



User's Guide

Release 1.1.0

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1 Features and history of AELAS

1.1 Overview

AELAS is an efficient open source command-line program for Automatic ELAStic constants derivations via high-throughput first-principles computation. It is designed by Dr. S. H. Zhang and Prof. R. F. Zhang at Beihang University. More details can be found at:

<https://sites.google.com/site/zrfbuaa/software/aelas>

1.2 Features of AELAS

The program has implemented the following methods

- Four filters to avoid the abnormal distortion
- The standardized unit cell (IEEE-format)
- The elastic constants of any crystal system for 3D materials
- The elastic constants of any crystal system for 2D materials
- The polycrystal elastic moduli in Voigt, Reuss and Hill average
- The ductility-brittleness transition, Pugh ratio
- The Cauchy pressure P_c
- The elastic stability criterion
- In-plane Young's (E_x and E_y) and shear (G_{xy}) moduli of 2D materials
- In-plane Poisson's ratios (ν_{xy} and ν_{yx}) of 2D materials
- etc.

1.3 Version history

v_1.0.0

(2017.3.12):

Four filters to avoid the unstable distortion

The standardized unit cell (IEEE-format)

>>> For 3D materials

The elastic constants of any crystal system

The Polycrystalline Young's, shear and bulk moduli and Poisson's ratio

The Pugh ratio (G/K)

The Cauchy pressure ($P_c=c_{12}-c_{44}$)

The elastic stability condition

>>> For 2D materials

The elastic constants of any crystal system

In-plane Young's (E_x and E_y) and shear (G_{xy}) moduli

In-plane Poisson ratios (ν_{xy} and ν_{yx})

Further development

Stress-strain method

Volume reservation elastic constant

Higher order elastic constants

Transform elastic tensors

Anisotropic elastic properties

More reliable polynomial fit

More available computer packages exciting VASP, QE, WIEN2K...

2 Theoretical background

2.1 Elasticity theory

Within the linear region, the response of solids to external loading are described using the generalized Hooke's law and the stress $\sigma=(\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5, \sigma_6)$ is related with the strain $\varepsilon=(e_1, e_2, e_3, e_4, e_5, e_6)$ in the normal form as:

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

where the coefficients c_{ij} are the elastic stiffness constants of the crystal and $e_1=e_{xx}$, $e_2=e_{yy}$, $e_3=e_{zz}$, $e_4=e_{xz}+e_{zx}$, $e_5=e_{zy}+e_{yz}$, $e_6=e_{yx}+e_{xy}$ are in Voigt notation [1] by simplifying a pair of Cartesian indices into a single integer $1 \leq i \leq 6$, *i.e.* $xx \rightarrow 1$, $yy \rightarrow 2$, $zz \rightarrow 3$, $yz \rightarrow 4$, $xz \rightarrow 5$, $xy \rightarrow 6$. Thus a 3×3 symmetric strain or stress matrix reduces to a vector with 6 independent components, and the elastic stiffness tensor is expressed by a 6×6 matrix. Eq. (1) is changed to the form

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

where s_{ij} are the elements of elastic compliance tensor that satisfies $[s_{ij}] = [c_{ij}]^{-1}$.

The internal energy of a crystal under strain ε can be represented by Taylor expansion in power of the strain tensor in the following equation:

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

where $E(V_0, 0)$ and V_0 are the energy and volume of the reference structure (usually the equilibrium one), respectively.

In general, there are two methods for the first-principles calculation of elastic constants: energy-strain method and stress-strain method. The energy-strain method is according to that

the elastic stiffness tensor is related to the second-order derivative of the total energies with respect to strain (*i.e.* Eq. (3)), while the stress-strain methodology is based on the first-order derivative of the stresses (*i.e.* Eq. (1)). The stress-strain method requires much smaller set of distortions than the energy-strain method, since there are six stress components that can be obtained for each calculation whereas only one energy for each fitting [2]. Nevertheless, a much higher computational precise is required for stress-strain method to achieve the same accuracy as energy-strain method [3], which makes the former method apply mainly for the determination of stability of a structure within minor distortion. To reduce the stress sensitivity, the energy-strain method is therefore applied in AELAS code. In this method, one first chooses a set of distortion modes, *e.g.* $\varepsilon_1=(0, 0, 0, \delta, \delta, \delta)$, $\varepsilon_2=(\delta, \delta, 0, 0, 0, 0)$ and $\varepsilon_3=(\delta, \delta, \delta, 0, 0, 0)$ for cubic system, and then the strain energies are calculated for each distorted structure. After that, the quadratic coefficients are determined by fitting the energy-distortion δ relationship, and finally the second order elastic constants c_{ij} are determined.

2.2 Polycrystalline bulk and shear moduli

In a polycrystalline material, the crystallites are randomly oriented, and such materials can be considered to be quasi-isotropic or isotropic in a statistical sense. The elastic response of an isotropic system is generally described by the bulk modulus K and the shear modulus G , which may be obtained by averaging the single-crystal elastic constants [4]. The averaging methods most widely used are the Voigt [1] bound, Reuss [5] bound, Hashin-Shtrikman [6] bound and Hill [7] average. Voigt's procedure assumes that the strain is uniform throughout an aggregate, while the Reuss's one takes the stress to be uniform [7]. In Voigt's approximation, the equation takes the following form:

$$\begin{cases} 9K_V = (c_{11} + c_{22} + c_{33}) + 2(c_{12} + c_{23} + c_{31}) \\ 15G_V = (c_{11} + c_{22} + c_{33}) - (c_{12} + c_{23} + c_{31}) + 4(c_{44} + c_{55} + c_{66}) \end{cases}, \quad (4)$$

while the Reuss bounds is that

$$\begin{cases} 1/K_R = (s_{11} + s_{22} + s_{33}) + 2(s_{12} + s_{23} + s_{31}) \\ 15/G_R = 4(s_{11} + s_{22} + s_{33}) - 4(s_{12} + s_{23} + s_{31}) + 3(s_{44} + s_{55} + s_{66}) \end{cases}. \quad (5)$$

The Young's modulus E , and Poisson's ratio ν for an isotropic material are given by

$$E = \frac{9KG}{3K+G} \text{ and } \nu = \frac{3K-2G}{2(3K+G)}, \text{ respectively.}$$

Hill [7] has demonstrated that the Voigt and Reuss bounds are rigorous upper and lower bounds, respectively. The arithmetic mean of the Voigt and Reuss bounds, *i.e.* $K_{VRH} = 1/2(K_V + K_R)$ and $G_{VRH} = 1/2(G_V + G_R)$, termed the Voigt-Reuss-Hill (VRH) average is also found as better approximation to the actual elastic behavior of a polycrystal material [7]. In weakly anisotropic materials, of course, all these averages lead to similar results for elastic moduli. Alternatively, one would prefer to use the geometric or harmonic means instead of the arithmetic average too.

2.3 Pugh ratio and Cauchy pressure

A well-established justification of whether a crystalline solid is ductile or brittle is if dislocation embryos can be more easily nucleated from a sharp crack tip prior to its propagation by cleavage [8, 9]. The bifurcation in mechanical behavior can be represented by the ratio of the shear modulus to the bulk modulus, *i.e.* Pugh ratio G/K , by simply considering K as the resistance to fracture and G as the resistance to plastic deformation [10]. The critical value of G/K ratio to separate ductile and brittle materials is around 0.57. That means if $G/K < 0.57$ the material is more ductile, otherwise the material behaves in a brittle

manner [10]. The higher G/K indicates the more brittleness of the material.

Cauchy pressure $P_C=(c_{12}-c_{44})$ is another quantity to describe the brittleness or ductility of a materials by counting for the angular character of atomic bonding in the metals and compounds [11]. For covalent materials with brittle atomic bonds, the Cauchy pressure is negative ($c_{12}<c_{44}$), because in this case material resistance to shear strain (c_{44}) is much more than that for volume change (c_{12}) [12]. In case of metallic-like bonding where the electrons are almost delocalized, however the Cauchy pressure should be positive ($c_{12}>c_{44}$) [11, 12].

2.4 Elastic anisotropy

To quantify the anisotropy of cubic crystals, Zener [13] introduced $A=2c_{44}/(c_{11}-c_{12})$, where c_{11} , c_{12} , and c_{44} are the three independent components of elastic stiffness constants. More recently, Chung and Buessem [14] proposed another empirical factor to measure elastic anisotropy of cubic crystals by a single-value as,

$$A^C = \frac{G_V - G_R}{G_V + G_R} = \frac{3(A-1)^2}{3(A-1)^2 + 25A}, \quad (6)$$

where G_V and G_R are the shear modulus with the Voigt and Reuss approximation, respectively, and A is the Zener anisotropy coefficient. Note that A^C is generally different if A^{-1} is used instead of A [15]. The two definitions of elastic anisotropy are helpful as long as one considers cubic crystals that exhibit an isotropic bulk resistance. For all other crystal types, the bulk response is in general anisotropic and one must account for such contributions in order to quantify the extent of anisotropy accurately. For this purpose, Ranganathan *et al.* [15] introduce a new universal anisotropy index that overcomes the above limitations:

$$A^U = 5 \frac{G_V}{G_R} + \frac{K_V}{K_R} - 6, \quad (7)$$

where K_V , K_R , G_V and G_R are the bulk and shear moduli with the Voigt and Reuss estimates, respectively. In the special case of cubic crystals, the relation between A^U and A takes the following form: $A^U = \frac{6}{5}(A^{1/2} - A^{-1/2})^2$ [15]. For an isotropic crystal, A^U is identically zero, and the departure of A^U from zero defines the extent of elastic anisotropy and accounts for both the shear and bulk contributions unlike all other existing anisotropy measures [15]. Thus, A^U represents a universal measure to quantify the single crystal elastic anisotropy [15].

2.5 Criterion of elastic stability

For a crystalline structure, the elastic stability criterion is defined as the elastic energy given by the quadratic form of Eq. (3). It is always positive [16] for a stable structure in the harmonic approximation [17]. As first noted by Born [18], it is mathematically equivalent to the following necessary and sufficient stability conditions: i) The second-order elastic stiffness tensor matrix \mathbf{C} is definitely positive, ii) all eigenvalues of \mathbf{C} are positive, iii) all the leading principal minors of \mathbf{C} are positive, and iv) an arbitrary set of minors of \mathbf{C} are all positive. These are four possible formulations of the Born elastic stability conditions for a crystal, which are valid regardless of the crystal symmetry.

Recently, Mouhat *et al.* [16] proposed necessary and sufficient elastic stability conditions as regards the elastic stability for various crystal systems. These more detailed criteria [16] can be used to identify elastic tensor that correspond to materials that are mechanically stable but are near an elastic instability with a small tolerance [19]. Taken cubic crystal system as an example, it is required that $c_{11}-c_{12}>0$, $c_{11}+2c_{12}>0$ and $c_{44}>0$ and a small tolerance could be used that $c_{11}-\varepsilon c_{12}>0$, where ε is a value slightly greater than one [19].

Under minor distortion, the elastic stability criterion considers mostly the pressure influence. The elastic constant tensor \mathbf{C} should be replaced by an new elastic stiffness tensor \mathbf{B} [20], *i.e.* $\mathbf{B}=\mathbf{C}+\Lambda$, where the tensor Λ depends only on the applied stress. For instance, the cubic crystal under the hydrostatic compression pressure ($P>0$) [21]: $c_{11}+2c_{12}+P>0$, $c_{11}-c_{12}-2P>0$, $c_{44}-P>0$.

2.6 Elasticity of 2D materials

For 2D materials, the elastic constants can also be derived from the Hooke's law under plane-stress condition [22]

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{16} \\ & c_{22} & c_{26} \\ & & c_{66} \end{bmatrix} \cdot \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_6 \end{bmatrix}. \quad (8)$$

Similar to 3D materials, the elastic stiffness constants can be calculated using the formula,

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

where A_0 is the area of simulation cell in the x - y plane. The relation between the Young's and shear moduli, Poisson's ratios and elastic stiffness constants for a 2D system can be derived [23]

$$E_x = \frac{c_{11}c_{22} - c_{12}c_{21}}{c_{22}}, \quad E_y = \frac{c_{11}c_{22} - c_{12}c_{21}}{c_{11}}, \quad \nu_{xy} = \frac{c_{21}}{c_{22}}, \quad \nu_{yx} = \frac{c_{12}}{c_{11}}, \quad G_{xy} = c_{66}, \quad (10)$$

where $E_i = \sigma_i / \varepsilon_i$ is the Young's modulus along the axis of i , $\nu_{ij} = -d\varepsilon_j / d\varepsilon_i$ is the Poisson's ratio with tensile strain applied in the direction i and the response strain in the direction j , and G_{xy} is the shear modulus in the x - y plane [23]. 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/m² or Pa). A method of effective thickness has been used in many literatures [24, 25]. 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 [25].

3 Workflow and automated scheme

For this section, please refer to our publication: S. H. Zhang and R. F. Zhang, AELAS: Automatic ELAStic constants derivations via high-throughput first-principles computation, in preparation.

4 Getting started

4.1 How to obtain AELAS

AELAS is an open source code and can be downloaded at:

<https://sites.google.com/site/zrfbuaa/software/aelas>

4.2 Necessary citations

Whenever using ADAIS in all publications and reports, you must cite the original papers, for example, in the following way:

The second-order elastic constants of two-dimensional and three-dimensional single crystal materials, and other derived elastic properties, *i.e.*, Young's, bulk and shear moduli as well as Poisson's ratio of polycrystal materials, Pugh ratio, Cauchy pressure, elastic anisotropy and elastic stability criterion, were calculation using the AELAS code [1], which is an automatic derivation of elastic property via high-throughput first-principles computation.

[1] S.H. Zhang and R.F. Zhang. "AELAS: Automatic ELAStic property derivations via high-throughput first-principles computation." *Computer Physics Communications* 220 (2017): 403-416.

4.3 How to install AELAS

The compiler "cmake" is needed before installing AELAS, and more information can be found via:

<https://cmake.org/>

After expanding source code, and go into the source code directory:

```
tar zxvf AELAS-x.x.x.tar.gz
cd AELAS-x.x.x
```

The current directory is PROJECT_SOURCE_DIR.

```
cd spglib-x.x.x
mkdir _build; cd _build
cmake ..
make
make install
```

The libraries are installed at PROJECT_SOURCE_DIR/spglib-x.x.x/lib and the header file is installed at PROJECT_SOURCE_DIR/spglib-x.x.x/include

```
cd ../../src
make -f makefile
```

4.4 How to run AELAS

For the AELAS runner, a number of user-friendly options are implemented for choice:

-g, --generate: to generate the distorted POSCAR files of 3D materials for the first-principles calculations.

-g2d, --generate2d: to generate the distorted POSCAR files of 2D materials for the first-principles calculations.

-d, --derive: to derive the elastic constants for 3D materials by quadratic polynomial fitting of the energy-strain relationships extracted from the "OSZICAR" files.

-d2d, --derive2d: to derive the elastic constants for 2D materials by quadratic polynomial fitting of the energy-strain relationships extracted from the "OSZICAR" files.

-e, --extract: to read the energies of distorted structures for 3D materials from the OSZICAR files.

-e2d, --extract2d: to read the energies of distorted structures for 2D materials from the OSZICAR files.

-i [pressure], --incar [pressure]: to create INCAR file with PSTRESS=pressure ([Integer], UNIT=GPa and =0000, if default).

-k [k1] [k2] [k3] [kscheme], --kmesh [k1] [k2] [k3] [kscheme]: to create the NEWKPT file in KPOINTS format according to the user's input. k1, k2 and k3 = [Integer] (no default value), kscheme=[MP | Gamma] (=Gamma, if default).

-ka [kppra] [kscheme], --kppra [kppra] [kscheme]: to create the NEWKPT file in KPOINTS format according to the K-Point Per Reciprocal Atom, kppra=[Integer] (=1000, if default), kscheme=[MP | Gamma] (=Gamma, if default).

-kv [kspacing] [kscheme], --kspac [kspacing] [kscheme]: to create the NEWKPT file in KPOINTS format according to the "kspacing", kspacing=[Real] (=0.5, if default), kscheme=[MP | Gamma] (=Gamma, if default).

-v, --version: to show the version information.

-h, --help: to show the help message.

-c, --clean: to clean the structure and OSZICAR file.

-l, --license: to show the license information.

4.5 Generation of INCAR and KPOINTS file using AELAS

For INCAR file

Two default INCAR files `incar_rlx` and `incar_stc` can be automatically created by AELAS code for structural relaxation and static calculation respectively. In order to calculate the

elastic properties under high pressure, one need to add the value of pressure in the command line, e.g.

```
% AELAS -i 500.
```

Note that when calculating the elastic properties at high pressure, the crystal structure needs to be fully relaxed at the corresponding pressure.

For KPOINTS file

In AELAS code, there are two automatic methods to specify the KPOINTS file: the k -points per reciprocal atom (KPPRA) [26] and the smallest allowed spacing between k -points (KSPACING). The KPPRA is a way to automatically set the k -point mesh while keeping the k -point density constant along the three axes despite of the variation of the unit cell. The number of mesh points along a given reciprocal lattice vector a_i is set proportional to $|a_i \cdot (a_2 \times a_3)| / |a_2 \times a_3|$, where a_2 and a_3 are the other two remaining reciprocal lattice vectors. The KSPACING is another automatic method that makes the mesh as uniform as possible. According to this method, the number of k -points in the direction of three reciprocal lattice vectors is determined by the equation: $|a_i| / KSPACING$. A generalized way to determine the KPOINTS file is also included in AELAS, by manually inputting the numbers of the subdivisions N_1 , N_2 and N_3 .

In order to create the KPOINTS file, one may simply input AELAS -ka, AELAS -kv or AELAS -k [N1] [N2] [N3] at command line and a file named NEWKPT will be created.

Notice that a file named **RECELL** in POSCAR-format is required if one use the two automatic generation methods for the KPOINTS file. The command AELAS -g or AELAS -g2d will generate RECELL file after analyzing the symmetry of the POSCAR input by user.

4.6 VASP&AELAS calculation

Pre-process

In pre-processing procedure, the standardized unit cell (IEEE-format) are defined from the input structure via SPGLIB and its derived structures are generated according to the crystal symmetry and the predefined distortion modes. Note that the input file named “INPOS” has the same format to the standard POSCAR.

To obtain the distorted structures, run AELAS:

For 3D materials

```
% AELAS -g
```

Or

```
% AELAS --generate
```

For 2D materials

```
% AELAS -g2d
```

Or

```
% AELAS --generate2d
```

These commands will generate the output files of RECELL, DEFMOD, and POS_{N₁}_{N₂}.vasp. The RECELL file is the redefined unit cell with the IEEE-format. The DEFMOD file contains the space group number, number of independence elastic stiffness constants, strain values and distortion mode. The POS_{N₁}_{N₂}.vasp files correspond to the distorted structures.

First-principles calculation using the structures with distortion

The energies of each POS_{N1}_{N2}.vasp file are calculated by the first-principles codes, *e.g.* VASP, and then the OSZICAR file will be saved to OSZICAR_{N1}_{N2} in sequence as follows:

```
% cp OSZICAR OSZICAR_{N1}_{N2}
```

To be noticed that no relaxation is allowed for the lattice constant.

Post-process

To derive the elastic constants by quadratic polynomial fitting of the energy-strain relationships that were extracted from the "OSZICAR" files. NOTE that the “**RECELL**” file is required for post-processing procedure.

For 3D materials

```
% AELAS -d
```

OR

```
% AELAS --derive
```

For 2D materials

```
% AELAS -d2d
```

OR

```
% AELAS --derive2d
```

After this command, ELADAT and EPVDAT will be generated if the calculation is successful. ELADAT gives a summary of the calculated elastic properties. EPVDAT contains the information of the space group number, number of independence elastic stiffness constants, the volume for 3D materials or the area for 2D materials, distortion mode, the energy values and the fitted parameters.

If the calculation is successful, there is a **‘SUCCESSFUL’** at the end of the RELAS file, while if the calculation is unsuccessful, an error or warning information will be shown in the RELAS file.

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