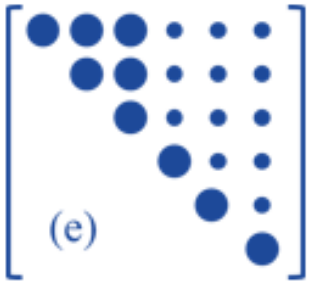
Monoclinic_1



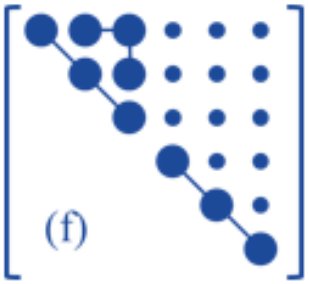
Monoclinic_2



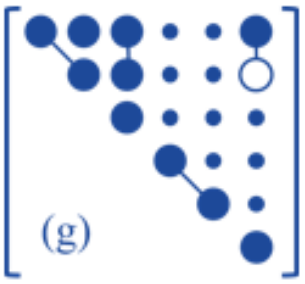
Orthorhombic



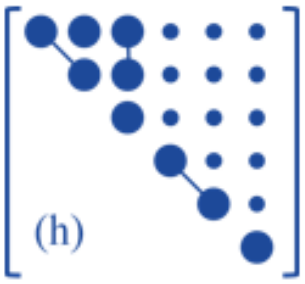
Cubic



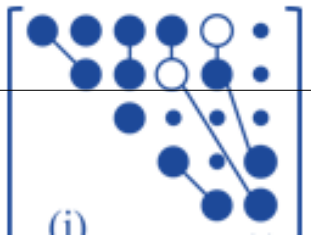
Tetragonal_1



Tetragonal_2



Trigonal_1



Trigonal_2

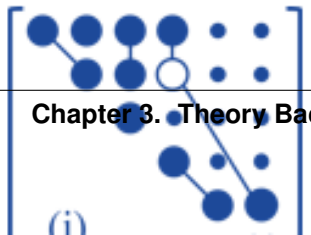


Fig. 2 The independent elastic constants in 3D crystals

- 2D crystal

The different crystal symmetry of 2D materials are illustrated in Fig. 3, and the corresponding independent elastic constants are shown in Fig. 4.

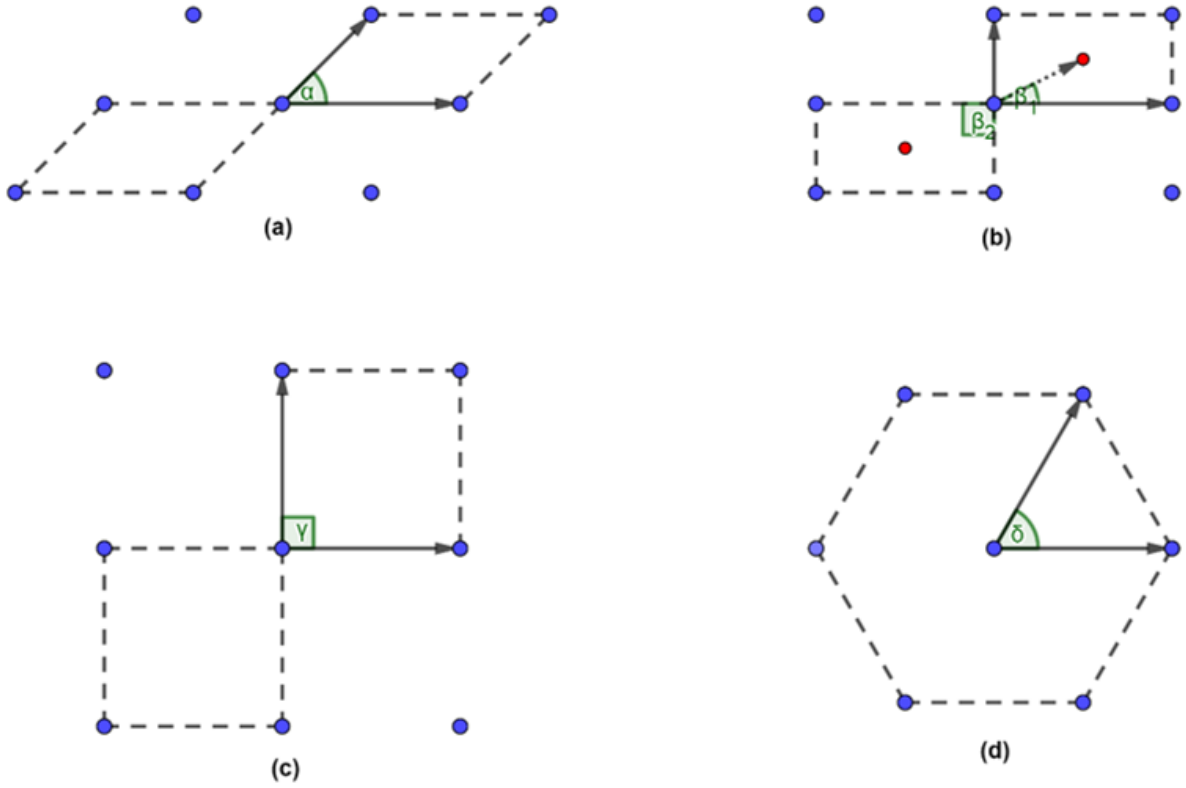


Fig. 3 Symmetry in 2D crystal

(a) Oblique; (b) Rectangular; (c) Square; (d)Hexagonal

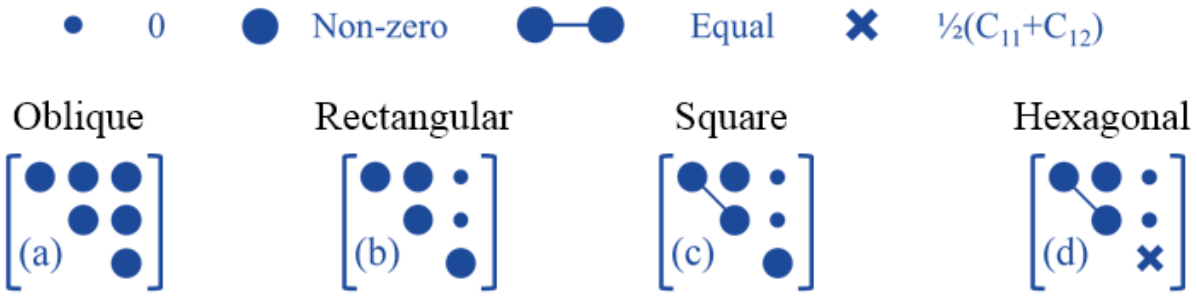


Fig. 4 The independent elastic constants in 2D crystals

CHAPTER 4

FAQ

TODO

CHAPTER 5

ElasticPOST API

TODO

CHAPTER 6

Citing

CHAPTER 7

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CHAPTER 8

Indices and tables

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