ElAM: A computer program for the analysis and representation of anisotropic elastic properties

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The continuum theory of elasticity has been used for more than a century and has applications in many fields of science and engineering. It is very robust, well understood and mathematically elegant. In the isotropic case elastic properties are obviously easily represented. However, for non-isotropic materials, even in the simple cubic symmetry, it can be difficult to visualise how, for instance, the Young's modulus or Poisson's ration vary with stress/strains orientation. The ElAM code carries out the required tensorial operations (inversion, rotation, diagonalisation) and creates 3D models of an elastic property's anisotropy. It can also produces 2D cuts in any given plane, compute averages following diverse schemes and query a database of elastic constants.

INTRODUCTION

In materials science, engineering or physics, the theory of elasticity is your typical undergraduate fare: it has been around for a very long time, works very well, is linear, and really is not very complicated. It also helps introducing interesting mathematical objects as more often than not, the first time someone encounters the magic of tensors is in a course on crystalline elasticity. Despite the familiarity, this old warhorse has been given a new life in the last two decades: there are materials out there that have very odd elastic properties indeed.

When a sample is stretched, it usually gets thinner, and materials behaving so familiarly have a positive Poisson's ratio. While negative Poisson's ratios (hereby NPR) are not theoretically prohibited, materials exhibiting them have only been produced or recognised recently. It is s easy to convince oneself of the theoretical possibility of NPR by considering the now canonical re-entrant honeycomb (see Figure 1).

The first NPR material to find wide recognition was indeed of the re-entrant type, a polymeric foam which had been compressed to generate concavity[1]. Since then, many other materials have been observed or postulated, and it has been observed that many crystals exhibit NPR, including most cubic metals[2]. This last result is very striking, and it is even more surprising that it was only established in 1998.

Some even rarer materials exhibit another unusual elastic property: when subjected to hydrostatic (isotropic) pressure, they expand in one direction[3, 4]. This property is referred to as Negative Linear Compressibility (NLC). It has been observed in only 14 materials.

Related NTE

It is not to say that the "negative" properties had not been noticed before… But it is only relatively recently that they have captured the imagination of materials scientist and that applications such as … have been dreamed of.

One of the problems with the full anisotropic elasticity theory is that, while beautifully symmetric and compact, it is not especially visualisable. First, the link between the interesting stuff (all the moduli and ratios) and the available data (usually the stiffness matrix) is not that obvious (it is more direct with the compliance matrix), and that is in the case of distortions on the principal axes. Worst even, for distortions in less symmetric directions, the number crunching is too dull to be carried by hand on a regular basis, and even exceed the potentiality of spreadsheet automation (for typical users at any rate). On the other hand, it is well adapted to programming as it is essentially linear algebra, for which many efficient algorithm are available.

It is therefore very surprising to note that there are no easily available code that would transpose the cold numbers of the stiffness matrix into 3D or 2D representations of elastic properties. 2D figures of, for instance, Poisson's ratio have been published, but it is almost certain that they have been produced with spreadsheets (limitation to principal planes and perpendicular strains). There are also examples in the literature of 3D plots for the young's modulus (by far the simplest property), but the authors do not indicate how they were produced[5, 6].

There lies the main motivation behind the present work: to offer a free, easy to use program capable of representing various elastic properties in any direction, for any crystal symmetry. A secondary goal is to allow the code to automatically query a database of elastic constants (as can be found in reviews such as [7]or [8]), in order to systematically investigate the occurrence of bizarre properties or possible correlations or trends.

The Methodology section first introduces the tensorial formalism behind the crystalline theory of elasticity and establishes the convention used for angles. It also presents various averaging scheme used in the field. It then details the algorithm used to compute the principal properties, namely

tensor rotation and dynamical matrix diagonalisation. The slightly more subtle case of the Poisson's ratio and shear modulus, which requires some optimisation if the results are to be visualisable in 3D, are treated separately.

We then describe the keywords and input files and present four cases studies, which illustrate some of E✓AM capabilities. The first two focus on the visualisation aspect and show that the cubic symmetry can still surprise and that some materials (Cristobalite, Lanthanum Niobate) have truly astonishing elastic properties. The last two examples display the database facilities by revisiting the NLC problem (identifying two new materials), and offering insight on how various definitions of elastic anisotropy are related.

METHODOLOGY

Elasticity Theory

At its most basic, the theory of elasticity linearly relates stresses to strains. This section introduces the various quantities, but without delving into subtleties. The interested reader is invited to consult standards text[9, 10].

Stress

The stress describes the surface forces acting on volume element in a continuum. It can be represented by a 2nd order tensor, with 6 independent coordinates.

Strain

The stain describes the state of deformation of solid body. It can also be represented by a 2nd order tensor, with 6 independent coordinates.

Stiffness

The stiffness tensor expresses the stress tensor in terms of the strain tensor:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} . \quad (1)$$

It is a property of the crystal. As a tensor, its coordinates depend on the choice of axis. Eq. (1) is the generalised Hooke's law.

Compliance

The compliance tensor is the inverse of the stiffness tensor and interprets the strain tensor in terms of the stress tensor:

$$\varepsilon_{ij} = S_{ijkl}\sigma_{kl} . \quad (2)$$

Young's modulus

Young's modulus, or modulus of elasticity is defined as the ratio of normal stress to linear normal strain (both in the direction of applied load).

Shear modulus

The shear Modulus, or modulus of rigidity is defined as the ratio of shear stress to linear shear strain.

Poisson's ratio

Poisson's ratio is defined as the ratio of transverse strain (normal to the applied load), to axial strain (in the direction of the applied load).

Linear compressibility

When the crystal is submitted to hydrostatic pressure, the linear compressibility is the ratio of the induced stretch, along a given line, by the pressure. Except for crystal of cubic or lower symmetry, it depends on the direction of the line.

Sound velocity

Something on symmetry ?

Voigt notation

Six components are sufficient to describe stress and strain. A scheme due to Voigt[11] uses this fact and replaces the cumbersome 2nd and 4th order tensors in a 3 dimension vector space by vectors and matrices of in a 6 dimension vector space.

Tensor notation	11	22	33	23,32	31,13	12,21	(3)
Voigt's notation	1	2	3	4	5	6	

$\varepsilon_{ii} = \varepsilon_p$

$\varepsilon_{ij} = \frac{1}{2}\varepsilon_p$ if i and j are different

$S_{ijkl} = S_{pq}$ if p and q are 1,2,3 only

$S_{ijkl} = \frac{1}{2}S_{pq}$ if either p or q are 4,5,6 (and the other is 1,2 or 3)

$S_{ijkl} = S_{pq}$ if p and q are 4,5,6 only (4)

Tensor rotation, Euler angles

A fourth order tensor transforms in a new basis set following the following rule

$$T'_{\alpha\beta\gamma\delta} = r_{\alpha i} r_{\alpha i} r_{\alpha i} r_{\alpha i} T_{ijkl}\,, \tag{5}$$

where Einsteins's summation rule is adopted and where the $r_{\alpha i}$ are the components of the rotation matrix (or direction cosines). They are expressed as the coordinates of the new basis set vectors in the old framework.

A direction in cartesian space, corresponding to an elastically significant distortion, for instance uniaxial stress or response to isotropic pressure, can be represented as a point on the unit sphere

(unit vector), and advantageously by two angle. We choose it to be first unit vector in the new basis set, *a*. It is fully characterised by the angles θ and φ, as illustrated in Fig. 1. The determination of some elastic properties (shear Modulus, Poisson's ratio) requires another, perpendicular, direction. This is defined by another unit vector, *b*, perpendicular to the first, and characterised by the angle χ. The coordinates of the two vectors are

$$a = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}, \text{ and } a = \begin{pmatrix} \cos\theta\cos\varphi\cos\chi - \sin\theta\sin\chi \\ \cos\theta\sin\varphi\cos\chi + \cos\theta\sin\chi \\ -\sin\theta\cos\chi \end{pmatrix} \tag{6}$$

By definition, the components of the first two columns of the rotation matrix are the coordinates of *a* and *b*. This is sufficient to obtain all the components of the fourth order in the subvectorial space defined by directions 1 and 2, for instance:

$$S'_{12} = S'_{1122} = r_{1i}r_{1j}r_{2k}r_{2l}S_{ijkl} = a_i a_j b_k b_l S_{ijkl}, \text{ and} \tag{7}$$

$$S'_{66} = S'_{1212} = r_{1i}r_{2j}r_{1k}r_{2l}S_{ijkl} = a_i b_j a_k b_l S_{ijkl}.$$

But by scanning θ, φ, and χ over the unit sphere, we can access all the components without having to take into account the third unit vector.

Averaging schemes

Traditionally, and for ease of manipulation, the elastic properties of an anisotropic material have been replaced by those of an "equivalent" isotropic material. These processes of averaging are especially important to treat materials consisting of crystalline grains of random orientation. There are four main schemes: Voigt[11], Reuss[12], Hill[13], and direct.

The Voigt averaging scheme is based on the stiffness matrix (assuming a given uniform strain) and the bulk modulus *K* and the shear modulus *G* are given by

$$K_V = \frac{A+2B}{3}, \qquad G_V = \frac{A-B+3C}{5}, \tag{8}$$

where

$$A = \frac{C_{11}+C_{22}+C_{33}}{3}, \qquad B = \frac{C_{23}+C_{13}+C_{12}}{3}, \qquad C = \frac{C_{44}+C_{55}+C_{66}}{3}.$$

Conversely, the Reuss averaging scheme is based on the compliance matrix (assuming a given uniform stress) and:

$$K_R = \frac{1}{3a+6b}, \qquad G_R = \frac{5}{4a-4b+3c}, \tag{9}$$

where

$$a = \frac{S_{11} + S_{22} + S_{33}}{3}, \qquad b = \frac{S_{23} + S_{13} + S_{12}}{3}, \qquad c = \frac{S_{44} + S_{55} + S_{66}}{3}.$$

In both case, the Young's modulus E and the Poisson's ratio *v* are given by

$$E = \left(\frac{1}{3G} + \frac{1}{9K} \right)^{-1}, \qquad \nu = \frac{1}{2}\left(1 - \frac{3G}{3K + G} \right). \tag{10}$$

The Hill average is the arithmetic average of the Voigt and Reuss values.

The direct averaging scheme is non analytical. It consists in integrating the desired quantity on the unit sphere. For instance, the young's modulus is given by

$$K_D = \frac{1}{4\pi} \iint E(\theta, \varphi) d\theta d\varphi . \tag{11}$$

Simple properties

Some properties can be simply expressed in terms of the compliance matrix.

The Young's modulus can be obtained by using a purely normal stress in Eq. 2 in its vector form and is given by

$$E(\theta, \varphi) = \frac{1}{S'_{11}(\theta, \varphi)} = \frac{1}{a_i a_j a_k a_l S_{ijkl}} . \tag{12}$$

The linear compressibility follows a slightly different scheme but is even simpler to compute. It is obtained by applying an isotropic stress (corresponding to pressure *p*) in tensor form, so that $\varepsilon_{ij} = -pS_{ijkk}$ and by considering that the extension in direction *a* is $\varepsilon_{ij} a_i a_j$, and that therefore

$$\beta(\theta, \varphi) = S_{ijkk} a_i a_j . \tag{13}$$

Shear modulus and Poisson's ratio: optimisation

Other properties depends on two directions (if perpendicular this corresponds two 3 angles), which makes them difficult to represent graphically. A convenient possibility is then to consider three representations: minimum, average and maximum. For each θ and φ, and doublet, the angle χ is scanned and the minimum, average and maximum values are recorded for this direction.

The shear ratio is obtained by applying a pure shear stress in the vector form of Eq. 2 and is results in

$$G(\theta, \varphi, \chi) = \frac{1}{4S'_{66}(\theta, \varphi, \chi)} . \tag{14}$$

Poisson's ratio can be obtained by using a purely normal stress in Eq. 2 in its vector form and is given by

$$\nu(\theta, \varphi, \chi) = -\frac{S'_{12}(\theta, \varphi, \chi)}{S'_{11}(\theta, \varphi)} = -\frac{a_i a_j b_k b_l S_{ijkl}}{a_i a_j a_k a_l S_{ijkl}} . \tag{15}$$

Sound velocities: diagonalisation

The dynamic matrix M, which describes the vibrational modes (phonons) in a crystal can be written in terms of the stiffness tensor (see for instance [14])

$$M_{ik} = C_{ijkl} k_j k_l , \tag{16}$$

where $k(k_x, k_y, k_z)$ is the wave vector (coordinates).

The dynamic matrix can be diagonalised, and its eigenvalues *w* are the square of the frequencies. From the *w*(**k**) dependence, we can extract the sound wave velocities.

MANUAL AND CASE STUDIES

This section introduces various ElAM input files, discusses parameters, and displays some of the results. It is hoped that the following examples will prove sufficiently explanatory for most users. The full list of Keywords is given in Appendix A.

Direct mode

Installation

Basic operations

One of the simplest input file is given in Ex. 1. The first line sets the symmetry type, the second line contains the corresponding stiffness constants, in the order given by the LB tables (C_{11}, C_{44}, C_{12} for cubic). The third line asks for Young's modulus to be graphically represented, and the last line finishes the input (`stop` must be present). The program would still be running in the absence of a property requirement. The order of the command is unimportant, with the obvious exception that if a keyword requires numerical values, these must be in the line immediately following it.

As is, this input produces two output files, `ElAM.log` and `ElAM_young.wrl`. The first file is a text summary of the calculations. It starts by the stiffness and compliance matrices, which is useful to check that the order of elastic constants was correct. It then recalls the meshing parameters and finally summarises the elastic properties in terms of averages, minimum/maximum values and their directions. The second file is in VRML (virtual reality modelling language) format and can be visualised and explored with a VRML capable browser. A screen copy is shown in Fig. 3.

It is not an especially good figure, and for many reasons. In fact, the previous input makes use of many default values, which are perfectly fine to obtain averages and quick indications in the .log files, but lack detail to produce good figures. This can be improved, as in Ex. 2 and the resulting Fig. 4. The first four lines give a title and an output root name. While the title is relatively unimportant, the output root name ease the organisation of files, now called `Ag_fcc.log` and `Ag_fcc_young.wrl`. The main difference with Ex. 1 is the refinement of the angular scanning

steps: `thet` and `phi` controls the steps for the calculations of optimum values and average, while `3dth` and `3dph` define the grid used for the graphical representation. The default values for these are 24, 24 ,12 and 12. The `3daxes` keyword facilitates orientation by adding arrows and labels for the three cartesian axes. Finally, the background color is changed to white with the `color_bg` keyword. Generally speaking, colour is coded in ElAM with four values (0. to 1.), red, green, blue, and transparency. Transparency being meaningless for the background, it is ignored in that case.

The other property codes are `shear`, `poisson`, `compress` and `sound`. The symmetry codes are self explanatory and are `cubi`, `hexa`, `tetr`, `trig`, `orth`, `mono` and `tric`. (Something on subtleties with tetr)

By default, the code interprets the elastic constants following the symmetry keyword as being components of the stiffness matrix. In order to force them to be components of the compliance matrix, one has to add the `compli` keyword to the input. It is also possible to input the elastic constant directly in 6x6 matrix form, following the keyword d `C` or `S` (note the capital).

This type of input file is sufficient to explore the elastic properties of a given materials and can already shed light on some interesting phenomena.

Case study 1: Poisson's ratio of cubic crystals

In 1998, B et al. did show that around two thirds of cubic metals (and alloys) do have negative poisson's ration, in the (110) direction. Up to this point, this property (also known as auxeticity) had been considered very rare. Fig. 5a and 5b displays screen copies of the VRML representation of Poisson's ratio for two cubic metals, Cesium and Aluminium.

The basic ElAM colour convention (transparent blue, maximum; green, minimum if positive, red, minimum when negative) makes it clear that these two metals have different elastic behaviour. Not only does aluminium appear much more isotropic, it also does not show any sign of auxeticity, which is confirmed by the numerical summary in the `.log` file. The convoluted shape for cesium is very interesting as it shows auxeticity, but also because it strongly hints that a visual inspection of this sort, even without the colour scheme could have identified negative Poisson's ratio in cubic metals a lot earlier than 1998.

The humble cubic symmetry is not without surprises, and the story does not stop here. From simple calculations, it was assumed that the extrema of Poisson's ratio for the cubic symmetry were along the [110] directions and permutations (for instance see [2]). If we consider the AuCd alloy in Fig. 5c, we can see that the negative minimum surface is concave at [110], and that therefore this direction is not the one of minimum Poisson's ratio. Recent analytic calculations[15, 16] have tackled this problem and pushed it even further, and shown that in some rare cases, the optima can occur in directions around [111]. Once again, this peculiarity (referred to as the "Ting & Chen

effect") could have been discovered much earlier, tipped off by graphical representations, such as Fig. 5d and 6d for InTl alloy (27% Tl).

Fine tuning and 2D graphics

As previously mentioned, the simplest properties are easy to represent, and a two-colour scheme is enough. The shear modulus and Poisson's ratio are more complex, with maximum, minimum and average surfaces. ElAM produces all four surfaces in a single VRML file, which could lead to overly rich 3D models. Control over which surfaces are represented is done by using the colour options. By default, the average surface colour is fully transparent and only maximum and minimum appear, minimum following the red/negative, green/positive convention, and maximum being blue and semi-transparent (to reveal the minimum surface underneath).The colour options are `color_bg`, `color_axis`, `color_pos`, `color_neg`, `color_max`, `color_minp`, `color_minn`, `color_aven`, and `color_avep`. They are followed by a line containing RGB numbers, and, with the exception of the first two, a transparency number (0 –opaque– to 1 –transparent–).

It is also possible to plot sections of the curves, in postscript format. The principles are very similar to those of the 3D curves. Whether a property is plotted or not is controlled by the following keywords: `2dyoun`, `2dshea`, `2dpois`, `2dcomp` and `2dsoun`. The plane in which the section is cut is defined by either `plane_xy` followed by a line containing the miller indices, or by `plane_an` followed by two angles defining the unit vector perpendicular to the plane. Other related keywords are of the type `2dyoung_tick` and `2dyoung_circ`; they control the presence of ticks on the axes or of circles to guide the eyes (see Ex. X and Fig. 7).

Case study 2: extreme crystalline auxeticity

Monoclinic Lanthanum niobates is remarkable for being one of few materials exhibiting negative linear compressibility, but it is also the crystal with the lowest observed Poisson's ratio (-3.01). It also has a very large maximum (3.96), interestingly in the same direction, along the y axis (see Fig.6a). α-Cristobalite is also an auxetic crytals, as can be seen from Fig. 7. The extreme values are more modest, at .10 and -.51, but for almost all direction, the absolute value for the minimum is larger than for the maximum (the reverse in transparency in Fig. 7b was achieved with the ElAM input from Ex. 3).

Both these crystals are considered very auxetic, yet their properties are strikingly different. Fig. 7c and 7d display the average Poisson's ratio (using input shown in Ex. 4). This value gives an indication of whether the section perpendicular to the stretch increases or decreases in area. It can be seen that while for α-Cristobalite, stretches in any direction results in decreasing section area,

Lanthanum niobate follows a much more normal pattern as the section area increases for any stretch. Both materials are certainly interesting, but would have different applications.

Database mode

This mode is geared towards the systematic discovery of unusual elastic properties. It does not use graphical representation; although the graphical keyword discussed previously can still be present, they will be ignored. The database mode requires an additional file, containing a list of materials name and elastic constants, as well as a list of properties to be tabulated. A simple input files is given in Ex. 5. The `database` keyword triggers the database mode and is followed by the database file name. The `data_prop` keyword is followed (on the same line) by the number of properties to appear in the output, and the next line contains their codes. The codes list is detailed in Appendix 2. In this example, the minimum and maximum of Young's modulus, linear compressibility, Poisson's ratio, as well as the bulk compressibility (inverse of bulk modulus) are requested.

The syntax of the database file is simple and is illustrated in Ex. 6. Each line contains first a identifier, then the type of data (C if stiffnesses, S if compliances), followed by a symmetry code and finally by the data (following the same order convention as LB, maybe in appendix ???). Anything after the last elastic constant will be ignored by the program, but can be used for comments or references. The last line must be `stop`.

ElAM has no sorting or parsing facilities, and the entirety of a database will be treated, which can take some time. We advise the user to keep their master database in a spreadsheet format to benefit from superior editing and sorting capabilities, and to export the relevant section in a text file when required.

Please note that the default value for the θ,φ grid is used (24, 24). If increased accuracy is desirable, `thet` and `phi` can still be used.

Case study 3: negative linear compressibility

In a celebrated article[3], Baughmann and coworkers used an early version of the ElAM methodology to scan a database of known elastic constants in order to identify those materials which exhibit negative linear compressibility. Out of around five hundred compounds, they suggested that thirteen did show negative linear compressibility: two trigonal, two tetragonal, six orthorhombic and three monoclinic, but no triclinic. The procedure was strangely indirect and consisted in looking for linear compressibility that exceeds the bulk compressibility (sign of negative area compressibility in the perpendicular plane). The reason for this choice are not clear, one can only postulate that as this methods samples a full plane for the cost of one direction, it is efficient if only the principal axis are investigated (which is implied, but never spelt in the article). We use ElAM to re-examine the data, with a full directional scan. We focus on the lower symmetry

crystals, and show that out of six triclinic present in LB, two do show clear signs of negative linear compressibility: ammonium tetroxalate dihydrate and potassium tetroxalate dihydrate. These compounds had been missed by the computationally simpler but less complete previous methodhology. The linear compressibility for ammonium tetroxalate dihydrate is shown in 3D and 2D in Fig. 8 and 9.

Case study 4: anisotropy measures

The original motivation for (and reason for the acronym of) ElAM's precursor was in fact an article by Ledbetter and Migliori[17] describing an extension to Zener's anisotropy measure[18]. They describe a straightforward method were the anisotropy is described by the ratio of ... and … which corresponds to the Zener measure for cubic crystals. It is for this reasons that the output contains a few lines with anisotropy results. But what is meant by elastic anisotropy? The Ledbetter definition is attractive for historical reasons as it links well with the Zener ratio (itself also a measure of shear ...),but also because it i of relevance in the field of geosciences, where transverse wave velocities in different rock layers help locating or predicting earthquakes[19] for instance. But other measures of anisotropy also suggests themselves, for instance a ration of maximum and minimum of Young's or shear modulus. Are these measures correlated and does "elastic anisotropy" means anything in the absence of reference to a given property? The analytical mathematical derivation might be doable for the higher symmetries, but are certainly very involved for hexagonal onwards. The database capabilities of ElAM permit a relatively pain free (once a database has been created) way of investigating this topic.

CONCLUSION

ACKNOWLEDGEMENTS

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Appendix 1: List of Keywords/options

Keywords are either stand alone (SA), require data on the following line(s) or (DFL), or must be accompanied by an integer on the same line AND data on following lines (I+FL)

Generic keywords

Keyword	Use	Default
`titl`	FL, title of the study, only appears in .log file	''
`outpu`	FL, root name for output files	'ElAM'
`verbose`	SA, triggers verbose mode and output too much information in .log	False
`stiff`	SA, elastic constants are read as components of stiffness matrix	True
`compli`	SA, elastic constants are read as components of compliance matrix	False
`thet`	FL,	24
`Phi`		24
`cubi`	FL, 3 elastic constants for cubic symmetry (C_{11}, C_{44}, C_{12})	
`hexa`	FL, 5 elastic constants for cubic symmetry (C_{11}, C_{44}, C_{12})	
`tetr`		
`trig`		
`orth`		
`mono`		
`tric`		
`C`		
`S`		
`stop`		

3D keywords

Keyword	Use	Default
`young`		False
`shear`		False
`compress`		False
`poisson`		False
`sound`		False
`3daxes`		False
`color_bg`		(0 0 0)
`color_front`		(1 1 1)
`color_pos`		(0 .8 0 0)

color_neg	(.8 0 0 0)
color_max	(0 0 .8 .5)
color_minp	(.8 0 0 0)
color_minn	(0 .8 0 0)
color_avep	(0 0 0 1)
color_aven	(0 0 0 1)

Appendix B: Elastic property codes

The property codes used in the database modes range from 1 to 999. With few exceptions, they consist in a three figure code. The first number refers to the property itself, as in Table B1.

The second two numbers refine the definition, see Table B2.

The leading 0 must be ommited for the stifnesses and compliances. Codes 1 to 21 comprise the stiffnesses in order 11, … 16, 22, … 26, …66. Codes 51 to 1 are the equivalent for the compliances.

Table B1: First figure code definition, for a code of the form Xnn

X=0	X=1	X=2	X=3	X=4
Stiffnesses or compliances	Young's modulus	Shear modulus	Compressibility	Poisson's ratio

Table B2: Second part code definition, for a code of the form Xnn

nn=00	nn=01	nn=02	nn=03	nn=04	
Direct average	Reuss average	Voigt average	Hill average	Bulk compressibility (only 304)	
nn=10	nn=11	nn=12	nn=13	nn=14	nn=15
minimums	θ at minimum	φ at minimum	x at minimum	y at minimum	z at minimum
nn=20	nn=21	nn=22	nn=23	nn=24	nn=25
maximum	θ at maximum	φ at maximum	x at maximum	y at maximum	z at maximum

Figure captions

Fig. 1: (a) 2D structure with positive (top) and negative (bottom) Poisson's ratio; (b) 2D illustration of one mechanism of NTE, increasing thermal agitation of linked, rigid squares reduces total area

Fig. 2: Definitions of angles used to describe directions in ElAM

Fig. 3: 3D representation of Young's modulus of Silver, using default setup.

Fig. 4: Improved 3D representation of Young's modulus of Silver, with finer angle mesh, white background and axes.

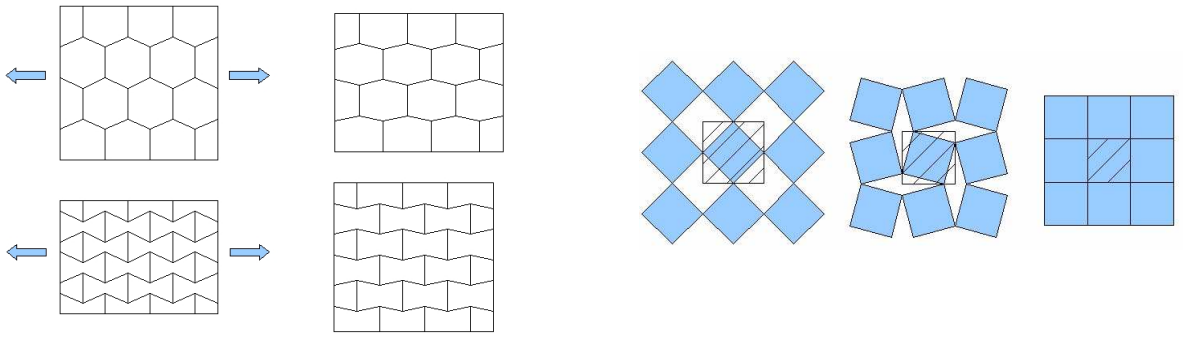
Fig. 5: 3D representation of Poisson's ratio for Aluminium (a), Cesium (b), AuCd alloy (c) and InTl alloy (d). maximum (blue), minimum positive (green) and minimum negative (red).

Fig. 6:2D representation of Poisson's ratio in the (-110) plane for Aluminium (a), Cesium (b), AuCd alloy (c) and InTl alloy (d). maximum (blue), minimum positive (green) and minimum negative (red).

Fig. 7: 3D representation of Poisson's ratio for lanthanum niobate (a, c) and α-Cristobalite (b, d). The top figures (a, b) show the maximum and minimum curves for each direction, while the bottom ones (c, d) show the rotationally averaged value. The scale, indicated by the length of the axes, is conserved for each material. The standard colour convention is used (note the, forced, reverse in transparency in the top left figure).

Fig.8: 3D representation of linear compressibility for ammonium tetroxalate dehydrate.

Fig.9: 2D representation of linear compressibility for ammonium tetroxalate dehydrate in the x-z plane.



(a) (b)

Fig. 1

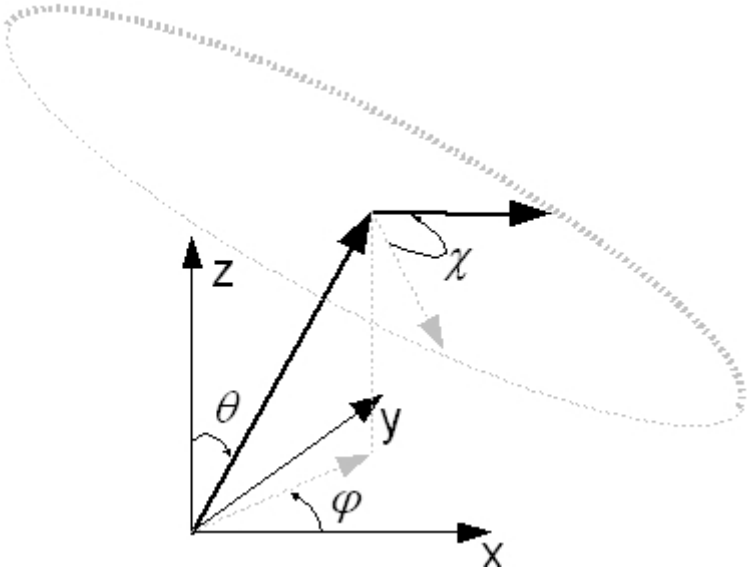


Fig. 2

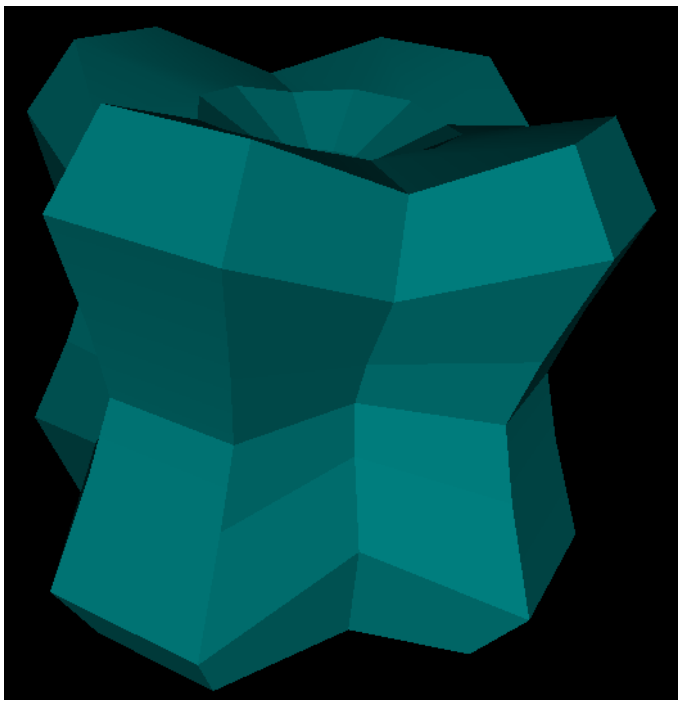


Fig. 3

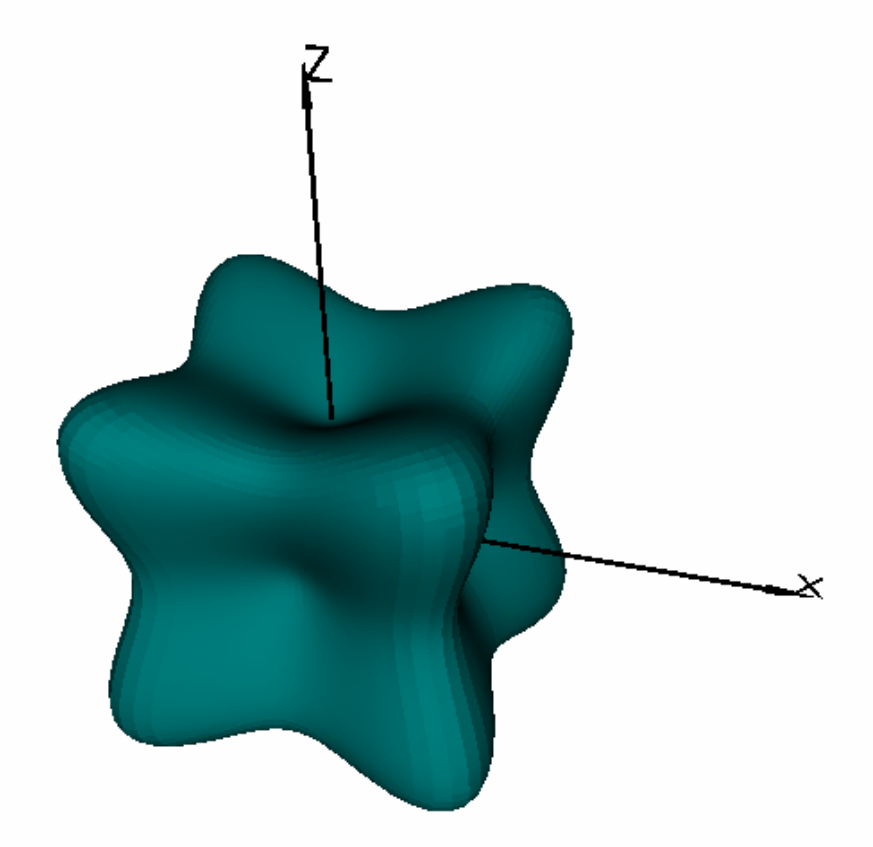
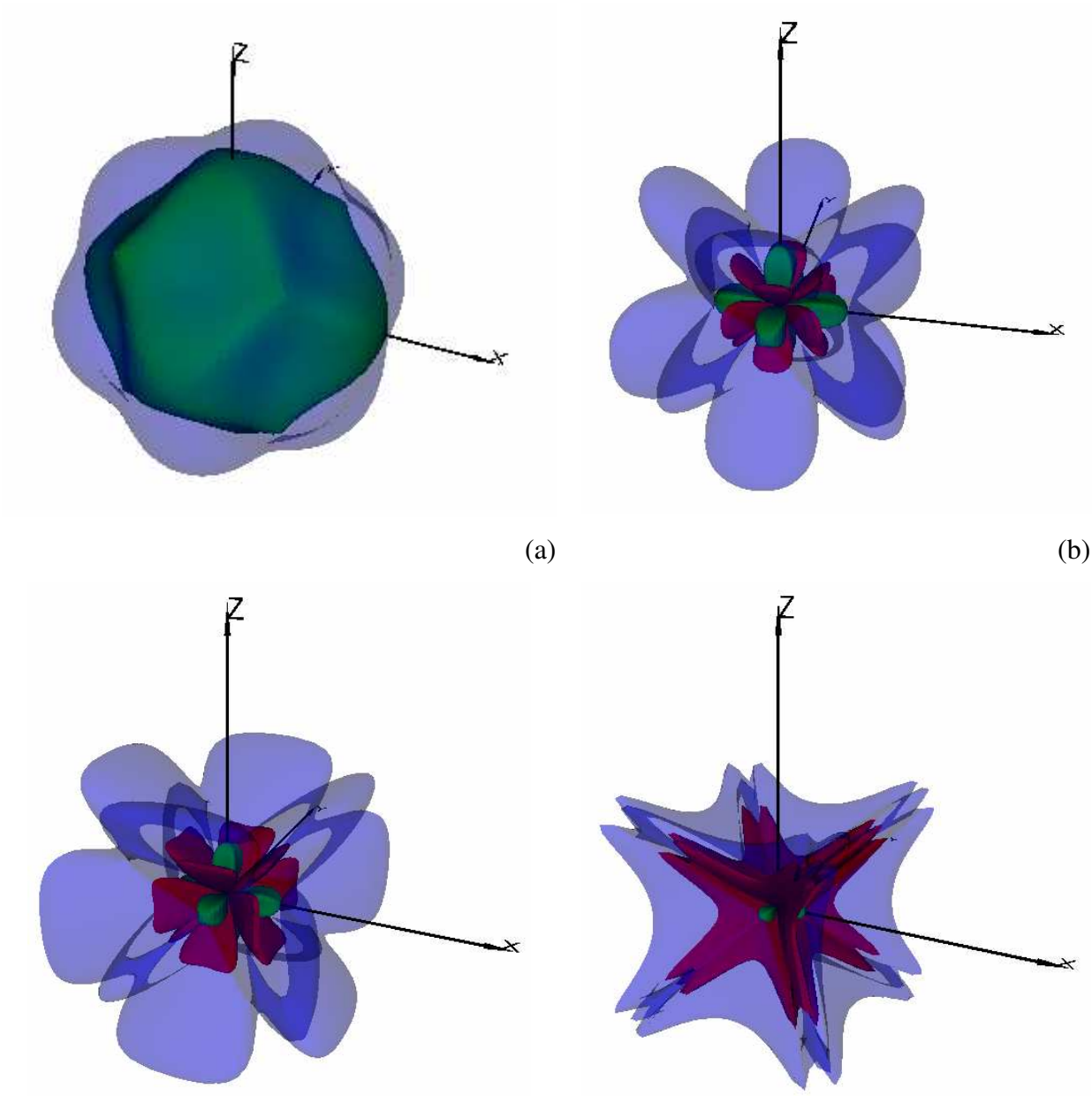


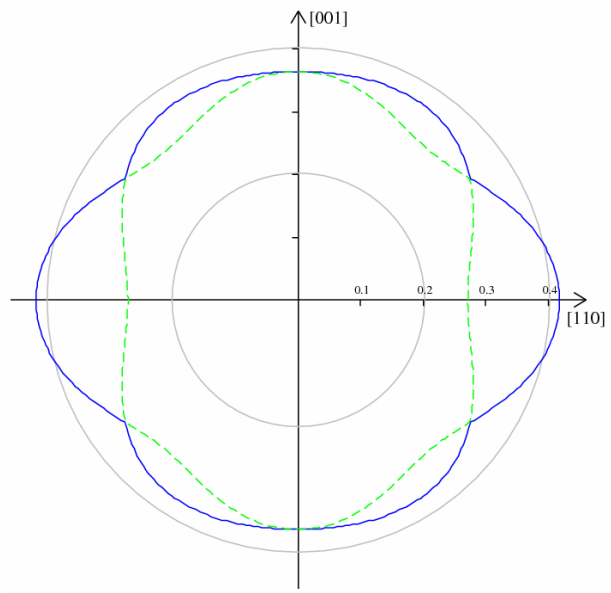
Fig. 4



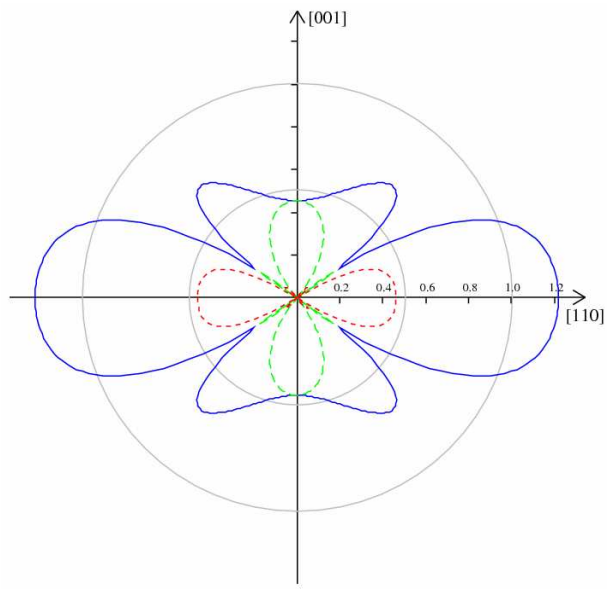
(a) (b)

(c) (d)

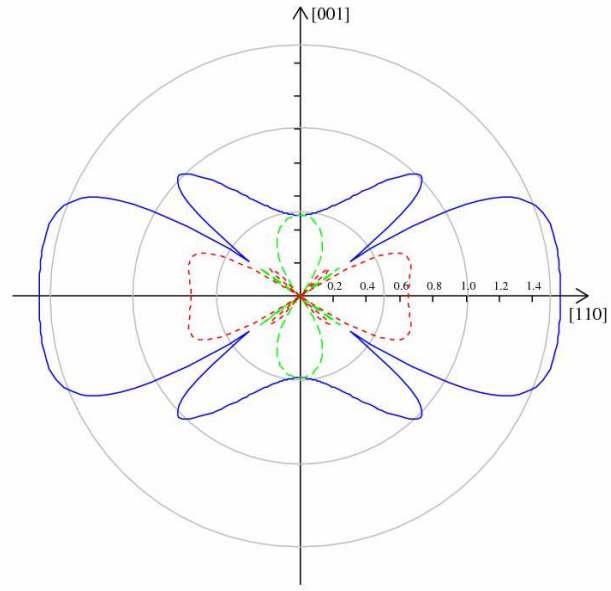
Fig. 5


[001]
0.1
0.2
0.3
0.4
[110]

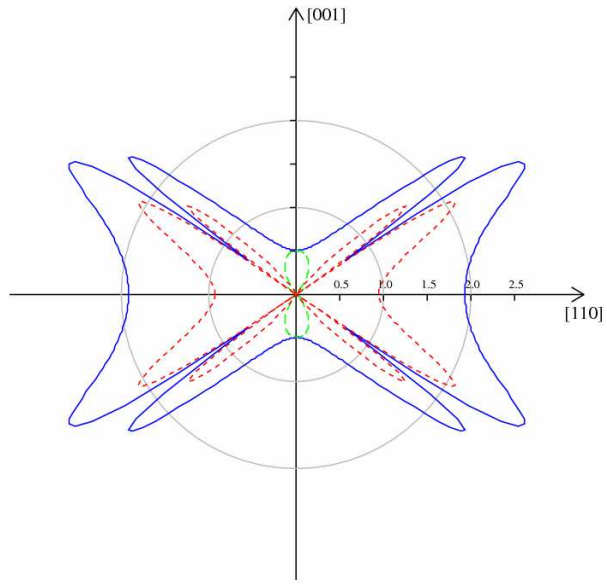
(a)


[001]
0.2
0.4
0.6
0.8
1.0
1.2
[110]

(b)

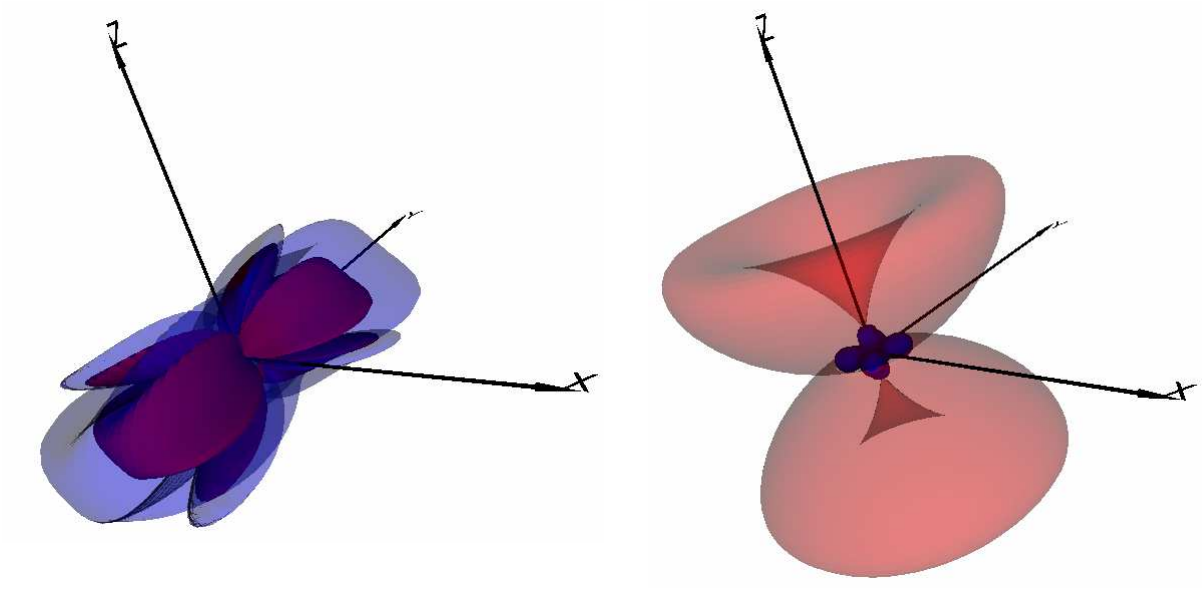

[001]
0.2
0.4
0.6
0.8
1.0
1.2
1.4
[110]

(c)

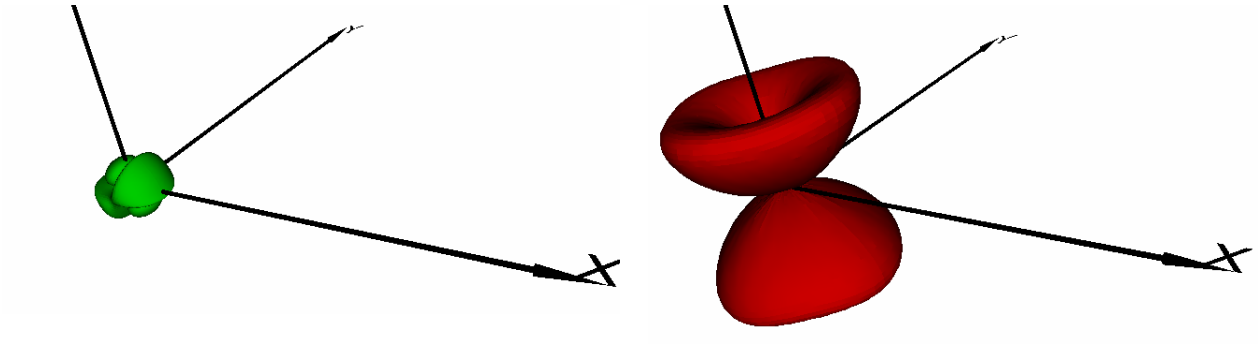

[001]
0.5
1.0
1.5
2.0
2.5
[110]

(d)

Fig. 6



(a) (b)



(c) (d)

Fig. 7

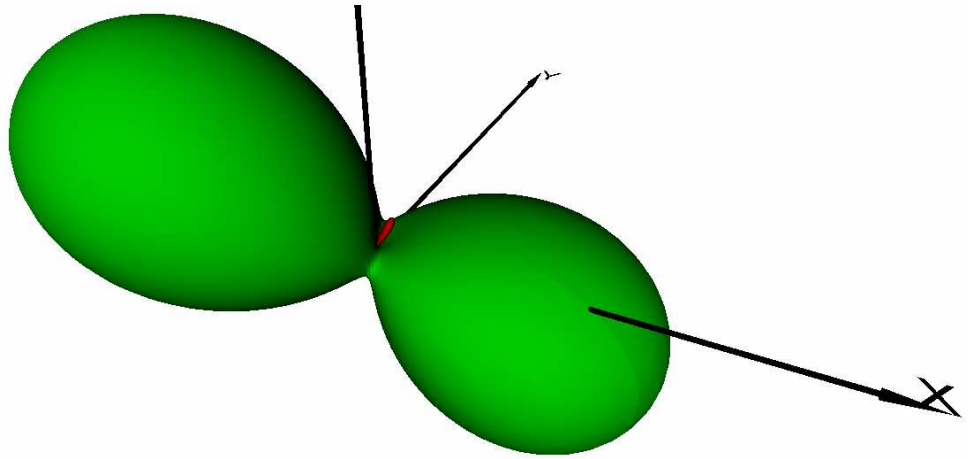


Fig. 8

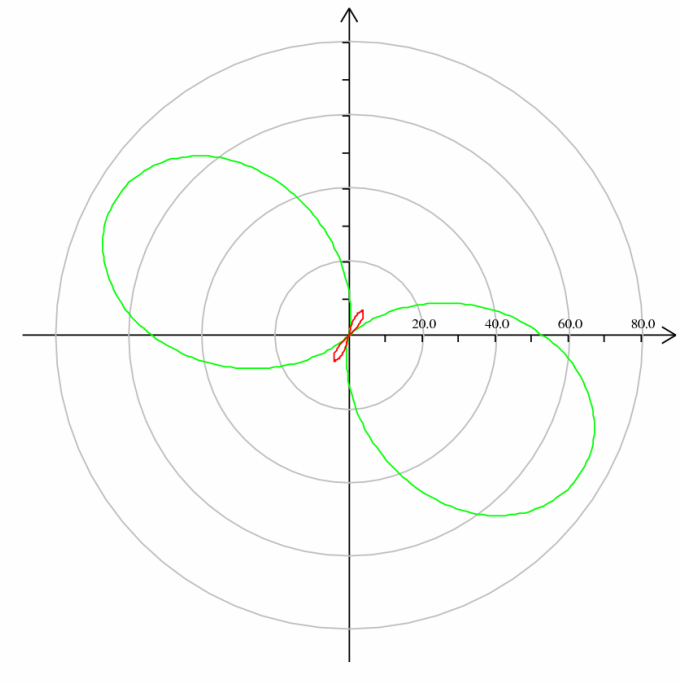


Fig. 9

Examples Captions

Ex. 1: Basic ElAM input for Young's modulus of Silver.

Ex. 1: Improved ElAM input for Young's modulus of Silver, with title, named outup, finer angle mesh, white background and axes.

Ex. 3 : Use of colour keywords for transparency reversal.

Ex. 4: Use of colour keywords to reveal average curves (α-Cristobalite).

Ex. 5: Typical database mode input file.

Ex. 6: Database file

```
cubi
 12.20 4.46 9.20
young
stop
```

Ex. 1

```
title
Silver fcc
output
Ag_fcc
cubi
 12.20 4.46 9.20
thet
200
phi
200
3dth
99
3dph
99
young
3daxes
color_bg
 0. 1. 1.
Stop
```

Ex. 2

```
…
color_max
   0. 0. .8 0.
Color_minp
.0 .8 .0 .5
color_minn
.8 .0 .0 .5
stop
```

Ex. 3

```
title
xtobal
tetr
59.4 42.4 67.2 25.7 3.8 -4.4 0.0
…
poisson
3daxes
color_bg
 1. 1. 1.
Color_max
   0. 0. .8 1.
Color_minp
.0 .8 .0 1.
Color_minn
.8 .0 .0 1.
Color_avep
.0 .8 .0 0.
Color_aven
.8 .0 .0 0.
Stop
```

Ex. 4

```
title
TST_DATABASE
database
triclinicLB.txt
data_prop 7
110 120 304 310 320 410 420
stop.
```

Ex. 5

```
Cristoballite C 5 59.4 42.4 67.2 25.7 3.8 -4.4 0.0
AuCd_Alloy C 7  110.8  40.7 104.9
Ag_FCC C 7 122 45.5 92.0
Cd_HCP C 6 114.1  49.9  19.0  41.0  40.3
Aluminium_pentaiodate_sexahydrate  C  6  42.9  38.7  16  15.7  21.9
stop.
```

Ex. 6