ELPWmat

USER GUIDE

USE PWMAT TO CALCULATE ELASTIC CONSTANTS

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1. Introduction

ELPWmat is an efficient open source python program using PWmat to calculate elastic constants, compliance constants, Young`s, shear and bulk moduli and Poisson`s ratio for 3D materials and 2D materials via high-throughput first-principles computation. For 3D materials, ELPWmat can calculate elastic constants, compliance constants, the polycrystalline Young`s, shear and bulk moduli and Poisson`s ratio, according to Voigt-Reuss-Hill`s approximations. For 2D materials, ELPWmat can calculate elastic constants, compliance constants, in-plane Young`s, shear moduli and in-plane Poisson`s ratio.

2. Theoretical background

Because crystals deform almost in a linear elastic manner at small strains, the response of solids to external loading can be described by the generalized Hooke`s law

$$\sigma_i = \sum_{j=1}^{6} c_{ij}\varepsilon_j \quad (1)$$

where σ_{ij} are the elements of stress tensor and ε_{ij} are the elements of strain tensor. Similarly the compliance tensor (s) can be written as

$$\varepsilon_i = \sum_{j=1}^{6} s_{ij}\sigma_j \quad (2)$$

where s_{ij} are the elements of elastic compliance tensor that satisfies $[s_{ij}] = [c_{ij}]^{-1}$ [1]. The internal energy $\mathrm{E}(\mathrm{V}, \{\varepsilon_{ij}\})$ of a crystal under a general strain ε_{ij} can be expressed by Taylor expansion in power of the strain tensor in the following equation:

$$\mathrm{E}(\mathrm{V},\{\varepsilon_i\}) = E(V_0,0) + V_0\sum_{i=1}^{6}\sigma_i\varepsilon_i + \frac{V_0}{2}\sum_{i,j=1}^{6}c_{ij}\varepsilon_i\varepsilon_j + \cdots \quad (3)$$

where $E(V_0,0)$ and V_0 are the energy and volume of the reference structure (usually the equilibrium one), respectively. And the strain tensor can be written as

$$\varepsilon = \begin{pmatrix} e_1 & \frac{1}{2}e_6 & \frac{1}{1}e_5 \\ \frac{1}{2}e_6 & e_2 & \frac{1}{2}e_4 \\ \frac{1}{2}e_5 & \frac{1}{2}e_4 & e_3 \end{pmatrix}$$

So, the elastic constants can be obtained by calculating the change of energy or stress with applying small strains to crystal. Direct calculation of elastic constants are possible from first principles total energy calculations and symmetry-general least-squares extraction method [2].

For polycrystalline materials, the crystallites are randomly, and such materials can be considered to be quasi-isotropic or isotropic in a statistical sense [1]. So, bulk modulus K and shear modulus G are generally used to describe the elastic response, and K, G can be obtained by averaging the single-crystal elastic constants. Voigt bound [3], Reuss bound [4] and Hill average [5] are most widely used averaging methods. For Voigt bounds are given by the following equations:

$$9K_v = (c_{11}+c_{22}+c_{33}) + 2(c_{12}+c_{23}+c_{31}) \quad (4)$$

$$15G_v = (c_{11}+c_{22}+c_{33}) - (c_{12}+c_{23}+c_{31}) + 4(c_{44}+c_{55}+c_{66}) \quad (5)$$

The Reuss bounds are given by:

$$1/K_R = (s_{11} + s_{22} + s_{33}) + 2(s_{12} + s_{23} + s_{31}) \quad (6)$$

$$15/G_R = 4(s_{11} + s_{22} + s_{33}) - 4(s_{12} + s_{23} + s_{31}) + 3(s_{44} + s_{55} + s_{66}) \quad (7)$$

Voigt and Reuss bounds are rigorous upper and lower bounds of K and G, respectively. Based on Voigt and Reuss bounds, Hill defined $K_{VRH} = \frac{1}{2}(K_v + K_R)$, $G_{VRH} = \frac{1}{2}(G_V + G_R)$, known as the Voigt-Reuss-Hill average. According to the values of bulk modulus K and shear modulus G, the Young`s modulus E and Poisson`s ratio v can be obtained by $\mathrm{E} = \frac{9KG}{3K+G}$, $\mathrm{v} = \frac{3K-2G}{2(3K+G)}$, respectively.

For 2D materials, the Hooke`s law evolved to the following form:

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ & c_{22} & c_{26} \\ & & c_{66} \end{bmatrix} . \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_6 \end{bmatrix} \quad (8)$$

The elastic constants can be obtained by:

$$c_{ij} = \frac{1}{A_0}\left(\frac{\partial^2 E}{\partial \varepsilon_i \partial \varepsilon_j}\right) \quad (9)$$

Where A_0 is the area of simulation cell in the x-y plane (vacuum layer along to z direction). The Young`s and shear moduli and Poisson`s ratios can be given by the following equations, respectively [1].

$$E_x = \frac{c_{11}c_{22} - c_{12}c_{21}}{c_{22}} \quad (10)$$

$$E_y = \frac{c_{11}c_{22} - c_{12}c_{21}}{c_{11}} \quad (11)$$

$$G_{xy} = c_{66} \quad (12)$$

$$v_{xy} = \frac{c_{21}}{c_{22}} \quad (13)$$

$$v_{yx} = \frac{c_{12}}{c_{11}} \quad (14)$$

Where E_i is the Young`s modulus along the axis of i; $G_{ij}$ is the shear modulus in the x-y planes; $v_{ij}$ is the Poisson`s ratio with strain applied

in the direction i and the response strain in the direction j. Note that since no particular thickness is assumed for a single atomic layer or a few atomic layers of 2D materials, the unit for the elastic stiffness tensor as well as the elastic moduli are actually force per unit length (N/m) rather than force per area (N/m^2 or Pa). A method of effective thickness has been used in many literatures. According to this method, the relationship between elastic stiffness constants c_{ij} (unit: Pa) and c_{ij} (unit: N/m) is that: $c_{ij}(Pa) = c_{ij}(N/m)/d_0$, where d_0 is the effective thickness of the system [1].

3. Install

ELPWmat can be obtained from http://www.pwmat.com/module.html. After download source code:

```
tar –zxvf ELPWmat.tar.gz
cd ELPWmat
./setup.py
```

4. Run ELPWmat

To run ELPWmat, etot.input (atomic relaxation), strain.config (completely optimized structure, you can copy final.config to strain.config) and *.PSP (pseudopotentials), job.pbs (PBS scripts) should be prepared and then run “ELPWmat.py” (for 3D materials) or “ELPWmat2d.py” (for 2D materials) in the current directory. In order to help users to use it, we provide four examples in “ELPWmat/examples”, “AlN” and “Si” for 3D materials, “graphene” and “phosphorene” for 2D materials. After all PBS tasks have finished, please run “ELTool.py” or

“ELTool2d.py”, you will obtain a file named “elastic.txt”. In this file, elastic constants, compliance constants, bulk and shear modulus and Poisson`s ratio will be exhibited.

Reference

[1] https://sites.google.com/site/zrfbuaa/softwares/aelas

[2] arXiv:cond-mat/0601216 [cond-mat.mtrl-sci]

[3] W. Voigt, Lehrbuch der Kristallphysik, Leipzig Berlin, 1928.

[4] A. Reuss, Z. Angew. Math. Mech 9 (1929) 49-58

[5] R. Hill, Proc. Phys. Soc. A 65 (1952) 349.