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A note on the computation of the extrema of Young's modulus for hexagonal materials: an approach by planar tensor invariants

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Abstract

A simple method to obtain the highest and lowest Young's modulus for a material of the hexagonal class is presented. It is based upon the use of tensor invariants of plane anisotropic elasticity; in fact, the cylindrical symmetry of the elastic tensor allows for transforming the 3D original problem into a planar one, with a considerable simplification.

Keywords: linear elasticity, anisotropy, polar formalism, bounds on elastic moduli

2010 MSC: 74B05, 74E10

1. Introduction

The problem of finding the extrema of the Young's modulus for materials belonging to the hexagonal class has been recently addressed by some authors, [1, 2, 3]. In particular, the last work by Cazzani clearly states some historical contributions going back to the XIX century, namely to the works of Saint Venant, [4, 5, 6].

The purpose of this paper is to show that, thanks to the particular elastic symmetry of hexagonal materials, the problem of finding the extrema of the Young's modulus, as well as of any other elastic parameter, can be found by a direct bi-dimensional approach, much easier and straightforward than the general approaches proposed in the cited papers. Such an approach is based

upon the *polar formalism*, where tensor invariants and angular variables are used to represent the elastic behavior of the material, in a way that reveals to be really powerful to state and solve the problem.

2. Statement of the problem by the polar formalism

Let us consider an elastic material having a hexagonal symmetry with X_3 as the axis of elastic symmetry. We address here the question of determining the extrema of the Young's modulus.

From a purely elastic point of view, a hexagonal symmetry cannot be distinguished from transverse isotropy: they share the same type of elastic tensors. This means also that for a hexagonal material, the elastic behavior is the same in all the meridian planes, i.e. those containing the X_3 axis.

For the purposes of this paper, this implies that it is sufficient to study the Young's modulus variation in any of such planes: the problem can be completely reduced from a three-dimensional to a planar one. For the sake of simplicity, we will indicate by x and y a couple of Cartesian axes in such a plane. Unlike what is commonly done in the literature, where the axis of symmetry for a material of the hexagonal symmetry class is labelled as the axis of X_3 , the remaining two axes of X_1 and X_2 laying in the transversal plane, the use of axes labelled x and y has been preferred here, for emphasizing the planar character of the approach. These axes lay in a meridian plane; the axis of x is rotated through an angle θ with respect to the transversal plane, hence, for instance, with respect to the X_1 or X_2 axes. For the sake of shortness, and for giving a particular importance to the couple of axes of orthotropy, we will name x_1 and x_2 the axes of x and y , respectively, when $\theta = 0$. Hence, for being more precise, $x_1 = X_1$ (or, indifferently, X_2) and $x_2 = X_3$, see Fig. 1. To remark that angle θ is here the *latitude*, i.e. $\theta = 0$ corresponds to the equator and $\theta = \pi/2$ to the pole.

It is worth to recall that the components of the compliance tensor $\mathbb{S}$ are exactly the same as those of the corresponding material in a planar state of stress. As $E(\theta)$ is given by (Voigt's notation is used throughout all this paper)

$$E(\theta) = \frac{1}{S_{xx}(\theta)}, \quad (1)$$

the final question is hence reduced to a planar elastic one, depending on only one variable: to find the extrema of the Young's modulus $E(\theta)$ of a planar

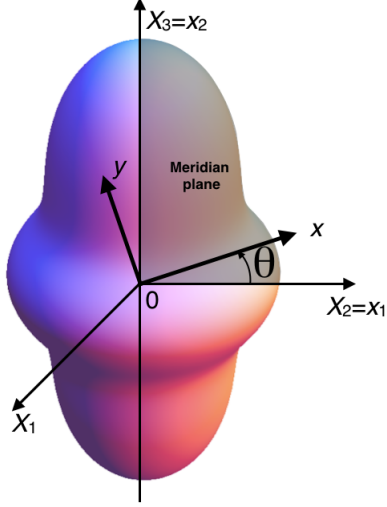


Figure 1: Sketch of the reference frames.

orthotropic material. For the mathematical symmetries, the study can be restricted to the set $0 \leq \theta < \pi/2$.

An interesting tool for the study of planar problems in anisotropic elasticity is the polar formalism, introduced by Verchery in 1979, [7]. This method is particularly effective in several situations, namely because a tensor is described making use of invariants and angles only, which reveals to be very useful for describing anisotropic properties. Restricting here the attention to the strict topic of this paper (the interested reader can find a detailed account of the polar formalism in [8]; here, due to the peculiarity of the matter, only the case of orthotropic materials is considered), it is

$$S_{xx}(\theta) = t_0 + 2t_1 + (-1)^k r_0 \cos 4(\varphi_1 - \theta) + 4r_1 \cos 2(\varphi_1 - \theta), \quad (2)$$

with t_0 and t_1 the *isotropy invariants*, r_0, r_1 and k the *anisotropy invariants*; all of them are non negative quantities. The last polar parameter, φ_1 , is an angle that fixes the frame.

The expressions of the above quantities are given as functions of the Cartesian components of $\mathbb{S}$ by the following relations (with the usual frame $\{X_1, X_2, X_3\}$ mentioned above, S_{22} should be S_{33} , S_{12} should be S_{13} or S_{23}

and S_{66} indifferently S_{44} or S_{55} , while S_{11} does not change of indexes):

$$\begin{aligned}
t_0 &= \frac{1}{8}(S_{11} - 2S_{12} + S_{66} + S_{22}), \\
t_1 &= \frac{1}{8}(S_{11} + 2S_{12} + S_{22}), \\
r_0 &= \frac{1}{8}|S_{11} - 2S_{12} - S_{66} + S_{22}|, \\
r_1 &= \frac{1}{8}|S_{11} - S_{22}|, \\
\cos 2\varphi_1 &= \frac{S_{11}-S_{22}}{|S_{11}-S_{22}|}.
\end{aligned} \tag{3}$$

It can be proved that the fifth invariant, k , can only be an integer; thanks to the periodicity of the Cartesian components, see for instance eq. (2), only two values are actually interesting, 0 and 1. For this reason, a suitable expression for uniquely determining k is:

$$k = \frac{1}{2} \left| \frac{S_{11} - 2S_{12} - S_{66} + S_{22}}{|S_{11} - 2S_{12} - S_{66} + S_{22}|} - 1 \right|; \tag{4}$$

k fixes the *type of planar orthotropy* and is of the greatest importance in the following, see also [9].

Incidentally, a glance at eq. (2) shows that the Cartesian components of $\mathbb{S}$ needed to describe the behavior of the material in a meridian plane are four, but that actually this behavior depends on all the five tensor invariants of the fictitious planar orthotropic material having the same Cartesian components of the hexagonal-symmetric material (i.e., with S_{22} corresponding to S_{33} , S_{66} to S_{44} and so on, as explained above). So, the planar analysis depends on the whole set of independent invariants and in this sense it is hence complete.

A remark, for the sake of precision: formulae in eq. (3) and (4) have been written as functions of the Cartesian components in the frame $x_1 - x_2$, i.e. for $\theta = 0$, and considering an orthotropic material, which is the case of concern here. More general formulae, using the Cartesian components in a generic frame $x - y$ rotated through an angle θ and concerning a completely anisotropic material, could be written as well, but have been omitted here for the sake of conciseness.

Of course, see eq. (1), the extrema of $S_{xx}(\theta)$ correspond to those of $E(\theta)$: a maximum for $S_{xx}(\theta)$ is a minimum for $E(\theta)$, and a minimum for $S_{xx}(\theta)$ is a maximum for $E(\theta)$. Hence, we will study $S_{xx}(\theta)$, the results for $E(\theta)$ will descend immediately.

Before proceeding with the search for the extrema of $S_{xx}(\theta)$, let us turn the attention on the choice of the frame. Fixing $\varphi_1 = 0$ corresponds to

put the axis of x_1 aligned with the direction giving the highest value of $S_{xx}(\theta)$, $\theta \in \{0, \pi\}$, and $\varphi_1 = \pi/2$ with the direction of the lowest value. Because these are the only two cases of concern here, it is worth to write eq. (2) in the equivalent form

$$S_{xx}(\theta) = t_0 + 2t_1 + (-1)^k r_0 \cos 4\theta + 4(-1)^h r_1 \cos 2\theta, \quad (5)$$

with $h = 0$ if $\varphi_1 = 0$ and $h = 1$ if $\varphi_1 = \pi/2$. A suitable Cartesian expression for h is

$$h = \frac{1}{2} \left| \frac{S_{11} - S_{22}}{|S_{11} - S_{22}|} - 1 \right|. \quad (6)$$

Looking at eq. (3₅), it can be easily noticed that for materials with $S_{11} > S_{22}$, $\varphi_1 = 0$ and $h = 0$. This is the case of a Young's modulus represented by a *prolate* surface, i.e. having $E(\theta = 0) < E(\theta = \pi/2)$; to remember that the x_1 axis belongs to the transversal plane and x_2 is the hexagonal axis of symmetry of the material. An *oblate* surface, i.e. with $E(\theta = 0) > E(\theta = \pi/2)$, corresponds to the case $S_{11} < S_{22}$, that gives $\varphi_1 = \pi/2$ and $h = 1$.

Though parameter h plays an algebraic role equivalent to that of k , nonetheless, these two quantities are really different, mathematically and mechanically: k is an invariant that determines the type of orthotropy regardless of the frame, h is a parameter linked to the frame choice that gives the form of the surface of E : prolate, for $h = 0$, oblate for $h = 1$.

The first derivative of $S_{xx}(\theta)$ is

$$S'_{xx}(\theta) = -8r_1 [(-1)^k \rho \cos 2\theta + (-1)^h] \sin 2\theta, \quad (7)$$

where

$$\rho = \frac{r_0}{r_1}. \quad (8)$$

The zeros of $S'_{xx}(\theta)$ are

$$\theta_1 = 0, \quad \theta_2 = \frac{1}{2} \arccos \frac{(-1)^{1+h-k}}{\rho}, \quad \theta_3 = \frac{\pi}{2}; \quad (9)$$

the second (intermediate) root, θ_2 , exists $\iff \rho > 1$. The second derivative of $S_{xx}(\theta)$ is

$$S''_{xx}(\theta) = -16r_1 [(-1)^k \rho \cos 4\theta + (-1)^h \cos 2\theta], \quad (10)$$

that gets the following values for the zeros of $S'_{xx}(\theta)$:

$$\begin{aligned} S''_{xx}(\theta_1) &= -16r_1 [(-1)^k \rho + (-1)^h], \\ S''_{xx}(\theta_2) &= -16(-1)^k r_1 \frac{1-\rho^2}{\rho}, \\ S''_{xx}(\theta_3) &= -16r_1 [(-1)^k \rho - (-1)^h]. \end{aligned} \quad (11)$$

When θ_2 exists, $\rho > 1$, so it is always

$$\frac{1-\rho^2}{\rho} < 0; \quad (12)$$

hence, the sign of $S''_{xx}(\theta_2)$ depends exclusively on k , because $r_1 \geq 0$, unlike what happens for $S''_{xx}(\theta_1)$ and $S''_{xx}(\theta_3)$, where it depends also on h , hence on the form of the surface representing E .

Considering the above equations and remarks, one can easily determine the nature of the stationary points of $S_{xx}(\theta)$ and hence of $E(\theta)$:

$$\begin{aligned} E(\theta_1) &= \frac{1}{t_0 + 2t_1 + (-1)^k r_0 + 4(-1)^h r_1}, \\ E(\theta_2) &= \frac{1}{t_0 + 2t_1 - (-1)^k (r_0^2 + 2r_1^2)/r_0}, \\ E(\theta_3) &= \frac{1}{t_0 + 2t_1 + (-1)^k r_0 - 4(-1)^h r_1}. \end{aligned} \quad (13)$$

The results for all the possible cases, eight on the whole, are summarized in Table 1, along with eight examples of materials, extracted from [3]; Be is Beryllium, Tc is Technetium, Ti is Titanium, CdS is Cadmium-Sulphide, Cd-Zn is a Cadmium-Zinc alloy, Zn is Zinc, InSe is Indium Selenide and Cd-Mg is a Cadmium-Magnesium alloy. It is worth noticing that the same extremal value of $E(\theta)$ can change its nature as a function of ρ , while $E(\theta_2)$ does not depend upon h , confirming the remark above.

The expressions of $E(\theta_i)$ in eq. (13) can be given in a completely Cartesian form using eq. (3):

$$\begin{aligned} E(\theta_1) &= \frac{1}{S_{11}}, \\ E(\theta_2) &= \frac{4(S_{11} - 2S_{12} - S_{66} + S_{22})}{4S_{11}S_{22} - (2S_{12} + S_{66})^2}, \\ E(\theta_3) &= \frac{1}{S_{22}}. \end{aligned} \quad (14)$$

It should be remarked that the difference between the cases $k = 0$ and $k = 1$ does not appear explicitly with the Cartesian formalism. Anyway, eq. (4), it is easy to check that

$$k = 0 \iff S_{11} - 2S_{12} - S_{66} + S_{22} > 0. \quad (15)$$

Table 1: Extrema of the Young's modulus: polar formulae.

	θ_1	θ_2	θ_3	Example	
$k = 0$					
$h = 0$	$\rho \leq 1$	min	-	max	Be
	$\rho > 1$	absolute min	max	local min	Tc
		$(\theta_2 \in \{\pi/4, \pi/2\})$			
	$E(\theta_i)$	$\frac{1}{t_0+2t_1+r_0+4r_1}$	$\frac{1}{t_0+2t_1-r_0-2r_1^2/r_0}$	$\frac{1}{t_0+2t_1+r_0-4r_1}$	
	$k = 1$				
$h = 1$	$\rho \leq 1$	min	-	max	Ti
	$\rho > 1$	local max	min	absolute max	CdS
		$(\theta_2 \in \{0, \pi/4\})$			
	$E(\theta_i)$	$\frac{1}{t_0+2t_1-r_0+4r_1}$	$\frac{1}{t_0+2t_1+r_0+2r_1^2/r_0}$	$\frac{1}{t_0+2t_1-r_0-4r_1}$	
	$k = 0$				
$h = 1$	$\rho \leq 1$	max	-	min	Cd-Zn
	$\rho > 1$	local min	max	absolute min	Zn
		$(\theta_2 \in \{0, \pi/4\})$			
	$E(\theta_i)$	$\frac{1}{t_0+2t_1+r_0-4r_1}$	$\frac{1}{t_0+2t_1-r_0-2r_1^2/r_0}$	$\frac{1}{t_0+2t_1+r_0+4r_1}$	
	$k = 1$				
$h = 1$	$\rho \leq 1$	max	-	min	InSe
	$\rho > 1$	absolute max	min	local max	Cd-Mg
		$(\theta_2 \in \{\pi/4, \pi/2\})$			
	$E(\theta_i)$	$\frac{1}{t_0+2t_1-r_0-4r_1}$	$\frac{1}{t_0+2t_1+r_0+2r_1^2/r_0}$	$\frac{1}{t_0+2t_1-r_0+4r_1}$	

About the angle θ_2 , its value is

$$\theta_2 = \frac{1}{2} \arccos \frac{(-1)^{1+h-k}}{\rho} = \frac{1}{2} \arccos \frac{S_{22} - S_{11}}{S_{11} - 2S_{12} - S_{66} + S_{22}}. \quad (16)$$

Its polar expression gives immediately that for $k \neq h$, $0 \leq \theta_2 < \pi/4$, while for $k = h$, $\pi/4 \leq \theta_2 < \pi/2$. Hence, the intermediate minimum of $E(\theta)$ is located between 0 and $\pi/4$, while the intermediate maximum between $\pi/4$ and $\pi/2$ for $h = 0$, prolate surfaces, and the exact contrary for the oblate surfaces, $h = 1$, see Table 1.

It is evident that angle θ_2 , and hence the second (intermediate) stationary value of the Young's modulus, exists if and only if the argument of function $\arccos$ in eq. (16) is admissible, i.e. if and only if

$$\rho > 1 \iff r_0 > r_1, \quad (17)$$

or equivalently if and only if

$$|S_{22} - S_{11}| < |S_{11} - 2S_{12} - S_{66} + S_{22}|. \quad (18)$$

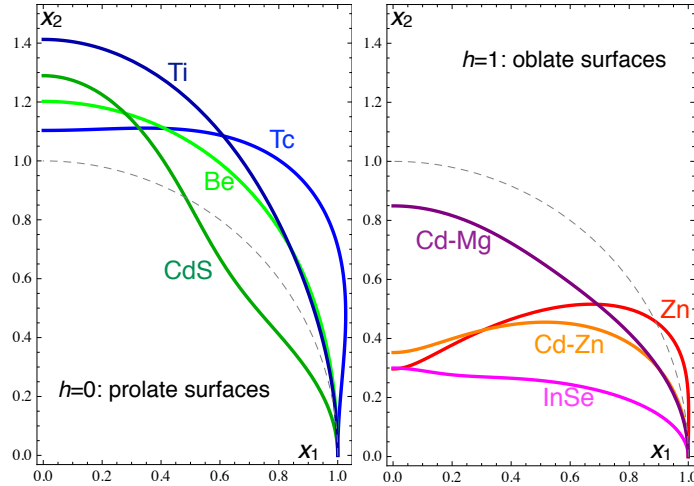


Figure 2: Normalized directional diagrams of $E(\theta)$ for the eight materials in Table 2. The dashed line represents the isotropic case

Eight examples, referring to the materials presented in Table 1, are presented in Table 2. The variation of the $E(\theta)$ for these eight cases is presented

Table 2: Numerical values for the eight materials cited in Table 1; the Young’s moduli are in GPa, the Cartesian and polar components of $\mathbb{S}$ in $\text{GPa}^{-1} \times 10^{-3}$.

	Be	Tc	Ti	CdS	Cd-Zn	Zn	InSe	Cd-Mg
S_{11}	3.45	3.20	9.69	20.50	12.55	8.22	11.60	24.20
S_{22}	2.87	2.90	6.86	15.90	35.62	27.70	38.70	28.50
S_{12}	-0.05	-0.90	-1.82	-5.30	-9.76	-7.00	-7.50	-6.20
S_{66}	6.16	5.70	21.50	66.70	49.78	25.30	85.50	75.10
t_0	1.57	1.70	5.21	14.21	14.68	9.40	18.85	17.53
t_1	0.78	0.54	1.61	3.23	3.58	2.74	4.41	5.04
r_0	0.03	0.28	0.16	2.46	2.24	3.08	2.53	1.25
r_1	0.07	0.04	0.35	0.58	2.88	2.44	3.39	0.54
k	0	0	1	1	0	0	1	1
h	0	0	0	0	1	1	1	1
ρ	0.45	7.33	0.46	4.28	0.78	1.26	0.75	2.33
θ_2 ($^\circ$)	-	48.92	-	38.25	-	18.85	-	57.73
$E(\theta_1)$	289.86	312.50	103.20	48.78	79.68	121.65	86.21	41.32
$E(\theta_2)$	-	401.64	-	42.75	-	125.76	-	34.12
$E(\theta_3)$	348.43	344.83	145.77	62.89	28.07	36.10	25.84	35.09

in Fig. 2; the diagrams have been normalized with respect to $E(\theta = 0)$. In Fig. 3 the three-dimensional surface diagram of E is presented for these eight materials; following a consolidated habitude, the symmetry axis has been put in the vertical direction.

3. Conclusion

The problem of determining the extrema of the Young’s modulus has been addressed in this paper; it has been shown that it can be reduced to the search for the maxima and minima of the component S_{xx} of the compliance tensor $\mathbb{S}$ of an ordinarily orthotropic planar material. In such a case, the use of the polar tensor invariants reduces the problem to an almost trivial one, with the advantage that the different possible cases, actually only eight, are determined by three non negative dimensionless parameters: k , an inte-

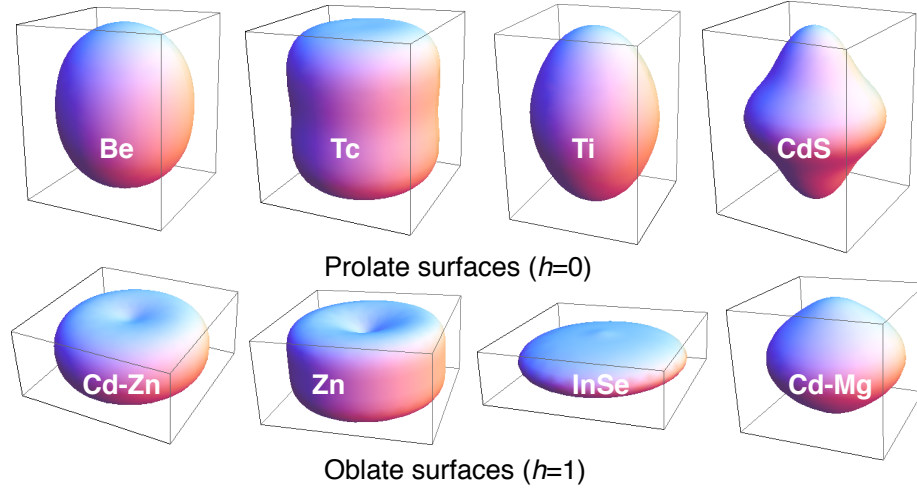


Figure 3: Normalized three-dimensional diagrams of E for the eight materials in Table 2.

ger invariant accounting for the type of planar ordinary orthotropy, h , still an integer, taking into account for the type of the surface representing E , and the ratio ρ , representing the relative importance of the two compliance anisotropy phases, r_0 and r_1 .

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