ElasticTools
Project

USERGUIDE

OF

AAEP

ANALYSIS OF ANISOTROPIC ELASTIC PROPERTIES

FROM ELASTICTOOLS PROJECT
v1.5.0
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1

SECTION

Features and Change Log of AAEP

AAEP is useful tool for the analysis of second-order elastic tensors of three-dimensional (3D) and two-dimensional (2D) crystal systems, which can be used for IRelat, ElaStic, AELAS codes, and so on. The AAEP (**A**nalysis of **A**nisotropic **E**lastic **P**roperties) has three powerful plotting and visualization tools that is conveniently interfaced with GNUPLOT, XMGRACE, and view3dscene, thus offering immediate visualization of the results. This code is an essential tool for identifying the anomalous mechanical properties, such as negative linear compressibility, negative Poisson's ratio, or highly-anisotropic elastic moduli in 2D and 3D materials.

There are currently two software packages available for analyzing second-order elastic stress and visualizing elastic properties of 3D materials that can investigate such properties. The first code is ELAM, and was developed by Marmier [3]. ElAM, implemented in Fortran90, is command-line driven and can output 2D cut figures in PostScript (PS) format and 3D surfaces in the Virtual Reality Modelling Language format (VRML). The following code is ELATE, and was developed by R. Gaillac *et al.* [4]. ELATE is a Python module for the manipulating of elastic tensors and a standalone online application for routine analysis of elastic tensors. In this code, a Python module is used to generate the HTML web page with embedded Javascript for dynamical plots. Notably, this code can also import elastic data directly by the use of the Materials API [2].

According to this explanation, the main motivation of the present work is a comprehensive and efficient program, AAEP (Analysis of Anisotropic Elastic Properties), that accommodates all the features of both codes, and eliminates their shortcomings. Hence, the most important features of AAEP are in the Sec. 1.2 .

1.1 Features of AAEP and its comparison with ELATE and ELAM codes

- Computes and display the main mechanical properties such as Bulk modulus, Young's modulus, Shear modulus, P-wave modulus, Universal anisotropy index [5], Chung-Buessem Anisotropy Index [5], Log-Euclidean anisotropy parameter [6], Cauchy pressure, Poisson's ratio, Pugh's ratio, according to the three averaging schemes, *i.e.*, Voigt, Reuss and Hill [7]: Many of these features are included in ELAM and ELATE codes.

- Investigation of mechanical stability using calculation of six (three) eigenvalues of the elastic tensor in 3D materials (2D materials): This option is only included in ELATE for 3D materials.

- Visualization of the 3D surfaces, as well as 2D projections on any desired plane for shear modulus, Poisson's ratio, linear compressibility, bulk modulus, Young's modulus in 3D materials: ELATE only depicts these features on XY, XZ, and ZY planes. Also, the Bulk modulus calculation is not included in ELAM and ELATE codes.

- Visualization of the 2D polar covers for Poisson's ratio, shear modulus, and Young's modulus in 2D materials: This option is not included in the ELATE and ELAM codes.

- The offline database contains more than 13000 elastic tensors taken from Materials API: This option is only available online in ELATE.

- Includes output files in different formats for custom drawing or display with various software: ".dat" files for custom drawing, ".wrl" files for visualization of the 3D surfaces by view3dscene software [8], ".agr" files for visualization of the 2D projections that are opened by XMGRACE [9], and ".gpi" script files for visualization of the 3D surfaces, 2D heat maps, and 2D projections that can be run by GNUPLOT [10]: ELAM only generates VRML (for 3D visualization) and PS formats (for 2D cut visualization), and ELATE code provides images online in PNG format.

1.2 Change Log

- v1.1.0 [14/07/2018] : Add a new funtion to calculate the bulk modulus properties for 3D system.

- v1.1.1 [20/12/2018] : Add a new funtion to check stability conditions for 3D system.

- v.1.2.0 [05/04/2019] : Add dat2gnu_lapw to plot by gnuplut.

- v.1.3.0 [12/05/2020] : Add a new funtion to calculate elsetic properties, and check stability conditions for 2D system.

- v.1.4.0 [10/06/2020] : The addition of a database includes more than 13,000 elastic tensors and a function for reading it.
- v.1.5.0 [01/07/2020] : Add a new funtion to calculate the phase and group velocities of the acoustic waves.
- v.1.5.1 [20/07/2020] : Add a new funtion to calculate the shear modulus for 2D system.
- v.1.5.2 [10/08/2020] : Add new options of dat2gnu to plot 2D heat maps.

2

SECTION

Theoretical Background

2.1 Hooke's law and elastic tensor of crystals

A solid material changes its shape when subjected to stress. Provided the stress is below a certain limiting value, the elastic limit (elastic regime); the strain is recoverable (Fig. 1). This means that the material returns to its original shape when the stress is removed. In this regime (elastic regime), according to Hooke's law, it can be stated that for sufficiently small stresses, the amount of strain is proportional to the magnitude of the applied stress:

$$\varepsilon = S\sigma, \tag{1}$$

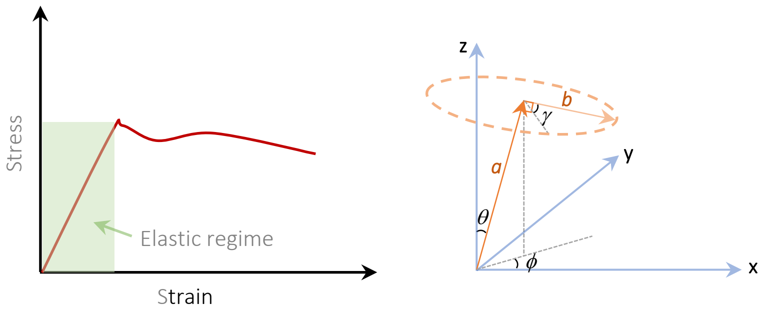


Figure 1: Schematic stress–strain curves and definitions of angles used to describe directions in the calculations related to AAEP. The elastic regime corresponds to the portion of the diagram where the strain is proportional to the stress.

where S is a constant. S is called the *elastic compliance constant* (ECC), or the *compliance*. Another form of this Eq. can be written as follows,

$$\varepsilon = C\sigma, \ E \equiv C = 1/s, \tag{2}$$

where C is the *elastic stiffness constant* (ESC), or the *stiffness*, and C is Young's modulus. The general form of Hooke's law can be rewritten in the form of tensor,

$$\varepsilon_{ij} = S_{ijkl}\sigma_{kl}, \tag{3}$$

where S_{ijkl} are the ECCs of the crystal. Also, as an alternative to Eq.(2),

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}, \tag{4}$$

where C_{ijkl} are the ESCs. Eq.(3) and Eq.(4) stands for nine equations, each with nine terms on the right-hand side. The S_{ijkl} or C_{ijkl} is a tensor of 4^{th}-rank, and ϵ_{ij} or σ_{ij} is a tensor of 2^{th}-rank. So, the C_{ijkl} (S_{ijkl}) are the 81 *stiffness* (*compliances*) constants of the crystal. Due to the inherent symmetries (translational and rotational symmetries) of ϵ_{ij}, σ_{ij}, and S_{ijkl} or $C_{ijkl,}$ the number of independent coordinates of the 4^{th}-rank tensor reduces to 21 for the least symmetric case. On the other hand, the symmetry of the crystal can further reduce this number: 21 for triclinic, 15 for monoclinic, 9 for orthorhombic, 7 for trigonal, 5 for tetragonal, 5 for hexagonal and 3 for cubic.

2.2 Transformation law and representation surfaces of elastic proprieties

A 4^{th}-rank tensor is defined (like tensors of lower rank) by its transformation law [11]. We know that the 81 tensor components A_{ijkl} representing a physical quantity are said to form a 4^{th}-rank tensor if they transform on change of axes to A'_{ijkl}, where

$$A'_{ijkl} = a_{im}\, a_{jn}\, a_{ko}\, a_{lp} A_{mnop}. \tag{5}$$

It can be shown that 4^{th}-rank tensor S_{ijkl} or C_{ijkl} also follows this rule [11]:

$$\left.\begin{aligned} \varepsilon'_{ij} &= a_{ik}a_{jl}\varepsilon_{kl}, \\ \varepsilon_{kl} &= S_{klmn}\sigma_{mn}, \\ \sigma_{mn} &= a_{om}a_{pn}\sigma'_{op}, \end{aligned}\right\} \varepsilon'_{ij} = a_{ik}a_{jl}\, S_{klmn}\, a_{om}a_{pn}\, \sigma'_{op}. \tag{6}$$

By comparing the Eq.(3) and the recent Eq.,

$$S'_{ijkl} = a_{im}a_{jn}a_{ko}a_{lp}S_{mnop}, \tag{7}$$

which is the necessary transformation law. To express the anisotropic form of Hooke's law in matrix notation, a notation called Voigt scheme is used. In the S'_{ijkl} and S_{mnop}, the first two suffixes are abbreviated into a single one running from 1 to 6, and the last two can be abbreviated in the same way, according to the following Voigt scheme:

$$\begin{array}{llllllll} \text{Tensor notation}: & 11 & 22 & 33 & 23,32 & 31,13 & 12,21 \\ \text{Matrix notation}: & 1 & 2 & 3 & 4 & 5 & 6 \end{array} \tag{8}$$

Therefore, the components of the stress (σ) and the strain (ϵ) tensors are written in a single suffix running from 1 to 6,

$$\sigma_{ij} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{pmatrix} \xrightarrow{\text{Voigt scheme}} \begin{pmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{pmatrix},$$
$$\varepsilon_{ij} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{pmatrix} \xrightarrow{\text{Voigt scheme}} \begin{pmatrix} \varepsilon_1 & \frac{1}{2}\varepsilon_6 & \frac{1}{2}\varepsilon_5 \\ \frac{1}{2}\varepsilon_6 & \varepsilon_2 & \frac{1}{2}\varepsilon_4 \\ \frac{1}{2}\varepsilon_5 & \frac{1}{2}\varepsilon_4 & \varepsilon_3 \end{pmatrix}. \tag{9}$$

According to this scheme, we have for the S_{mnop} [11],

$$S_{mnop} = S_{ij}, \text{ when } i \text{ and } j \text{ are 1; 2 or 3,}$$
$$2S_{mnop} = S_{ij}, \text{ when either } i \text{ or } j \text{ are 4; 5 or 6,}$$
$$4S_{mnop} = S_{ij} \text{ when both } i \text{ and } j \text{ are 4; 5; or 6.}$$

In general, therefore, Eq.(3) takes the shorter form

$$\varepsilon_i = S_{ij}\sigma_j \;\; (i, j = 1, 2, ..., 6). \tag{10}$$

In fact, the Voigt scheme replaces the cumbersome 2^{nd} and 4^{th}-rank tensors in a 3-dimension vector space by vectors and matrices in a 6-dimension vector space. The reason for introducing the factors of 0.5 in Eq.(9) and the factors of 2 and 4 into the definitions of the S_{ij} is to make it possible to write Eq.(10) in a compact form.
Using S_{ij} in Eq.(10) and Eq.(5), we can get a general and simple compliance transformation relation for any crystal from the old systems (T') to measurement systems (T)

$$T'_{ijkl} = r_{i\alpha}\, r_{j\beta}\, r_{k\gamma}\, r_{l\delta}\, T_{\alpha\beta\gamma\delta}, \tag{11}$$

where the r are the components of the rotation matrix (or direction cosines). In general, the tension produces, not only longitudinal, and lateral strains but shear strains as well. Therefore, spherical coordinates are suitable for such stresses and the responses that materials give to stresses. We choose $\boldsymbol{r}\equiv\boldsymbol{a}$ to be the first unit vector in the new basis set [3, 4],

$$\boldsymbol{a} = \begin{pmatrix} \sin(\theta)\cos(\varphi) \\ \sin(\theta)\sin(\varphi) \\ \cos(\theta) \end{pmatrix}; \quad 0 \le \theta \le \pi, \; 0 \le \varphi \le \pi, \tag{12}$$

This unit vector ($\boldsymbol{a}$) is required to determine Young's modulus, linear compressibility (β) and Bulk modulus (B). But some elastic properties such as shear modulus (G) and Poisson's ratio (ν) require another, perpendicular, direction. Therefore, we define unit vector $\boldsymbol{b}$, which is perpendicular to $\boldsymbol{a}$ (see Fig. 1), as follows [3, 4]:

$$\boldsymbol{b} \equiv \begin{pmatrix} \cos(\theta)\cos(\varphi)\cos(\gamma) - \sin(\theta)\sin(\gamma) \\ \cos(\theta)\sin(\varphi)\cos(\gamma) - \cos(\theta)\sin(\gamma) \\ -\sin(\theta)\cos(\gamma) \end{pmatrix}, \; 0 \le \gamma \le 2\pi.0 \tag{13}$$

Therefore, by defining these two vectors, Eq.(11) is as follows:

$$T'_{\alpha\beta\gamma\delta} = a_{\alpha i}\, a_{\beta j}\, b_{\gamma k}\, b_{\delta l}\, T_{ijkl}, \tag{14}$$

Using this equation, we can calculate the representation surfaces for elastic properties. For instance, from Eq.(10), we know that Young's modulus can be obtained by using purely normal stress (see Fig. **??**(c)),

$$\begin{aligned} E(\mathbf{a}) \equiv \tfrac{1}{S'_{1111}} &= \textstyle\sum_{ijkl}^{6} \tfrac{1}{a_{1i}a_{1j}a_{1k}a_{1l}S_{ijkl}} \\ &= \tfrac{1}{S'_{11}} = \tfrac{1}{a_i a_j a_k a_l S_{ijkl}} \ \ (\mathrm{by\,Einstein's\,summation\,rule}), \end{aligned} \tag{15}$$

The volume compressibility of a crystal is the proportional decrease in volume of a crystal when subjected to unit hydrostatic pressure, but the linear compressibility is the relative decrease in length of a line when the crystal is subjected to unit hydrostatic pressure (HP). Hence, it is obtained by applying isotropic stress (P$_{HP}$) in tensor form, so that ε_{ij}=-(P$_{HP}$)S_{ijkk} [3, 11], and by considering that the extension in a direction is $\varepsilon_{ij}a_i a_j$, and for this reason,

$$\beta(\boldsymbol{a}) = a_i a_j a_k a_k S_{ijkk} = a_i a_j S_{ijkk}; \ \ a_k.\, a_k = 1 \tag{16}$$

On the other hand, the relationship between β and B can be expressed as follows [11],

$$B(\boldsymbol{a}) = \frac{1}{\beta(\mathbf{a})} = \frac{1}{a_i a_j S_{ijkk}} \tag{17}$$

As mentioned, the G and ν are not as straightforward to represent and depends on two directions ($\boldsymbol{a}$ and $\boldsymbol{b}$). The shear ratio (Poisson's ratio) is obtained by applying a pure shear (Fig. **??**(d)) (a purely normal) stress in the vector form of Eq.(3), and results in

$$G(\boldsymbol{a}, \boldsymbol{b}) = \frac{1}{4S_{1212}} = \frac{1}{4S_{66}} = \frac{1}{4}\frac{1}{a_i b_j a_k b_l S_{ijkl}}, \tag{18}$$

$$\nu(\boldsymbol{a}, \boldsymbol{b}) = -\frac{S'_{1212}}{S'_{1111}} = -\frac{S'_{12}}{S'_{11}} = -\frac{a_i a_j b_k b_l S_{ijkl}}{a_i a_j a_k a_l S_{ijkl}}. \tag{19}$$

To better understand these equations, we obtain Young's modulus of a cubic crystal. As for cubic crystal, because of lattice symmetry, there are three independent variables C_{11}, C_{12}, C_{44} in C_{ij}, and S_{11}, $S_{12,}$ and S_{33} in S_{ij}. Using Eq.(15) and Eq.(12), we have,

$$\begin{aligned} S'_{1111} = {} & a_{11}a_{11}a_{11}a_{11}S_{1111} + a_{12}a_{12}a_{12}a_{12}S_{2222} + a_{13}a_{13}a_{13}a_{13}S_{3333} + \\ & a_{11}a_{11}a_{12}a_{12}S_{1122} + a_{11}a_{11}a_{13}a_{13}S_{1133} + a_{12}a_{12}a_{13}a_{13}S_{2233} + \\ & a_{11}a_{11}a_{12}a_{12}S_{2211} + a_{11}a_{11}a_{13}a_{13}S_{3311} + a_{12}a_{12}a_{13}a_{13}S_{3322} + \\ & \tfrac{1}{4}[a_{12}a_{13}a_{12}a_{13}S_{2323}] + \tfrac{1}{4}[a_{13}a_{11}a_{13}a_{11}S_{3131}] + \tfrac{1}{4}[a_{11}a_{12}a_{11}a_{12}S_{1212}] \\ = {} & S_{11}(a_{11}^4 + a_{12}^4 + a_{13}^4) + (\tfrac{1}{4}S_{44} + 2S_{12})[a_{12}^2 a_{13}^2 + a_{11}^2 a_{13}^2 + a_{11}^2 a_{12}^2], \end{aligned} \tag{20}$$

with a little simplification,

$$\frac{1}{E} = S'_{1111} = S_{11} - 2(S_{11} - S_{12} - \frac{1}{2}S_{44})(a_{11}^2 a_{12}^2 + a_{11}^2 a_{13}^2 + a_{12}^2 a_{13}^2) \tag{21}$$

To calculate the orientation-dependent Poisson's ratio, shear modulus and Young's modulus in 2D material, Eq.(12) and Eq.(13) are used again and changed as follows:

$$\mathbf{a} = \begin{pmatrix} \cos(\varphi) \\ \sin(\varphi) \\ 0 \end{pmatrix}; \ \mathbf{b} = \begin{pmatrix} -\sin(\varphi) \\ \cos(\varphi) \\ 0 \end{pmatrix}; \quad 0 \le \varphi \le 2\pi. \tag{22}$$

For 2D system, according to Hooke's law (Eq.(3) and Eq.(4)), the relationship between σ and the corresponding strain tensor ε can be described as the stiffness tensor C_{ij}, for orthogonal symmetry under plane stress conditions is [12],

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \end{pmatrix}, \tag{23}$$

where Voigt notation has been used for C_{ij}. Here C_{11} (S_{11}), C_{22} (S_{22}), C_{12}=C_{21} (S_{12}=S_{21}), and C_{66} (S_{66}) represent C_{1111} (S_{1111}), C_{2222} (S_{2222}), C_{1122} (S_{1122}), and C_{1212} (S_{1212}), respectively. So, using the previous equations, the in-plane Young's modulus, shear modulus, and Poisson's ratio, defined as:

$$E(\varphi) = \frac{1}{S_{11}\cos^4(\varphi) + S_{22}\sin^4(\varphi) + (2S_{12} + S_{66})\cos^2(\varphi)\sin^2(\varphi)} \tag{24}$$

$$\nu(\varphi) = -\frac{[S_{22} - S_{33} + S_{22}]\cos^2(\varphi)\sin^2(\varphi) + S_{12}\cos^4(\varphi) + S_{12}\sin^4(\varphi)}{[2S_{12} + S_{66}]\cos^2(\varphi)\sin^2(\varphi) + S_{11}\cos^4(\varphi) + S_{22}\sin^4(\varphi)} \tag{25}$$

$$\frac{1}{G(\varphi)} = [S_{11} + S_{22} - S_{12}]\cos^2(\varphi)\sin^2(\varphi) + \frac{1}{4}S_{66}[\cos^4(\varphi) + \sin^4(\varphi) - 2\sin^2(\varphi)\cos^2(\varphi)] \tag{26}$$

2.3 Basic proprieties and averaging schemes

From elastic constants, other basic elastic properties, including elastic moduli, can be obtained. The elastic response of an isotropic system is generally described by the B and the G, which may be obtained by averaging the single-crystal elastic constants. The averaging methods most usually used are the Voigt [13], Reuss [14] and Hill [7] bounds. In Voigt's and, Reuss's approximations, the equation takes the following form:

$$\begin{aligned} B_V &= \tfrac{1}{9}([C_{11} + C_{22} + C_{33}] + 2[C_{12} + C_{23} + C_{31}]), \\ G_V &= \tfrac{1}{15}([C_{11} + C_{22} + C_{33}] - [C_{12} + C_{23} + C_{31}] + 4[C_{44} + C_{55} + C_{66}]), \\ B_R &= \tfrac{1}{9}([S_{11} + S_{22} + S_{33}] + 2[S_{12} + S_{23} + S_{31}]), \\ G_R &= \tfrac{1}{15}([S_{11} + S_{22} + S_{33}] - 4[S_{12} + S_{23} + S_{31}] + 3[S_{44} + S_{55} + S_{66}]). \end{aligned} \tag{27}$$

Also, the arithmetic mean of the Voigt and Reuss bounds, termed the Voigt-Reuss-Hill (VRH) average is also found as a better approximation to the actual elastic behavior of a polycrystal material,

$$\begin{aligned} B_{VRH} &= \tfrac{1}{2}(B_V + B_R), \\ G_{VRH} &= \tfrac{1}{2}(G_V + G_R) \end{aligned} \tag{28}$$

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

$$E = \frac{9BG}{3B+G}, \quad \nu = \frac{3B-2G}{2(3B+G)}. \tag{29}$$

The elastic anisotropy is a crucial measurement of anisotropy of chemical bonding, and can be calculated by elastic constants. For all crystal systems, the bulk response is in general anisotropic, and one must account for such contributions to quantify the extent of anisotropy accurately. For this purpose, Ranganathan *et al.* [5] introduce a new universal anisotropy index (A^U),

$$A^U = 5\frac{G_V}{G_R} + \frac{B_V}{B_R} - 6. \tag{30}$$

It is noteworthy that in weakly anisotropic materials, *i.e.,* isotropic material, all these averages lead to similar results for elastic moduli. The mechanical behavior such as ductile or brittle can be represented by the ratio of the G to the B, *i.e.,* the Pugh ratio G/B, by simply considering B as the resistance to fracture and G as the resistance to plastic deformation. The critical value of Pugh ratio to separate *ductile* and *brittle* materials is around 0.57. If $G/B < 0.57$, the material is more *ductile*; otherwise the material behaves in a *brittle* manner [1, 15]. So, the higher the Pugh ratio indicates the more brittleness of the material. Cauchy pressure (P_c) is another characteristic to describe the brittleness and ductility of the metals and compounds as defined [16],

$$P_c = C_{12} - C_{44} \tag{31}$$

For covalent materials with brittle atomic bonds, the P_c is negative, because in this case, material resistance to shear strain, *i.e.*, C_{44}, is much more than that for volume change, *i.e.*, C_{12}. However, the P_c must be positive if the metallic-like bonding, where the electrons are almost delocalized. For an isotropic crystal, A^U is zero. The departure of A^U from zero defines the extent of elastic anisotropy.

In this work, the relation between the E, G, ν, and elastic stiffness constants for a 2D system can be derived,

$$\begin{aligned} E_x &= \tfrac{C_{11}C_{22}-C_{12}C_{21}}{C_{22}}, \\ E_y &= \tfrac{C_{11}C_{22}-C_{12}C_{21}}{C_{11}}, \\ \nu_{xy} &= \tfrac{C_{21}}{C_{22}}, \\ \nu_{yx} &= \tfrac{C_{12}}{C_{11}}, \\ G_{xy} &= C_{66}, \end{aligned} \tag{32}$$

where E_l= σ_l/ε_l is the Young's modulus along the axis of l, v_{lk} =-$d\varepsilon_k/d\varepsilon_l$ is the Poisson's ratio with tensile strain applied in the direction l and the response strain in the direction k, and G_{xy} is the shear modulus in the xy-plane.

3

SECTION

Workflow of AAEP

For this section, please refer to our paper.

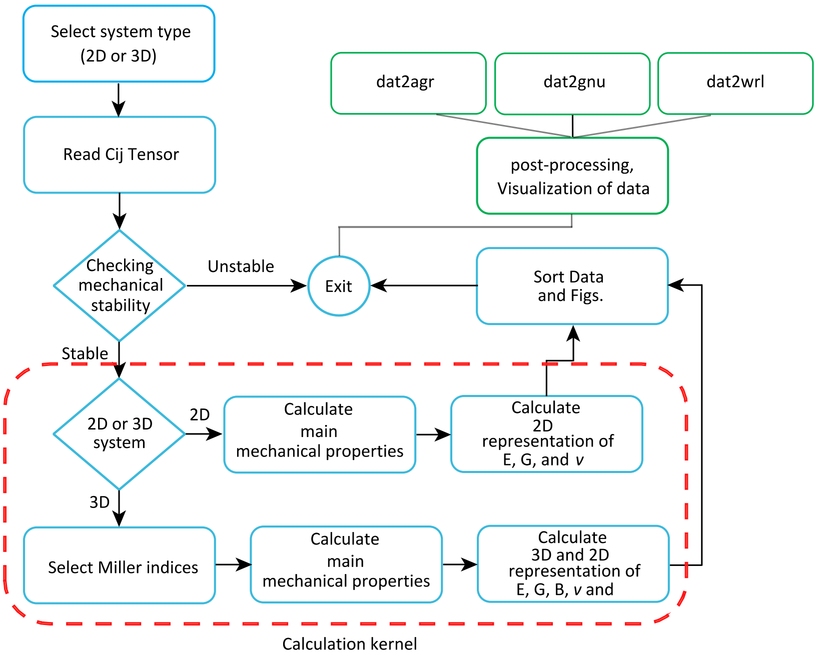

Select system type (2D or 3D)
Read Cij Tensor
Checking mechanical stability
Unstable
Exit
Stable
dat2agr
dat2gnu
dat2wrl
post-processing, Visualization of data
Sort Data and Figs.
2D or 3D system
2D
Calculate main mechanical properties
Calculate 2D representation of E, G, and v
3D
Select Miller indices
Calculate main mechanical properties
Calculate 3D and 2D representation of E, G, B, v and
Calculation kernel

Figure 2: The flowchart of AAEP. The red dashed line represents the Calculation Kernel (CK) block.

4

SECTION

Getting started

4.1 How to obtain AAEP

AAEP is an open source code with MIT license and can be downloaded by sending an email to yalameha93@gmail.com [Shahram Yalameha]

4.2 How to install AELAS

AAEP is written in Fortran90 and is installed with Intel Fortran (ifort) or gnu fortran (gfortran) compiler. But before the installation of AAEP, the necessary libraries and packages should be installed first: GNUPLOT, LAPACK, and LaTeX libraries. LAPACK libraries are for numerical calculations and are used to calculate elastic compliance constant and so on. LaTeX and GNUPLOT are used to plot temporary figures and the post-processing stages. One of the packages IRelast, Elast, AELAS, and ElaStic can calculate the elastic stiffness constant (C_{ij}). AAEP supports the output of these packages.
AAEP is distributed in a compressed tar file aaep_1.**.tar.gz, which uncompresses into several directories: soc, doc, db, and bin. The soc directory contains the f90 files and Makefile. For the compilation, you need to modify Makefile for your system. The doc directory contains a copy of this paper, short userguide, and the examples directory. The db directory contains the elastic constant database file. The path of these files must be specified before installation. For this purpose, you can use run_path.sh script to path these files. This script is located in the soc directory and runs as follows:

```
chmod +x run_path.sh ; ./run_path.sh
```

Then you need the complete path (example: /home/.../soc/db/) of the elastic constant database files (Cijs.binery and All_2ID_cop.csv) in the db directory, which is different for the user system.

After installation, which is done with make command, the executable files (AAEP, dat2gnu, dat2agr, and dat2wrl) are saved in bin directory. Finally, the code will run by executing AAEP. You can put this path to the system PATH with

```
export PATH=/home/.../aaep_1.**/bin:$PATH
```

to the .bashrc file in your home directory.

4.3 How to use AAEP

You must prepare one of the following files for C_{ij} tensor:

INVELC-matrix: output file of IRelast

elast.output: output file of Elast

ELADAT: output file of AELAS

ElaStic_2nd.out: output file of ElaStic

Cij.dat (3D system) or Cij-2D.dat (2D system) file for any other outputs.

After the preparation of these files, you can just run AAEP.

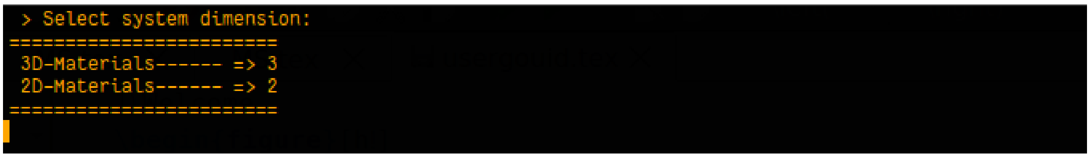
4.4 Run AAEP and Results data

After running AAEP, you must follow the steps below:

1) Welcome

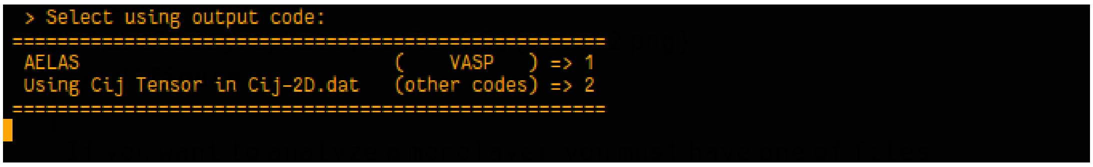
```
===========================================
 Analysis Anisotropic Elastic Properties
 -        -          -          -

              41 41 45 50
======= Shahram Yalameha (c) 2018 ========
                v1.5.0
                 From
          ElasticTools Project
```

2) Select 2D or 3D crystal system :



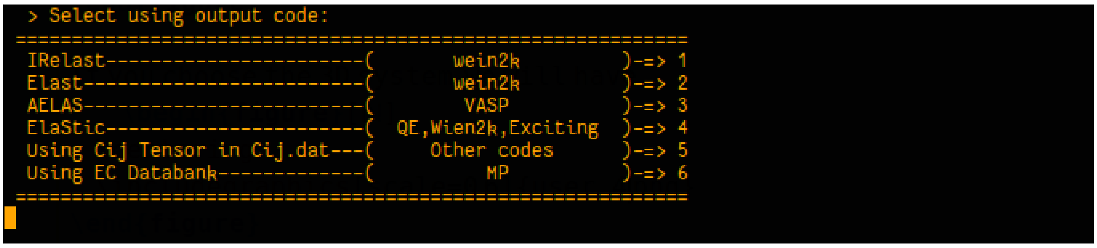
```
 > Select system dimension:
========================
 3D-Materials------ => 3
 2D-Materials------ => 2
========================
```

If you want to analyze a monolayer, you must have one of files ELADAT or Cij-2D.dat in the executable directory.



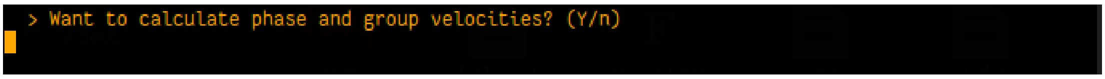
```
 > Select using output code:
=====================================================
 AELAS                           (    VASP   ) => 1
 Using Cij Tensor in Cij-2D.dat  (other codes) => 2
=====================================================
```

If you choose the 3D system, we will have



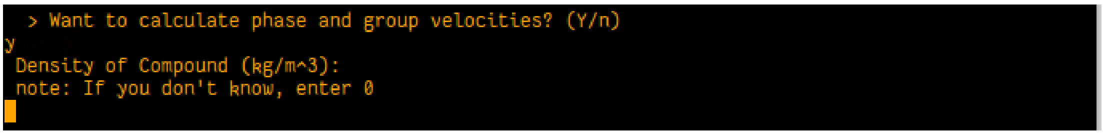
```
 > Select using output code:
============================================================
 IRelast-----------------------(       wein2k         )-=> 1
 Elast-------------------------(       wein2k         )-=> 2
 AELAS-------------------------(        VASP          )-=> 3
 ElaStic-----------------------(  QE,Wien2k,Exciting  )-=> 4
 Using Cij Tensor in Cij.dat---(     Other codes      )-=> 5
 Using EC Databank-------------(         MP           )-=> 6
============================================================
```

4) Calculate phase and group velocities.



```
 > Want to calculate phase and group velocities? (Y/n)
```

This option has been entered in the code since version 1.5.0. If you select this option we will have:

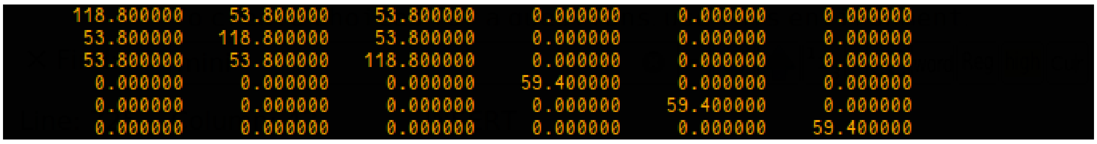


```
  > Want to calculate phase and group velocities? (Y/n)
y
 Density of Compound (kg/m^3):
 note: If you don't know, enter 0
```

You need to know or calculate the density of compound. If you know the density of the compound, enter its value, otherwise enter the number 0. If you enter the value 0, the program calculates the density of the composition by taking the crystal lattice parameters from you.

4.4.1 Calculation Kernel (CK)

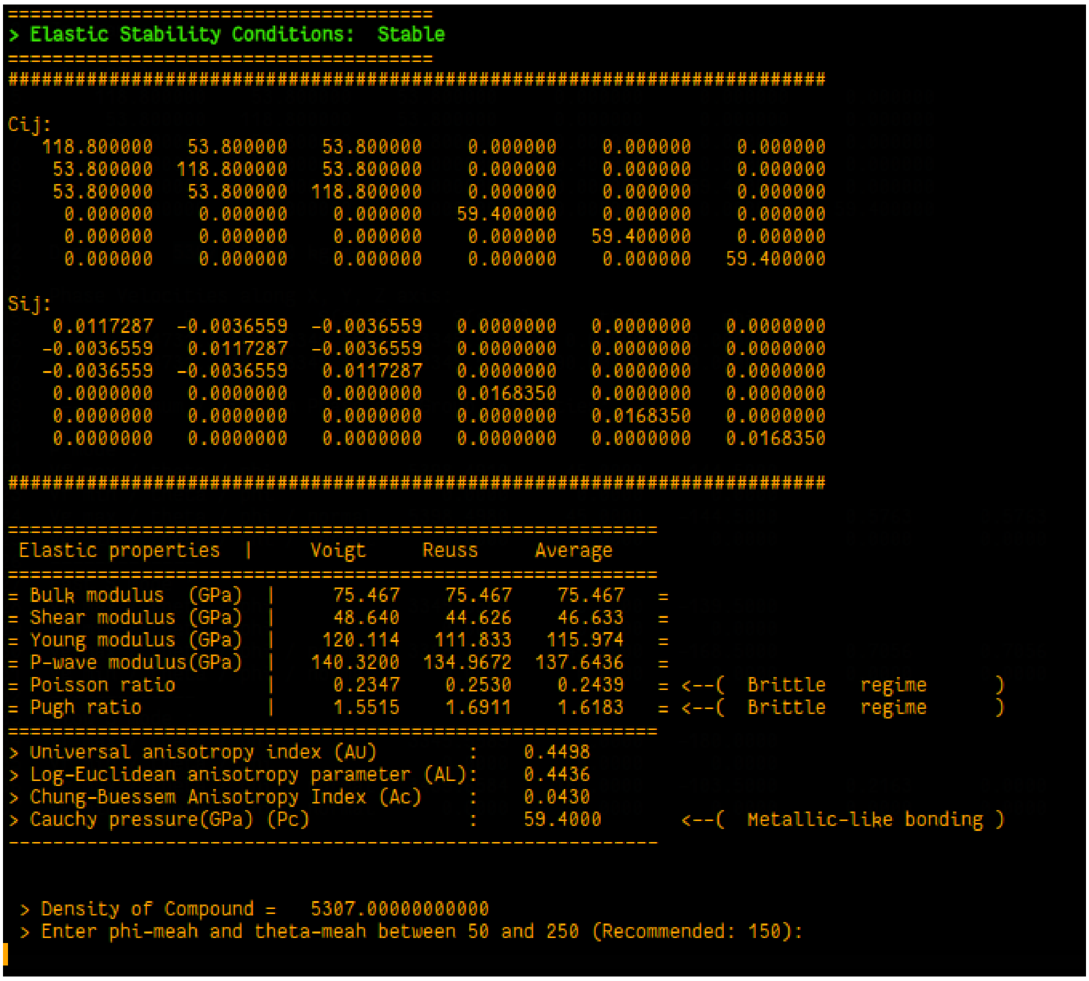
To explain this section, we analyze the GaAs Cubic compound. Cij tensor of this compound (in Cij.dat file) is equal to:



```
  118.800000    53.800000    53.800000     0.000000     0.000000     0.000000
   53.800000   118.800000    53.800000     0.000000     0.000000     0.000000
   53.800000    53.800000   118.800000     0.000000     0.000000     0.000000
    0.000000     0.000000     0.000000    59.400000     0.000000     0.000000
    0.000000     0.000000     0.000000     0.000000    59.400000     0.000000
    0.000000     0.000000     0.000000     0.000000     0.000000    59.400000
```

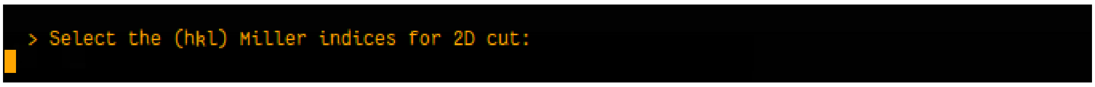
Also, the density of this compound is 5307 kg/m^3.

Before entering step CK, AAEP examines the mechanical stability condition. As can be seen, it is marked in green color. It then calculates and displays the S_{ij}, calculating the main properties.



```
======================================
> Elastic Stability Conditions:  Stable
======================================
#########################################################################

Cij:
   118.800000   53.800000   53.800000    0.000000    0.000000    0.000000
    53.800000  118.800000   53.800000    0.000000    0.000000    0.000000
    53.800000   53.800000  118.800000    0.000000    0.000000    0.000000
     0.000000    0.000000    0.000000   59.400000    0.000000    0.000000
     0.000000    0.000000    0.000000    0.000000   59.400000    0.000000
     0.000000    0.000000    0.000000    0.000000    0.000000   59.400000

Sij:
    0.0117287  -0.0036559  -0.0036559   0.0000000   0.0000000   0.0000000
   -0.0036559   0.0117287  -0.0036559   0.0000000   0.0000000   0.0000000
   -0.0036559  -0.0036559   0.0117287   0.0000000   0.0000000   0.0000000
    0.0000000   0.0000000   0.0000000   0.0168350   0.0000000   0.0000000
    0.0000000   0.0000000   0.0000000   0.0000000   0.0168350   0.0000000
    0.0000000   0.0000000   0.0000000   0.0000000   0.0000000   0.0168350

#########################################################################

==========================================================
 Elastic properties  |     Voigt     Reuss     Average
==========================================================
= Bulk modulus  (GPa)  |     75.467    75.467    75.467   =
= Shear modulus (GPa)  |     48.640    44.626    46.633   =
= Young modulus (GPa)  |    120.114   111.833   115.974   =
= P-wave modulus(GPa)  |   140.3200  134.9672  137.6436   =
= Poisson ratio        |     0.2347    0.2530    0.2439   = <--(  Brittle   regime      )
= Pugh ratio           |     1.5515    1.6911    1.6183   = <--(  Brittle   regime      )
==========================================================
> Universal anisotropy index (AU)         :    0.4498
> Log-Euclidean anisotropy parameter (AL):    0.4436
> Chung-Buessem Anisotropy Index (Ac)     :    0.0430
> Cauchy pressure(GPa) (Pc)               :    59.4000      <--(  Metallic-like bonding )
----------------------------------------------------------


 > Density of Compound =    5307.00000000000
 > Enter phi-meah and theta-meah between 50 and 250 (Recommended: 150):
```

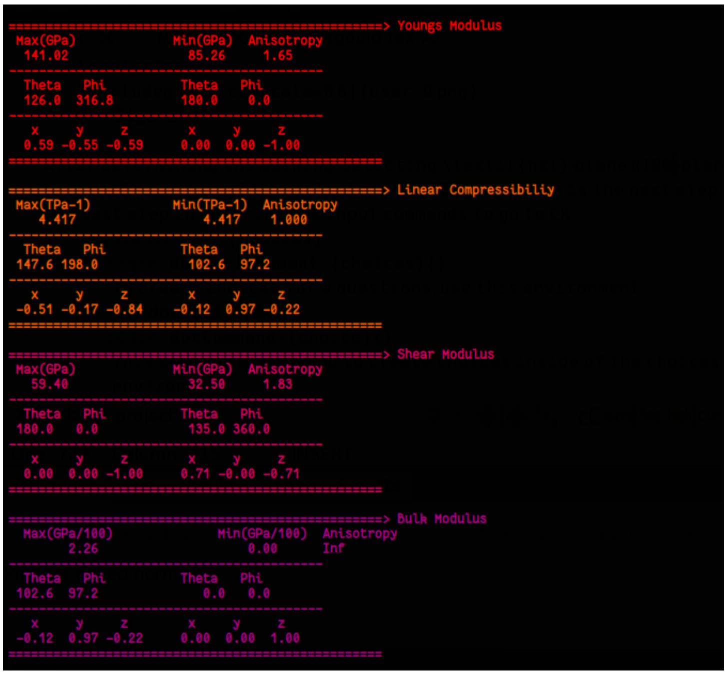
After this process, you need to specify the meshes of ϕ and θ angles. We recommend **150** for both angles.



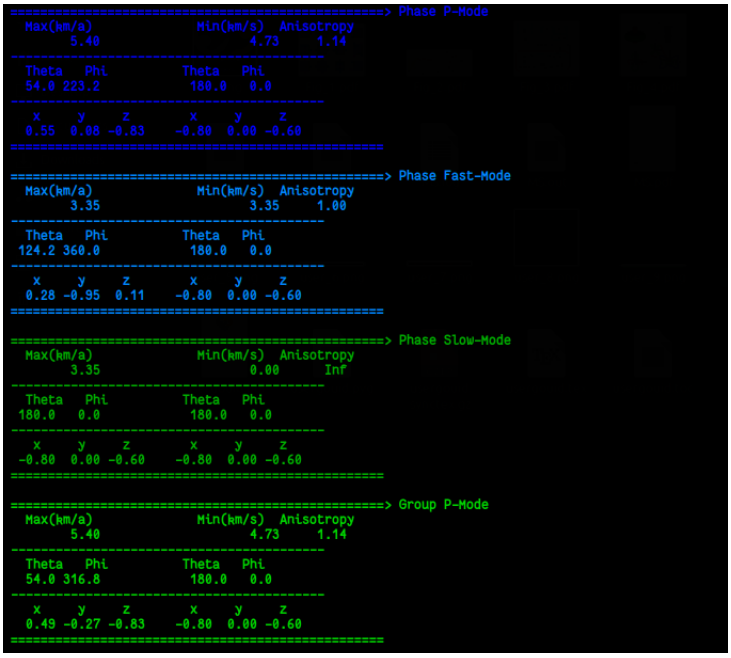
```
 > Select the (hkl) Miller indices for 2D cut:
```

After determining the meshing, selecting *hkl*-plane ((100)-plane was selected as an example) to calculate the 2D projection is the next step. This is the last step in entering the input commands to go to CK.

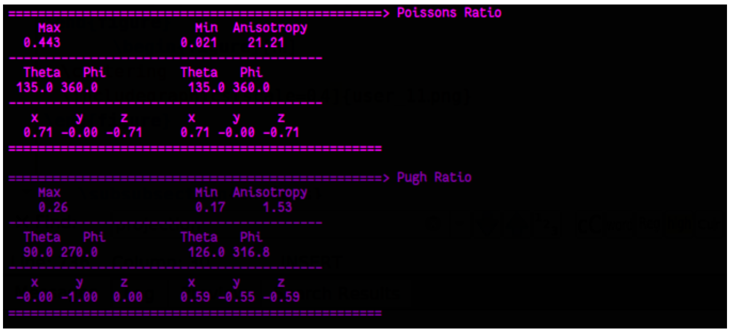
At the end of CK step, the minimum and maximum value of properties and their coordinates and anisotropic index (A_M) are calculated and displayed. These results are also stored in DATA.dat file.



```
==================================================> Youngs Modulus
 Max(GPa)             Min(GPa)  Anisotropy
  141.02                85.26     1.65
------------------------------------------
  Theta   Phi          Theta   Phi
  126.0  316.8         180.0    0.0
------------------------------------------
   x     y     z        x     y     z
  0.59 -0.55 -0.59     0.00  0.00 -1.00
==================================================

==================================================> Linear Compressibiliy
 Max(TPa-1)           Min(TPa-1)  Anisotropy
    4.417                 4.417    1.000
------------------------------------------
  Theta   Phi          Theta   Phi
 147.6 198.0            102.6  97.2
------------------------------------------
   x     y     z        x     y     z
 -0.51 -0.17 -0.84    -0.12  0.97 -0.22
==================================================

==================================================> Shear Modulus
 Max(GPa)             Min(GPa)  Anisotropy
   59.40                32.50     1.83
------------------------------------------
  Theta   Phi          Theta   Phi
 180.0   0.0            135.0 360.0
------------------------------------------
   x     y     z        x     y     z
  0.00  0.00 -1.00     0.71 -0.00 -0.71
==================================================

==================================================> Bulk Modulus
  Max(GPa/100)              Min(GPa/100)  Anisotropy
        2.26                    0.00      Inf
------------------------------------------
  Theta   Phi          Theta   Phi
 102.6  97.2              0.0   0.0
------------------------------------------
   x     y     z        x     y     z
 -0.12  0.97 -0.22     0.00  0.00  1.00
==================================================
```



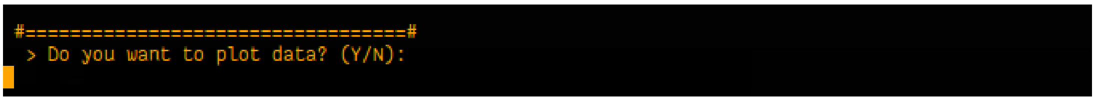
```
==================================================> Phase P-Mode
  Max(km/a)              Min(km/s)  Anisotropy
        5.40                    4.73     1.14
------------------------------------------
  Theta   Phi          Theta   Phi
  54.0 223.2            180.0   0.0
------------------------------------------
   x     y     z        x     y     z
  0.55  0.08 -0.83    -0.80  0.00 -0.60
==================================================

==================================================> Phase Fast-Mode
  Max(km/a)              Min(km/s)  Anisotropy
        3.35                    3.35     1.00
------------------------------------------
  Theta   Phi          Theta   Phi
 124.2 360.0            180.0   0.0
------------------------------------------
   x     y     z        x     y     z
  0.28 -0.95  0.11    -0.80  0.00 -0.60
==================================================

==================================================> Phase Slow-Mode
  Max(km/a)              Min(km/s)  Anisotropy
        3.35                    0.00      Inf
------------------------------------------
  Theta   Phi          Theta   Phi
 180.0   0.0            180.0   0.0
------------------------------------------
   x     y     z        x     y     z
 -0.80  0.00 -0.60    -0.80  0.00 -0.60
==================================================

==================================================> Group P-Mode
  Max(km/a)              Min(km/s)  Anisotropy
        5.40                    4.73     1.14
------------------------------------------
  Theta   Phi          Theta   Phi
  54.0 316.8            180.0   0.0
------------------------------------------
   x     y     z        x     y     z
  0.49 -0.27 -0.83    -0.80  0.00 -0.60
==================================================
```



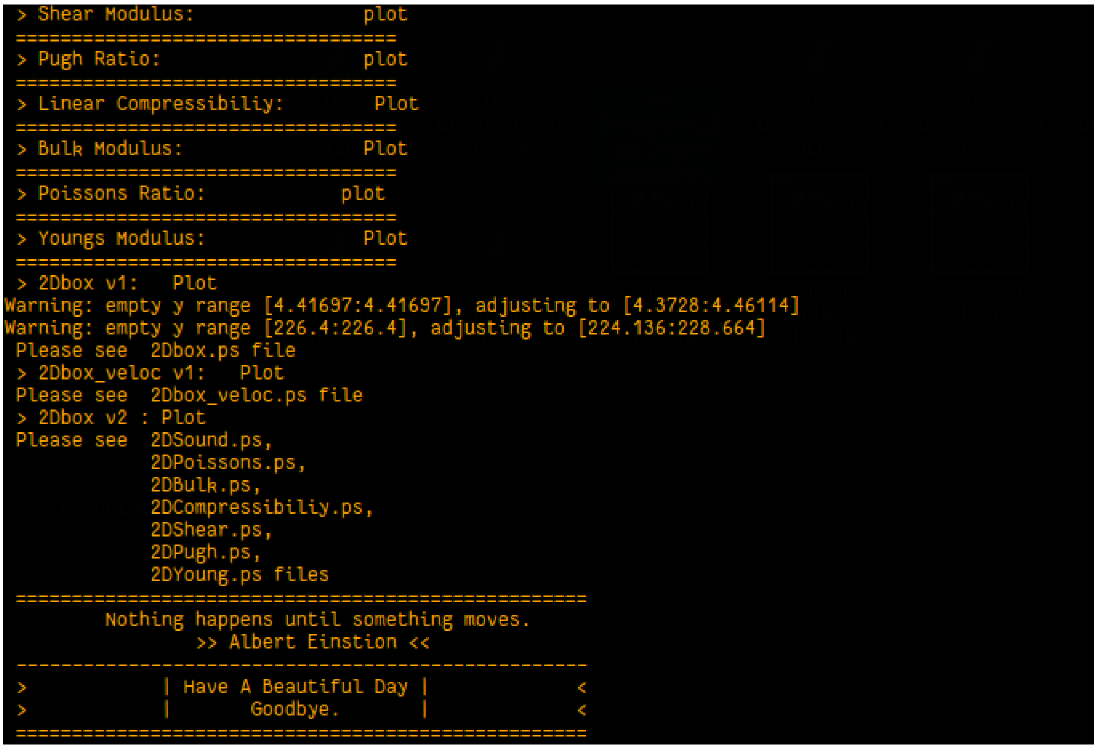
```
==================================================> Poissons Ratio
    Max                  Min  Anisotropy
  0.443                0.021    21.21
------------------------------------------
  Theta   Phi          Theta   Phi
 135.0 360.0            135.0 360.0
------------------------------------------
   x     y     z        x     y     z
  0.71 -0.00 -0.71     0.71 -0.00 -0.71
==================================================

==================================================> Pugh Ratio
    Max                  Min  Anisotropy
    0.26                 0.17     1.53
------------------------------------------
  Theta   Phi          Theta   Phi
  90.0 270.0            126.0 316.8
------------------------------------------
   x     y     z        x     y     z
 -0.00 -1.00  0.00     0.59 -0.55 -0.59
==================================================
```

4.4.2 Temporary images

After passing CK step, you will be asked to plot temporary images.



```
 #==================================#
  > Do you want to plot data? (Y/N):
```



```
 > Shear Modulus:               plot
 ==================================
 > Pugh Ratio:                  plot
 ==================================
 > Linear Compressibiliy:        Plot
 ==================================
 > Bulk Modulus:                Plot
 ==================================
 > Poissons Ratio:            plot
 ==================================
 > Youngs Modulus:              Plot
 ==================================
 > 2Dbox v1:   Plot
Warning: empty y range [4.41697:4.41697], adjusting to [4.3728:4.46114]
Warning: empty y range [226.4:226.4], adjusting to [224.136:228.664]
 Please see  2Dbox.ps file
 > 2Dbox_veloc v1:   Plot
 Please see  2Dbox_veloc.ps file
 > 2Dbox v2 : Plot
 Please see  2DSound.ps,
             2DPoissons.ps,
             2DBulk.ps,
             2DCompressibiliy.ps,
             2DShear.ps,
             2DPugh.ps,
             2DYoung.ps files
 ===================================================
         Nothing happens until something moves.
                 >> Albert Einstion <<
 ---------------------------------------------------
 >             | Have A Beautiful Day |             <
 >             |       Goodbye.       |             <
 ===================================================
```

By accepting this request, temporary images are plot and stored in a folder called PicFile-hkl (here, hkl is 100). The data files for post processing step are also listed in DatFile-hkl folder, and **END**.

5

SECTION

Post processing

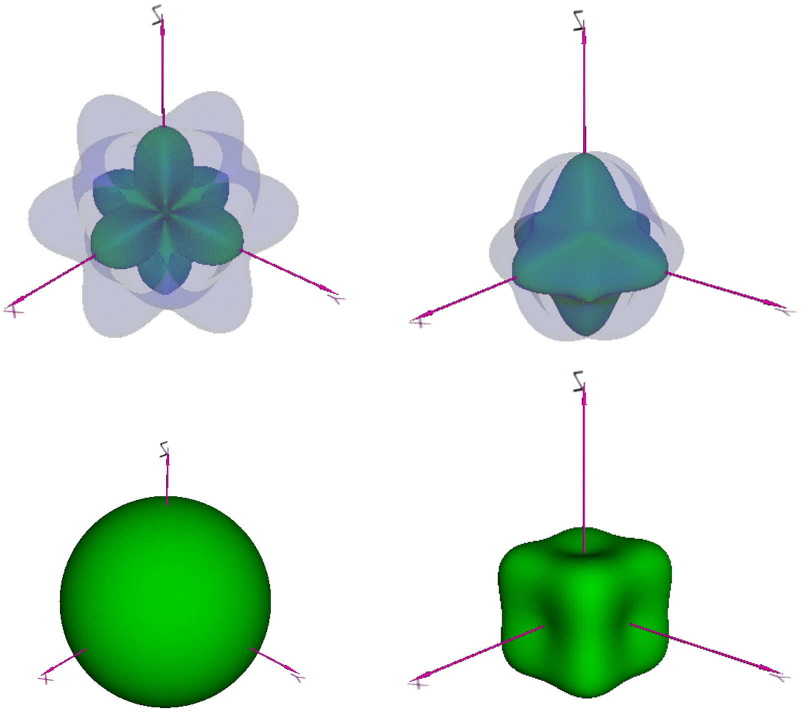
In the post-processing, three powerful program dat2gnu, dat2agr and dat2wrl are designed to visualize these results, which produce files in gpi, agr and wrl formats, respectively.

5.1 dat2wrl

dat2wrl is prepared for 3D graphical representations of elastic properties, capable of producing files in "wrl” format. This format can be visualized and explored with a VRML capable browser, such as View3dscene [8]. Input commands and output files for this program:

Input command to run	Properties	Ouput file
dat2wrl poi	Poisson's ratio	Poisson.wrl
dat2wrl shear	Shear modulus	Shear.wrl
dat2wrl young	Young's modulus	Young.wrl
dat2wrl bulk	Bulk modulus	Bulk.gpi
dat2wrl comp	Linear compressibility	Compress.wrl
dat2wrl pp	Phase velocity: P-mode	Phase-P.wrl
dat2wrl ps	Phase velocity: Slow-mode	Phase-Slow.wrl
dat2wrl pf	Phase velocity: Fast-mode	Phase-Fast.wrl
dat2wrl gp	Group velocity: P-mode	Group-P.wrl
dat2wrl gs	Group velocity: Slow-mode	Group-Slow.wrl
dat2wrl gf	Group velocity: Fast-mode	Group-Fast.wrl
dat2wrl pfp	Power Flow angle (PFA): P-mode	Power-Flow-P.wrl
dat2wrl pfs	Power Flow angle: Slow-mode	Power-Flow-Slow.wrl
dat2wrl pff	Group velocity: Fast-mode	Power-Flow-Fast.wrl

Some output files are displayed by View3dscene software:



5.2 dat2gnu

dat2gnu is responsible for generating files for 2D projections and 2D heat mapes representations of elastic properties, and generate files in "gpi" format, which can be run by

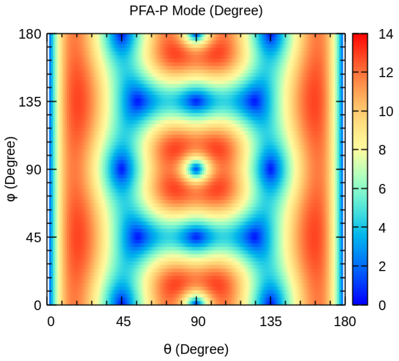
GNUPLOT program. Input commands and output files this program for 3D materials:

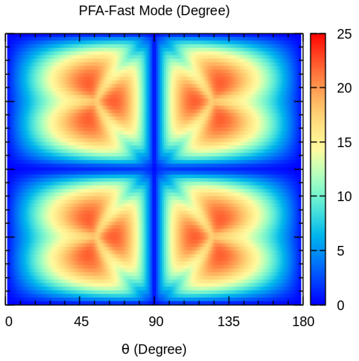
Input command to run	Properties	Ouput file
dat2gnu poi	Poisson's ratio	poissons.gpi
dat2gnu shear	Shear modulus	shear.gpi
dat2gnu young	Young's modulus	young.gpi
dat2gnu bulk	Bulk modulus	bulk.gpi
dat2gnu comp	Linear compressibility	compressibiliy.gpi
dat2gnu pp	Phase velocity: P-mode	phase-p.gpi
dat2gnu ps	Phase velocity: Slow-mode	phase-slow.gpi
dat2gnu pf	Phase velocity: Fast-mode	phase-fast.gpi
dat2gnu gp	Group velocity: P-mode	group-p.gpi
dat2gnu gs	Group velocity: Slow-mode	group-p.gpi
dat2gnu gf	Group velocity: Fast-mode	grouphase-p.gpi
dat2gnu pall	Phase and PFA: all-mode	phase.gpi
dat2gnu gall	Group and PFA all-mode	group.gpi
dat2gnu hmpoi	2D heat mape of Poisson's ratio	poissons_smap.gpi
dat2gnu hmcomp	2D heat mape of Linear compressibility	compressibiliy_smap.gpi
dat2gnu hmshear	2D heat mape of Shear modulus	shear_smap.gpi
dat2gnu hmbulk	2D heat mape of Bulk modulus	bulk_smap.gpi
dat2gnu hmyoung	2D heat mape of Young's modulus	young_smap.gpi
dat2gnu hmpall	2D heat mape of Phase velocity: all-mode	phase_smap.gpi
dat2gnu hmgall	2D heat mape of Group velocity: all-mode	group_smap.gpi
dat2gnu hmpfall	2D heat mape of PFA: all-mode	powerflow_smap.gpi

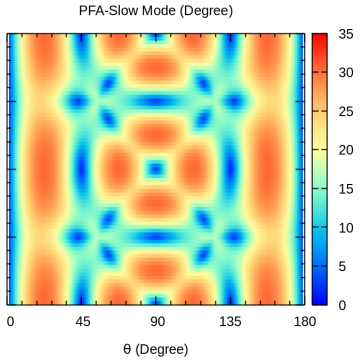
Input commands and output files this program for 2D materials:

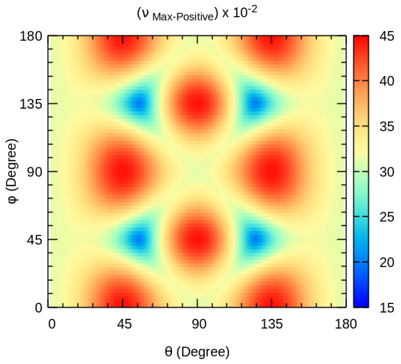
Input command to run	Properties	Ouput file
dat2gnu 2dpoi	Poisson's ratio	2Dpoissons.gpi
dat2gnu 2dyoung	Young's modulus	2Dyoung.gpi
dat2gnu 2dshear	Shear modulus	2Dshear.gpi
dat2gnu 2d	Generate all propreites	2Dshear/2Dyoung/2Dpoissons.gpi

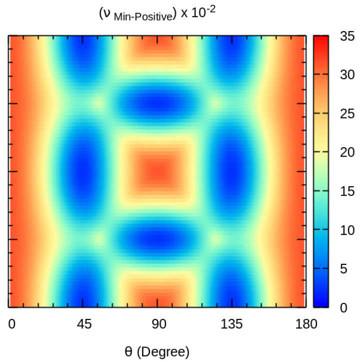
Some output files are displayed by GNUPLOT software:

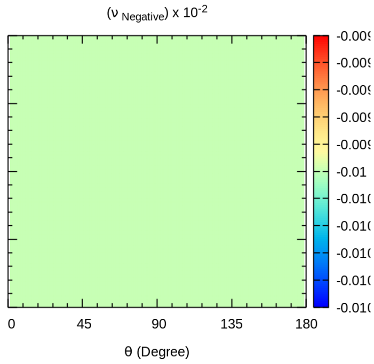


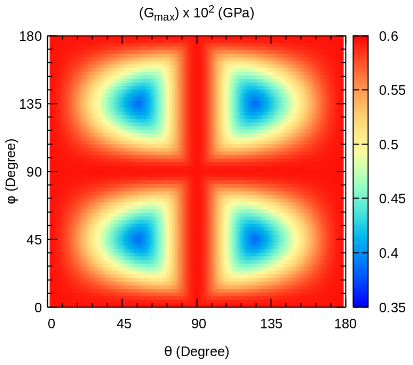


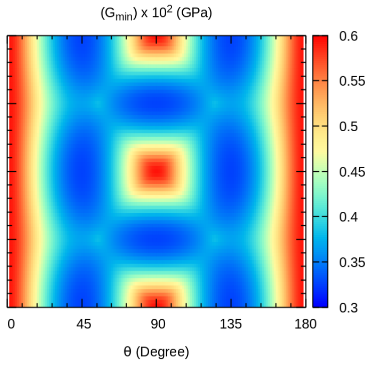


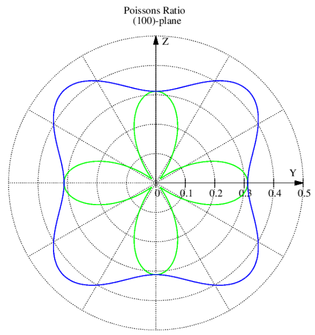


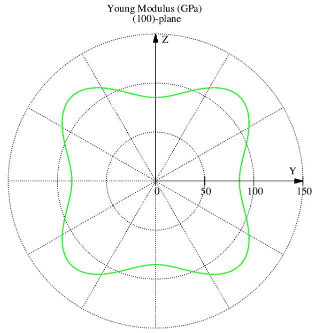










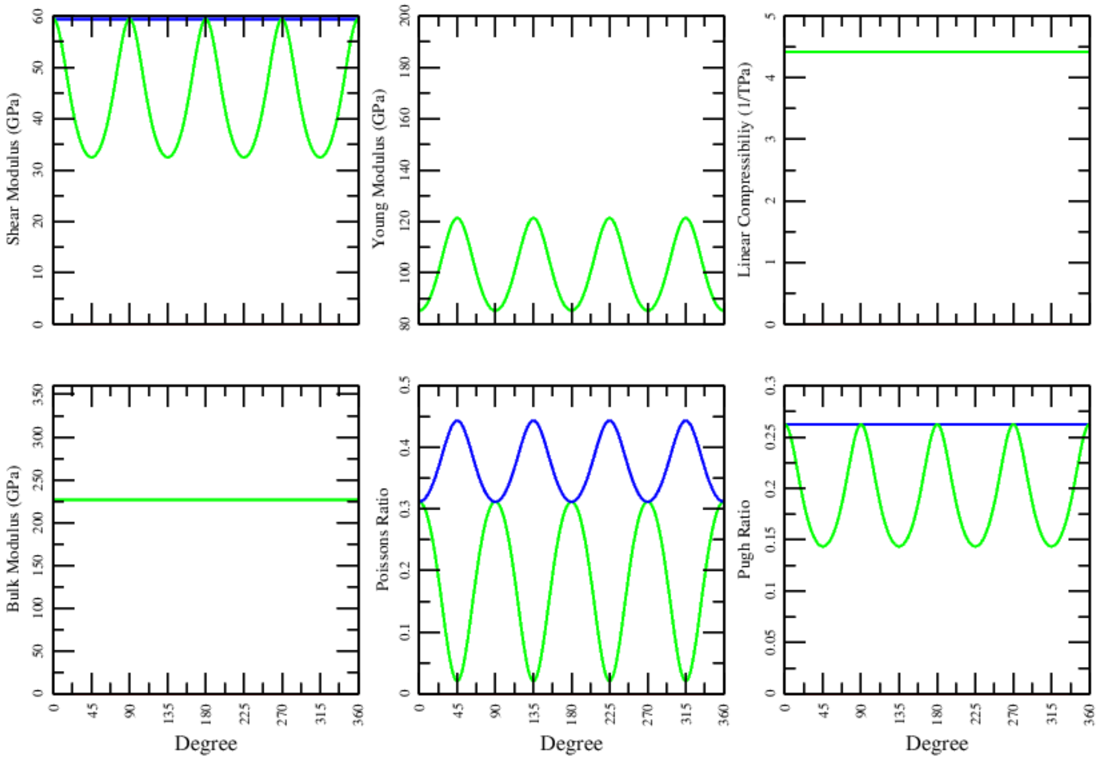


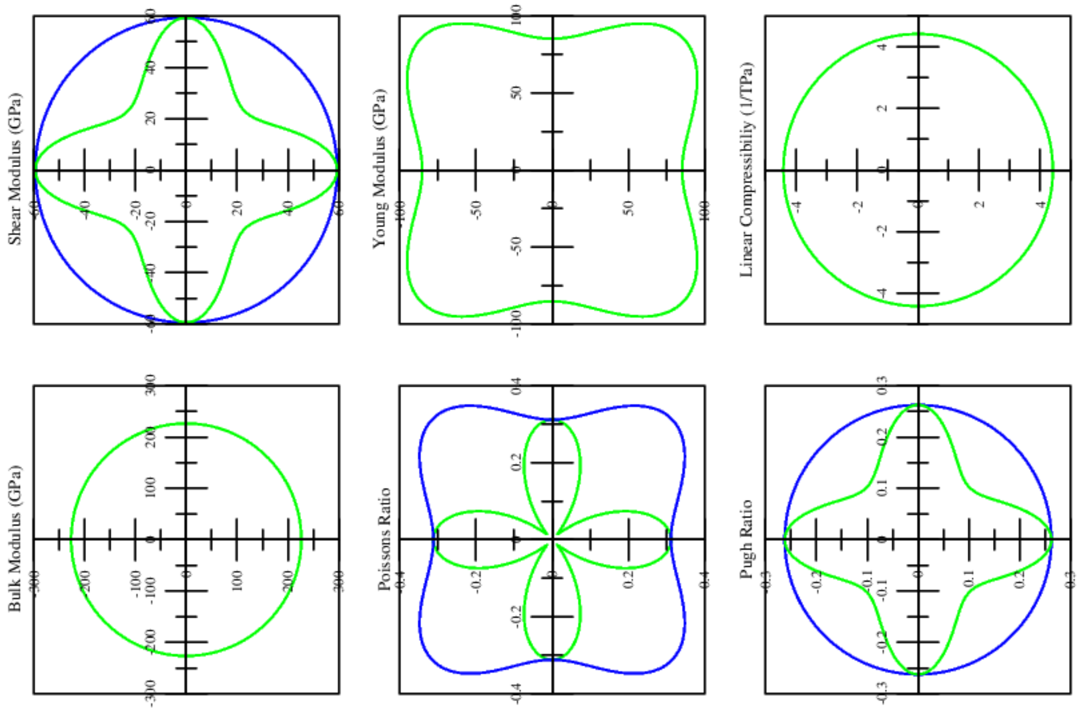
5.3 dat2agr

dat2agr is responsible for generating files for 2D projections representations of elastic properties, and generate files in "agr” format, which can be run by XMGRACE program. Input commands and output files this program for 3D materials:

Input command to run	Properties	Ouput file
dat2agr box	All elastic properties in Cartesian coordinates	2Dbox.agr
dat2agr polar	All elastic properties in polar coordinates	2Dpolar.agr

Two output files are displayed by XMGRACE software:





5

SECTION

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