

Irreducible Parts of Elastic Compliance Tensor and Anisotropy

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Abstract: Irreducible parts of elastic compliance (modulus) tensor are presented. It is shown that Voigt average (polycrystalline) elastic constant can be obtained from the scalar parts of the elastic constant irreducible parts. It is also shown that the volumetric compressibility is directly related to the first irreducible scalar part of the elastic compliance tensor and this relation holds for all symmetries of the linearly anisotropy materials. Norm concept of Cartesian Tensor is given. The norm of a Cartesian Tensor is used as a criterion for representing and comparing the overall effect of a certain property of the same or different symmetry. The norm of elastic compliance tensor and the norms of the irreducible parts for different materials are calculated. The relation of the scalar parts norm and the other parts norms and the anisotropy of the material are presented.

Key Words: Irreducible tensor, Norm, Isotropic, Anisotropy, Elastic Compliance

Elastic Compliance Tensor Decomposition:

The constitutive relation characterizing linear anisotropic solids is the generalized Hook's law Nye, 1964:

$$\sigma_{ij} = C_{ijkl} \epsilon_{kl}, \quad \epsilon_{ij} = S_{ijkl} \sigma_{kl} \quad (1)$$

Where σ_{ij} and ϵ_{kl} are the symmetric second rank stress and strain tensors, respectively C_{ijkl} is the fourth-rank elastic stiffness tensor (elastic constant tensor) and S_{ijkl} is the elastic compliance tensor.

There are three index symmetry restrictions on these tensors. These conditions are:

$$S_{ijkl} = S_{jikl}, \quad S_{ijkl} = S_{ijlk}, \quad S_{ijkl} = S_{klij} \quad (2)$$

which the first equality comes from the symmetry of stress tensor, the second one from the symmetry of strain tensor, and the third one is due to the presence of a deformation potential. In general, a fourth-rank tensor has 81 elements. The index symmetry conditions (2) reduce this number to 21. Consequently, for most asymmetric materials (triclinic symmetry) the elastic constant tensor has 21 independent components. Elastic

constant tensor C_{ijkl} possesses the same symmetry properties as the elastic constant tensor S_{ijkl} and their connection is given by Teodosio, 1982:

$$C_{ijkl} S_{klmr} = \frac{1}{2} (\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}) \quad (3)$$

Where δ_{ij} is the Kronecker delta

The Einstein summation convention over repeated indices is used and indices run from 1 to 3 unless otherwise stated. Schouten (1954) has shown that: C_{ijkl} can be decomposed into two scalars, two deviators, and

one-nonor parts. The same decomposition in terms of the irreducible representations of the three-dimensional rotation group has been given in Heine (1960) as:

$$2D_0 + 2D_2 + D_4 \quad (4)$$

where the subscripts denote the weight of the representation. By applying the symmetry conditions (2) to the decomposition results obtained for a general fourth-rank tensor, the following reduction spectrum for the elastic compliance tensor is obtained. It contains two scalars, two deviators, and one-nonor parts:

$$S_{ijkl} = S_{ijkl}^{(0;1)} + S_{ijkl}^{(0;2)} + S_{ijkl}^{(2;1)} + S_{ijkl}^{(2;2)} + S_{ijkl}^{(4;1)} \quad (5)$$

Where

$$S_{ijkl}^{(0;1)} = \frac{1}{9} \delta_{ij} \delta_{kl} S_{ppqq} \quad (6)$$

$$S_{ijkl}^{(0;2)} = \frac{1}{90} (3\delta_{ik} \delta_{jl} + 3\delta_{il} \delta_{jk} - 2\delta_{ij} \delta_{kl}) (3S_{ppqq} - S_{ppqq}) \quad (7)$$

$$S_{ijkl}^{(2;1)} = \frac{1}{5} (\delta_{ik} S_{jplp} + \delta_{jk} S_{iplp} + \delta_{il} S_{jpkp} + \delta_{jl} S_{ipkp}) - \frac{2}{15} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) S_{ppqq} \quad (8)$$

$$S_{ijkl}^{(2;2)} = \frac{1}{7} \delta_{ij} (5S_{klpp} - 4S_{kplp}) + \frac{1}{7} \delta_{kl} (5S_{ijpp} - 4S_{ijlp}) - \frac{2}{35} \delta_{ik} (5S_{jlp} - 4S_{jlp}) - \frac{2}{35} \delta_{jl} (5S_{ikpp} - 4S_{iklp})$$

$$- \frac{2}{35} \delta_{il} (5S_{jkpp} - 4S_{jlp}) - \frac{2}{35} \delta_{jk} (5S_{ilpp} - 4S_{ilp}) + \frac{2}{105} (2\delta_{jk} \delta_{il} + 2\delta_{ik} \delta_{jl} - 5\delta_{ij} \delta_{kl}) (5S_{ppqq} - 4S_{ppqq}) \quad (9)$$

Radwan: Irreducible Parts of Elastic Compliance Tensor and Anisotropy

$$S_{ijkl}^{(4)} = \frac{1}{3}(S_{ijkl} + S_{ikjl} + S_{iljk}) - \frac{1}{21}[\delta_{ij}(S_{kipp} + 2S_{kplp}) + \delta_{ik}(S_{jppp} + 2S_{jplp}) + \delta_{il}(S_{jkpp} + 2S_{jpkp}) + \delta_{jk}(S_{iipp} + 2S_{iplp}) + \delta_{jl}(S_{ikpp} + 2S_{ipkp}) + \delta_{kl}(S_{ijpp} + 2S_{ijpl})] + \frac{1}{105}[(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})(S_{ppqq} + 2S_{ppqq})] \quad (10)$$

The scalar parts of the elastic constant tensor C_{ijkl} are:

$$C_{ijkl}^{(0,1)} = \frac{1}{9}\delta_{ij}\delta_{kl}C_{ppqq} \quad (11)$$

$$C_{ijkl}^{(2)} = \frac{1}{90}(3\delta_{ik}\delta_{jl} + 3\delta_{il}\delta_{jk} - 2\delta_{ij}\delta_{kl})(3C_{ppqq} - C_{ppqq}) \quad (12)$$

These parts are orthonormal to each other. Using Voigt's notation Nye (1964) for C_{ijkl} and S_{ijkl} can be expressed in 6 by 6 reduced matrix notation, where the matrix coefficients $C_{\mu\lambda}$ and S_{mn} are connected with the tensor

components C_{ijkl} and S_{ijkl} respectively by the recalculation rules:

$$C_{ijkl} = C_{\mu\lambda} \quad (ij \leftrightarrow \mu = 1, \dots, 6, kl \leftrightarrow \lambda = 1, \dots, 6):$$

That is:

$$11 \leftrightarrow 1, 22 \leftrightarrow 2, 33 \leftrightarrow 3, 23 \leftrightarrow 32 \leftrightarrow 4, 31 \leftrightarrow 13 \leftrightarrow 5, 12 \leftrightarrow 21 \leftrightarrow 6,$$

and

$$S_{ijkl} = S_{mn} \quad \text{When } m \text{ and } n \text{ are } 1, 2 \text{ or } 3,$$

$$2S_{ijkl} = S_{mn} \quad \text{When either } m \text{ or } n \text{ are } 4, 5 \text{ or } 6,$$

$$4S_{ijkl} = S_{mn} \quad \text{When both } m \text{ and } n \text{ are } 4, 5 \text{ or } 6.$$

Voigt Average (Polycrystalline) Elastic Constants: Elastic constants of a macroscopically isotropic polycrystalline aggregate in terms of the elastic constants of the constituent single crystals was first given by Voigt (1989), who assumed uniform strain throughout the aggregate and derived average elastic constants in terms of the single crystal elastic constants averaged over all possible orientations. Reuss (1980) assumed uniform stress and obtained average compliances in terms of the single crystal averaged over all directions. A different method was used in Leibfried (1953) and Povolo and Bolmaro (1987) to obtain the same average elastic constants by employing linear combinations of invariants

of C_{ijkl} . The above average elastic constants can be obtained from the scalar part of

C_{ijkl} , i.e. from the sum of (11) and (12) as follows

$$C_{ijkl} = \frac{1}{9}C_{ppqq}\delta_i\delta_j\delta_k\delta_l + \frac{1}{90}(C_{ppqq} - \frac{1}{3}C_{ppqq})[\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}] - \frac{1}{90}\delta_i\delta_j\delta_k\delta_l \quad (13)$$

where \bar{C}_{ijkl} denotes the macroscopically isotropic

polycrystalline elastic constant tensor. Using Voigt's

notation Nye (1964) for \bar{C}_{ijkl} , (13) can be expressed in

6 by 6 reduced matrix notation as:

$$\begin{pmatrix} \bar{c}_{11} & \bar{c}_{12} & \bar{c}_{13} & 0 & 0 & 0 \\ \bar{c}_{12} & \bar{c}_{22} & \bar{c}_{23} & 0 & 0 & 0 \\ \bar{c}_{13} & \bar{c}_{23} & \bar{c}_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{c}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \bar{c}_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & \bar{c}_{66} \end{pmatrix} = K_v \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$2G_v \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix} \quad (14)$$

From (14), we have:

$$\bar{c}_{11} = K_v + \frac{4}{3}G_v, \quad (15)$$

$$\bar{c}_{12} = K_v - \frac{2}{3}G_v \quad (16)$$

Where the Voigt average polycrystalline bulk and shear moduli are:

$$K_v = \frac{1}{9}C_{ppqq} = \frac{1}{3}(\bar{c}_{11} + 2\bar{c}_{12}) \quad (17)$$

and

$$G_v = \frac{1}{10}\left(C_{ppqq} - \frac{1}{3}C_{ppqq}\right) = \frac{1}{2}(\bar{c}_{11} - \bar{c}_{12}) = \bar{c}_{44} \quad (18)$$

The above results are the same as those given in Voigt (1989) and Hearmon (1961). Thus, we have established the macroscopically isotropic polycrystalline elastic constants, which were obtained by Voigt in 1889, can be

obtained directly from the scalar irreducible parts of C_{ijkl}

Isotropic Elastic Constant Tensor and Stress-Strain

Relation: A material is isotropic with respect to certain properties if these properties are the same in all directions. The isotropic elastic constant tensor elements in matrix form are:

$$\begin{pmatrix} c^{11} & c^{12} & c^{12} & 0 & 0 & 0 \\ c^{12} & c^{11} & c^{12} & 0 & 0 & 0 \\ c^{12} & c^{12} & c^{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}(c^{11} - c^{12}) & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}(c^{11} - c^{12}) & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c^{11} - c^{12}) \end{pmatrix}$$

Radwan: Irreducible Parts of Elastic Compliance Tensor and Anisotropy

For isotropic elastic materials, there are only two irreducible parts, they are the following two scalar parts:

$$C_{ijkl}^{(0,1)} = \frac{1}{9} \delta_{ij} \delta_{kl} C_{ppqq} \quad (11)$$

$$C_{ijkl}^{(0,2)} = \frac{1}{90} (3\delta_{ik}\delta_{jl} + 3\delta_{il}\delta_{jk} - 2\delta_{ij}\delta_{kl}) (3C_{ppqq} - C_{ppqq}) \quad (12)$$

Their 6 by 6 reduced matrix form are:

$$C_{\mu\lambda}^{(0,1)} = K \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (19)$$

$$C_{\mu\lambda}^{(0,2)} = \frac{G}{3} \begin{pmatrix} 4 & -2 & -2 & 0 & 0 & 0 \\ -2 & 4 & -2 & 0 & 0 & 0 \\ -2 & -2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix} \quad (20)$$

Where

$$K = \frac{1}{3}(c_{11} + 2c_{12})$$

is the bulk modulus and

$$G = \frac{1}{2}(c_{11} - c_{12})$$

is the shear modulus, here c_{11} and c_{12} are the elastic constants in two indices notation.

The sum of (11) and (12) becomes:

$$C_{ijkl} = K\delta_{ij}\delta_{kl} + 2G \left[\frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) - \frac{1}{3}\delta_{ij}\delta_{kl} \right] \quad (21)$$

Equation (21) is an expression for C_{ijkl} in terms of

K and G which is different than the traditionally known

$$\text{form: } C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \quad (22)$$

Where $\mu (=G)$ and λ are the Lamé's constants.

From (1) and (21) the stress-strain relation, for isotropic solids, can be defined as:

$$\sigma_{ij} = Ke_{rr}\delta_{ij} + 2G \left(e_{ij} - \frac{1}{3}e_{rr}\delta_{ij} \right) \quad (23)$$

This is also different than the traditionally known form:

$$\sigma_{ij} = \lambda e_{rr}\delta_{ij} + 2\mu e_{ij} \quad (24)$$

Equation (23) was obtained in Landau and Lifshits (1959) by a different method, which was based on the expansion of the strain energy density function in powers

of ϵ_{ij} . The decomposition of

σ_{ij} into spherical and deviatoric parts is:

$$\sigma_{ij} = \frac{1}{3}\sigma_{rr}\delta_{ij} + \left(\sigma_{ij} - \frac{1}{3}\sigma_{rr}\delta_{ij} \right) \quad (25)$$

The resultant equation, which is obtained by writing the hand sides of (23) and (25) equal to each other, can be broken down into independently operating physically meaningful parts Borodich (1963):

$$J_1 = 3KI_1 \quad (26)$$

and

$$\left(\sigma_{ij} - \frac{1}{3}\sigma_{rr}\delta_{ij} \right) = 2G \left(\epsilon_{ij} - \frac{1}{3}\epsilon_{rr}\delta_{ij} \right) \quad (27)$$

Where

$J_1 = \sigma_{ii}$ and $I_1 = \epsilon_{ii}$ are the first fundamental invariants of

stress and strain tensors, respectively.

It is known Landau and Lifshits (1959) and Borodich (1963) that (26) represents volume-change without distortion under hydrostatic stress and (27) represents shape-change without volume-change under deviatoric stress (or pure shear stress).

Similarly, the strain energy density W can be separated into two independently operating parts Fraijs and deVeubeke (1979):

$$W = W_1 + W_2 = \frac{1}{2}KI_1^2 - 2G\Gamma_2 \quad (28)$$

Where

Γ_2 is the second fundamental invariant of strain

deviator,

energy part, $W_1 = \frac{1}{2}KI_1^2$ is the volume-change

Radwan: Irreducible Parts of Elastic Compliance Tensor and Anisotropy

$$W_2 = -2G\Gamma_2$$

is the shape-change energy part.

We conclude that the separation of (23) and (28) into two independently operating meaningful parts is a direct consequence of (22) and of the two irreducible

orthonormal scalar parts (11) and (12) of C_{ijkl}

Volumetric Compressibility of Anisotropic Materials: Volumetric compressibility is defined as the relative reduction of material's volume under unit hydrostatic pressure.

The uniform stress tensor or hydrostatic compression is:

$$\sigma_{kl} = -p\delta_{kl}$$

The strains due to hydrostatic compression are:

$$\varepsilon_{ij} = -pS_{ijkl}\delta_{kl} = -pS_{ijkk}$$

and volumetric compression is:

$$\Delta = \Delta V / V = \varepsilon_{ii} = -pS_{iikk}$$

Where V is the volume of the crystal.

Consequently the volumetric compressibility is:

$$-\frac{\Delta}{p} = S_{iikk} = s_{11} + s_{22} + s_{33} + 2(s_{12} + s_{23} + s_{13}) = S_{ppqq}$$

which implies that the volumetric compressibility is related to the first scalar part of elastic compliance tensor for anisotropic materials.

The Norm Concept: Generalizing the concept of the modulus of a vector, norm of a Cartesian tensor (or the modulus of a tensor) is defined as the square root of the contracted product over all indices with itself:

$$N = \|T\| = \left\{ T_{ijkl} \dots T_{ijkl} \dots \right\}^{1/2}$$

Denoting rank-n Cartesian $T_{ijkl} \dots$, by T_n , the square of the norm is expressed as Jerphagnon *et al.* (1978):

$$N^2 = \|T\|^2 = \sum_{j,q} \|T^{(j,q)}\|^2 = \sum_{(n)} T_{(n)} T_{(n)} = \sum_{(n),j,q} T_{(n)}^{(j,q)} T_{(n)}^{(j,q)}$$

This definition is consistent with the reduction of the tensor in tensor in Cartesian formulation when all the irreducible parts are embedded in the original rank-n tensor space.

Since the norm of a Cartesian tensor is an invariant quantity, we suggest the following:

Rule1. The norm of a Cartesian tensor may be used as a criterion for representing and comparing the overall effect of a certain property of the same or different

symmetry. The larger the norm value, the more effective the property is.

It is known that the anisotropy of the materials, i.e., the symmetry group of the material and the anisotropy of the measured property depicted in the same materials may be quite different. Obviously, the property, tensor must show, at least, the symmetry of the material. For example, a property, which is measured in a material, can almost be isotropic but the material symmetry group itself may have very few symmetry elements. We know that, for isotropic materials, the elastic compliance tensor has two irreducible parts, i.e., two scalar parts, so the norm of the elastic compliance tensor for isotropic materials depends only on the norm of the scalar parts,

i.e., $N = N_s$. Hence, the ratio $\frac{N_s}{N} = 1$ for isotropic

materials. For anisotropic materials, the elastic constant tensor additionally contains two deviator parts and one

nonor part, so we can define $\frac{N_d}{N}$ for the deviator irreducible parts and

$\frac{N_n}{N}$ for nonor parts. Generalizing this to irreducible

tensors up to rank four, we can define the following

norm ratios: $\frac{N_s}{N}$ for scalar parts, $\frac{N_v}{N}$ for vector parts, $\frac{N_d}{N}$

for deviator parts, $\frac{N_{sc}}{N}$ for septor parts, and $\frac{N_n}{N}$

for nonor parts. It is to be noted that we calculate norms for weights only, i.e., for values of $j = 0, 1, 2, 3, 4$. Although norm ratios of different irreducible parts represent the anisotropy of that particular irreducible part, they can also be used to assess the anisotropy degree of a material property as a whole, we suggest the following two more rules:

Rule 2. When N_s is dominating among norms of

irreducible parts: the closer the norm ratio $\frac{N_s}{N}$ is to one, the closer the material property is isotropic.

Rule3. When N_s is not dominating or not present, norms of the other irreducible parts can be used as a criterion. But in this case the situation is reverse; the larger the norm ratio value we have, the more anisotropic the material property is.

The square of the norm of the elastic compliance tensor

S_{mn} , is:

$$\|N\|^2 = \sum_{mn} \{s_{mn}^{(01)}\}^2 + \sum_{mn} \{s_{mn}^{(02)}\}^2 + 2 \sum_{mn} \{s_{mn}^{(01)} s_{mn}^{(02)}\} + \sum_{mn} \{s_{mn}^{(21)}\}^2 + \sum_{mn} \{s_{mn}^{(22)}\}^2$$

$$+ 2 \sum_{mn} \{s_{mn}^{(21)} s_{mn}^{(22)}\} + \sum_{mn} \{s_{mn}^{(41)}\}^2 \quad (29)$$

Radwan: Irreducible Parts of Elastic Compliance Tensor and Anisotropy

Table 1: Compliances at room temperature (unit = $10^{-12} \text{ cm}^2 / \text{dync}$)

Crystal	Class	S_{11}	S_{12}	S_{44}	S_{33}	S_{13}	S_{14}	S_{66}
Sodium Chloride	m3m	2.21	-0.45	07.83	-	-	-	-
Aluminum	m3m	1.59	-0.58	03.52	-	-	-	-
Copper	m3m	1.49	-0.63	01.33	-	-	-	-
Nickel	m3m	0.79	-0.31	00.84	-	-	-	-
Tungsten	m3m	0.25	-0.07	00.66	-	-	-	-
Sodium Chlorate	23	2.20	-0.60	80.60	-	-	-	-
Tin	4/mmm	1.85	-0.99	05.70	1.18	-0.25	-	13.5
ADP	42m	1.80	00.70	11.30	4.30	-1.10	-	16.2
Zinc	6/mmm	0.84	00.11	02.64	2.87	-0.78	-	-
Cadmium	6/mmm	1.23	-0.15	05.40	3.55	-0.93	-	-
Quartz	32	1.27	-0.17	02.01	0.97	-0.15	-0.430	-
Tourmaline	3m	0.40	-0.10	01.51	0.63	-0.01	00.058	-

ADP: Ammonium dihydrogen phosphate. By using Table 1 and the decomposition of the elastic tensor, we calculated the norms and norm ratios as in Table 2.

Table 2: The norms and norm ratios (the anisotropy degree)

Crystal	N_1	N_2	N_3	N	N_1/N	N_2/N	N_3/N
Tungsten	01.2397162	0	0	01.2397262	1.000000	0	0
Aluminum	07.2117795	0	0.6661711	07.2424822	0.995761	0	0.9198100
Sodium Chloride	12.837292	0	2.0391336	12.998236	0.987618	0	0.1568777
Sodium chlorate	13.8802020	0	2.4372115	14.0925510	0.9849318	0	0.1729432
Nickel	02.6160401	0	1.1194925	02.8455103	0.9193571	0	0.3934241
Copper	04.6715122	0	2.3640952	05.2356444	0.8922516	0	0.4515385
ADP	19.2765000	1.387309	7.7853870	20.8355500	0.9251730	0.066583	0.3736580
Tin	12.5106800	4.310237	4.3698460	13.9352400	0.8977730	0.309305	0.3135820
Cadmium	09.0989770	3.319803	0.9211400	09.7293900	0.9352100	0.341210	0.0946800
Zinc	05.5425590	2.641131	1.9535371	06.4430200	0.8602400	0.409920	0.3032300
Tourmaline	00.3162510	0.318069	0.3618600	02.3658200	0.9790500	0.134440	0.1529500
Quartz	04.6469620	0.566354	1.1244600	04.8145000	0.9652000	0.117630	0.2335600

From Table (2) we can notice that in the first six crystals (which are cubic symmetry) the most isotropic material is Tungsten, in the next two crystals (which are Tetragonal symmetry) ADP is more isotropic than Tin, in the next two crystals (which are Hexagonal symmetry) Cadmium is more isotropic than Zinc, and in the next two crystals (which are Trigonal symmetry) Tourmaline is more isotropic than Quartz.

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