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A general elastic-anisotropy measure

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We propose an elastic-anisotropy measure. Zener's familiar anisotropy index $A=2C_{44}/(C_{11}-C_{12})$ applies only to cubic symmetry [*Elasticity and Anelasticity of Metals* (University of Chicago Press, Chicago, 1948), p. 16]. Its extension to hexagonal symmetry creates ambiguities. Extension to orthorhombic (or lower) symmetries becomes meaningless because $C_{11}-C_{12}$ loses physical meaning. We define elastic anisotropy as the squared ratio of the maximum/minimum shear-wave velocity. We compute the extrema velocities from the Christoffel equations [M. Musgrave, *Crystal Acoustics* (Holden-Day, San Francisco, 1970), p. 84]. The measure is unambiguous, applies to all crystal symmetries (cubic-triclinic), and reduces to Zener's definition in the cubic-symmetry limit. The measure permits comparisons between and among different crystal symmetries, say, in allotropic transformations or in a homologous series. It gives meaning to previously unanswerable questions such as the following: is zinc (hexagonal) more or less anisotropic than copper (cubic)? is alpha-uranium (orthorhombic) more or less anisotropic than delta-plutonium (cubic)? The most interesting finding is that close-packed-hexagonal elements show an anisotropy near 1.3, about half that of their close-packed-cubic counterparts. A central-force near-neighbor model supports this finding. © 2006 American Institute of Physics. [DOI: 10.1063/1.2338835]

I. INTRODUCTION

In the 1930s, Zener began to emphasize the importance of elastic anisotropy in mechanical-physical processes.¹ For cubic-symmetry crystals, Zener defined an elastic-anisotropy index,

$$A = 2C_{44}/(C_{11} - C_{12}). \quad (1)$$

Here, the three C_{ij} denote the three independent cubic-symmetry elastic-stiffness coefficients, the Voigt coefficients. C_{44} represents resistance to shear on $\{100\}$ in $\langle 0kl \rangle$, while $(C_{11}-C_{12})/2$ represents resistance to shear on $\{110\}$ in $\langle -110 \rangle$. Thus, A represents the ratio of the two extreme elastic-shear coefficients. For most materials, $A > 1$; but for many bcc elements and for many compounds, $A < 1$. Except accidentally, one never expects isotropic behavior, $A = 1$.

Elastic anisotropy plays a key role in many mechanical-physical properties. These properties include unusual phonon modes,² phase transformations,³ precipitation,⁴ dislocation dynamics,⁵ anisotropic plastic deformation,⁶ anomalous bcc slip,⁷ mechanical yield points,⁸ crack behavior,⁹ elastic instability,¹⁰ internal friction,¹¹ and strenuous tests of *ab initio* theory calculations.¹² A fascinating elastic-anisotropy application occurs in geophysics: some Earth models take the inner core as a gigantic cph-iron monocrystal with its c axis aligned with Earth's magnetic poles.¹³ In geophysics, seismic anisotropy constitutes a huge topic, focusing on many problems, for example, aligned olivine (orthorhombic) crystals in the upper mantle, amounting essentially to an Earth-encircling monocrystal.¹⁴

Applying Eq. (1) to other crystal symmetries produces immediate difficulties. For example, hexagonal-symmetry crystals possess more than two independent shear moduli.

Beside C_{44} and $C_{66}=(C_{11}-C_{12})/2$, there exists a third independent principal shear coefficient given by¹⁵

$$C = (1/6)(C_{11} + C_{12} + 2C_{33} - 4C_{13}). \quad (2)$$

Thus, no unique shear-coefficient ratio exists. For zinc, for example, taking the three possible ratios of these three shear elastic coefficients yields anisotropies of 0.61, 2.64, and 3.36.¹⁵ For orthorhombic symmetry, other difficulties arise: mainly $C_{11}-C_{12}$ loses physical meaning; it fails to correspond to any wave with a propagation direction \mathbf{n} and a polarization direction \mathbf{p} .

Here, we generalize Eq. (1) to any symmetry, including triclinic. Basically, we solve Christoffel's equations for the minimum and maximum quasishear-wave velocities. Here, *quasi* means the three orthogonal vibration (polarization) directions do not contain the wave-propagation direction. Physically, except along high-symmetry crystallographic directions, waves propagate in one direction; the elastic-energy flux propagates in a slightly different direction.¹⁶ In extremely anisotropic crystals, the quasishear/quasilongitudinal distinction breaks down; a quasishear velocity may exceed the quasilongitudinal velocity in some crystal directions. These cases need special care, and we ignore them here.

II. ANALYSIS

We invoke the well-known relationship connecting elastic-stiffness coefficient with mass density and sound velocity,

$$C = \rho v^2. \quad (3)$$

Substitution into Eq. (1) gives

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TABLE I. Elastic anisotropies and crystallographic aspect ratios of cph crystals.

	A^*	c/a
Be	1.22	1.58
Cd	2.18	1.89
α -Co	1.49	1.62
α -Dy	1.12	1.57
α -Er	1.13	1.57
α -Gd	1.17	1.59
α -Hf	1.18	1.58
Ho	1.12	1.57
α -Lu	1.04	1.58
Mg	1.19	1.62
α -Nd (dcph)	1.37	1.62
α -Pr (dcph)	1.47	1.61
Re	1.37	1.62
Ru	1.17	1.58
α -Sc	1.33	1.59
α -Tb	1.15	1.58
α -Ti	1.49	1.59
α -Tl	3.39	1.60
Y	1.18	1.57
Zn	2.39	1.86
α -Zr	1.38	1.59
Average (21)	1.45 ± 0.56	
Average (18)	1.31 ± 0.26	

$$A^* = v_2^2/v_1^2. \quad (4)$$

Here, v_1 and v_2 denote the minimum and maximum shear-sound-wave velocities among all propagation directions \mathbf{n} and polarization directions \mathbf{p} . Equation (4) applies to all seven crystal symmetries, from cubic through triclinic.

We solve for v_1 and v_2 numerically by considering many \mathbf{n} vectors and simply noting the two extrema values obtained from the Christoffel equations,¹⁶

$$\det(C_{ijkl}n_i n_j - \rho v^2 \delta_{ij}) = 0 \quad (\text{usual Einstein summation convention}). \quad (5)$$

Here, C_{ijkl} denotes the full fourth-order elastic-stiffness tensor, n_i the components of the wave-propagation vector, ρ the mass density, v the sound-wave velocity, and δ_{ij} the Kronecker operator. [Note that we use the same indices for C_{ij} and C_{ijkl} , believing that the contracted two-index ($i=1-6$) case creates no confusion with the four-index ($i=1-3$) case.] In solving Eq. (5), we used 10 000 vectors generated randomly. Equation (5) yields three (usually distinct) eigenvalues ρv^2 , one for a quasilongitudinal wave and two for quasitransverse waves, fast and slow. We use only two: the fast and slow quasishear-wave velocities. Using Voigt's contracted notation, defining $\Gamma_{ij} = C_{ijkl}n_k n_l$, then the most general (lowest symmetry, triclinic) set of Christoffel coefficients becomes¹⁶

$$\Gamma_{11} = C_{11}n_1^2 + C_{66}n_2^2 + C_{55}n_3^2 + 2(C_{16}n_1n_2 + C_{15}n_1n_3 + C_{56}n_2n_3), \quad (6a)$$

TABLE II. Elastic anisotropies of cubic-hexagonal allotropes.

	A_{cubic}	$A_{\text{hexagonal}}^*$
Co	3.49	1.49
Co-Ni	3.15	1.66
Ti	5.0	1.49
Zr	2.07	1.38

$$\Gamma_{22} = C_{66}n_1^2 + C_{22}n_2^2 + C_{44}n_3^2 + 2(C_{26}n_1n_2 + C_{46}n_1n_3 + C_{24}n_2n_3), \quad (6b)$$

$$\Gamma_{33} = C_{55}n_1^2 + C_{44}n_2^2 + C_{33}n_3^2 + 2(C_{45}n_1n_2 + C_{35}n_1n_3 + C_{34}n_2n_3), \quad (6c)$$

$$\Gamma_{12} = C_{16}n_1^2 + C_{26}n_2^2 + C_{45}n_3^2 + (C_{12} + C_{66})n_1n_2 + (C_{14} + C_{56})n_1n_3 + (C_{25} + C_{26})n_2n_3, \quad (6d)$$

$$\Gamma_{13} = C_{15}n_1^2 + C_{46}n_2^2 + C_{35}n_3^2 + (C_{14} + C_{56})n_1n_2 + (C_{13} + C_{55})n_1n_3 + (C_{36} + C_{45})n_2n_3, \quad (6e)$$

$$\Gamma_{23} = C_{56}n_1^2 + C_{24}n_2^2 + C_{34}n_3^2 + (C_{25} + C_{46})n_1n_2 + (C_{36} + C_{45})n_1n_3 + (C_{23} + C_{44})n_2n_3. \quad (6f)$$

Here, the gammas show symmetry: $\Gamma_{ij} = \Gamma_{ji}$.

III. RESULTS

Table I shows calculated anisotropies for 21 cph metals. We omit references to the original C_{ij} , which occur elsewhere,¹⁷ and because exact C_{ij} values are unimportant for present discussion and arguments. Table II shows anisotropies for four cases where C_{ij} exist for both cubic and hexagonal allotropes. Table III shows results for homologous electron-configuration pairs. Table IV shows Mendeleev-table adjacent pairs that show both fcc and cph structures. Table V shows results for lanthanides-actinides.

IV. DISCUSSION

First, we discuss the cph results in Table I. These elements show an average value of 1.45 ± 0.56 . (Eliminating the three outliers Cd, Tl, and Zn yields much smaller deviations.) Previous results for fcc metals¹⁸ show a much higher average of 2.76 ± 0.80 . Although both crystal structures are close packed, cubic materials show twice the anisotropy of hex-

TABLE III. Anisotropies of Mendeleev-table homologous fcc-cph and bcc-cph pairs.

	A (cubic)	A^* (hexagonal)
Ca-Mg	3.40	1.12
Sr-Mg	2.39	1.12
Ir-Co	1.56	1.49
Pb-Sn	4.08	4.13 (tetragonal)
Ba-Mg	1.34	1.12
Fe-Ru	2.41	1.17

TABLE IV. Anisotropies of Mendeleev-table adjacent pairs, fcc-cph.

	A (fcc)	A* (cph)
Ca-Sc	3.40	1.33
Cu-Zn	3.16	2.39
Sr-Y	2.39	1.18
Ag-Cd	2.88	2.18

agonal materials. [The hexagonal case is close packed only for the ideal c/a ratio $(8/3)^{1/2}$.] Relaxing the structure from cubic to hexagonal (introducing a c/a ratio) lowers the anisotropy. This finding presents a big surprise because the structures show the same 1 and 2 nn numbers and relative distances, and even the 3 nn numbers and distances differ only slightly. What explains the large fcc-cph anisotropy difference?

To try to understand the low elastic anisotropy, we use a central-force interatomic potential $\phi(r)$ and consider only nearest-neighbor interactions, thus a single “spring constant.” In such a model, the total energy is given by

$$U = (1/2V^0) \sum \phi(r). \quad (7)$$

Here V^0 denotes the undeformed atomic volume and summation occurs over all atomic pairs. The fourth-rank-tensor Brugger elastic coefficients are given by¹⁹

$$C_{ijkl} = \frac{\partial^2 U}{\partial \eta_{ij} \partial \eta_{kl}} = \frac{1}{2V^0} \left[\sum D^2 \phi(r) r_i^0 r_j^0 r_k^0 r_l^0 \right]. \quad (8)$$

Here $D\phi(r)$ denotes $(1/r)[\partial\phi(r)/\partial r]$, r_i^0 components of the interatomic-distance vector, and η_{ij} components of the Lagrangian elastic-strain matrix. Further details on this type of calculation occur elsewhere.^{20,21} Close-packed-hexagonal lattices possess 12 neighbors at distance r , six neighbors at $\sqrt{2}r$ and 21 neighbors at $\sqrt{8/3}r$. Then, using Eq. (8), as described by Johnson,²⁰ but ignoring the volume-dependent term, we obtain the following Voigt-contraction ($C_{ijkl} \rightarrow C_{ij}$) matrix representation of the elastic-stiffness coefficients:

TABLE V. Anisotropies of lanthanides-actinides, in increasing atomic number.

	Structure	A*
γ -Ce	fcc	2.96
α -Pr	dcph	1.47
α -Nd	dcph	1.37
α -Gd	cph	1.59
α -Tb	cph	1.58
α -Dy	cph	1.57
Ho	cph	1.57
α -Er	cph	1.57
α -Lu	cph	1.04
α -Th	fcc	3.62
α -U	orthorhombic	2.08
δ -Pu (Ga)	fcc	7.03

$$C_{ij} = \frac{f}{12\sqrt{2}d} \begin{pmatrix} 29 & 11 & 8 & 0 & 0 & 0 \\ & 29 & 8 & 0 & 0 & 0 \\ & & 32 & 0 & 0 & 0 \\ & & & 8 & 0 & 0 \\ & & & & 8 & 0 \\ & & & & & 9 \end{pmatrix}. \quad (9)$$

Here f denotes the 1 nn spring constant, whose magnitude can be neglected because we shall focus on elastic-stiffness ratios, and d denotes the interatomic distance (the sphere diameter for close-packed spheres). (The spring constant's magnitude can be calculated from $f = \sqrt{2}Bd/4$, where B denotes bulk modulus.) This result can be found in both the classic Born-Huang book on crystal-lattice dynamics and in Leibfried's classic review on lattice theory of crystalline mechanical and thermal properties.^{22,23} Using Eq. (9), and calculating the elastic anisotropy as described above in Eq. (4) gives

$$A^* (\text{cph, central force, 1 nn}) = 1.40. \quad (10)$$

This theoretical result agrees surprisingly well with the average of measurements for 21 cph metals: 1.45 ± 0.56 .

The conclusion that cph metals show near elastic-isotropy emerged previously from Fast *et al.*,²⁴ who studied the hexagonal transition metals using first-principles electronic-structure calculations. They noted also that these materials nearly satisfy the Cauchy (central force) relationships: $C_{12} = C_{66}$ and $C_{13} = C_{44}$. Equation (9) breaks the $C_{12} = C_{66}$ condition because the cph primitive cell contains two atoms and the model allows for internal displacements: one sublattice moving against the other. Basically, this internal displacement explains the different elastic responses of the cph lattice compared with the fcc lattice, which possesses a one-atom primitive cell, thus no internal displacements during deformation. Although this internal displacement affects c/a , it is independent in the sense that one could calculate c/a -change effects without allowing internal displacement, that is the homogeneous-deformation case.

Lower elastic anisotropy means tighter bounds (Voigt-Reuss, Hashin-Shtrikman, and Kroner-upper-lower) when reducing the monocrystal C_{ij} to effective (average over direction) quasi-isotropic polycrystal averages. Thus, simple formulas suffice for most hexagonal materials, while highly anisotropic cubic metals require more sophisticated and complicated approaches.²⁵

Another perspective on the fcc-cph anisotropy difference comes from considering allotropes. For a few materials, we know the monocrystal elastic constants for both cubic and hexagonal phases. Table II summarizes these cases. We see a general result: for the same material, the cubic-symmetry anisotropy always exceeds the hexagonal-symmetry anisotropy. Omitted from the table, TI provides an exception to the rule, indicating either singular behavior or perhaps an error in its measured elastic coefficients. (TI shows another related oddness: against thermodynamic expectations, the lower-temperature hexagonal phase shows a lower elastic Debye temperature than the higher-temperature cubic phase.)

Another perspective comes from considering homologous elements, elements with same (or similar) electron configurations, and elements in the same column in Mendeleev's table. As shown in Table III, again we see lower anisotropy in the hexagonal case. The Pb–Sn result in Table III suggests that going to a lower symmetry such as tetragonal or orthorhombic may not decrease anisotropy, that reducing anisotropy requires changing point groups to one possessing a sixfold-rotation symmetry operator. For the rhombohedral crystals Bi, Hg, and Sb (threefold rotation), we calculated $A^* = 1.7, 3.6$, and 1.8 , much higher than the hexagonal case, a subgroup of rhombohedral.

Considering adjacent-atom pairs leads to the same result, as shown in Table IV. For all four cases where adding one electron effects a fcc-cph transformation, the hexagonal phase shows lower anisotropy.

The lanthanide-actinide elements shown in Table V share a common feature: f -electrons whose itinerant-localized balance affects strongly the material's elastic stiffness.²⁶ δ -Pu shows the highest-known elastic anisotropy of any fcc element. Among the elements in Table V, the lowest anisotropy appears in the hexagonal structures, which are double close packed. Several lanthanides-actinides (Am, Ce, La, Nd, and Pr) show a double-close-packed-hexagonal crystal structure. This structure shows stacking sequence $ABAC\dots$, versus the usual close-packed hexagonal $AB\dots$, and face-centered-cubic $ABC\dots$, hence a doubled c axis. Both close-packed and double-close-packed hexagonal structures show the same space group: $P6_3/mmc$ (No. 94). Thus, we expect the single and double hexagonal structures to show the same elastic and elastic-anisotropy behaviors. Thus, among the actinides, we expect Am to show low elastic anisotropy. As summarized by Young,²⁷ except for Eu, all 15 elements in the La–Lu series show hexagonal crystal structures at ambient temperature and pressure. Whether Sm with a nine-atom hexagonal unit cell fits the present pattern remains to be studied. Considering the early actinides, if close-packed structures occur they are fcc. Later actinides, beginning with Am, show cph structures. Alpha-plutonium may also show low elastic anisotropy. Although α -Pu shows a monoclinic crystal structure (space group No. 11), several studies emphasized its strong correspondence to a close-packed-plane-stacking crystal structure.²⁸ Choosing an alternative monoclinic unit cell reveals a connection to close packing.²⁹ Although orthorhombic (eight-atom unit cell) γ -Pu may show low elastic anisotropy because its layers along the c axis strongly resemble cph; they would be cph if the b/a ratio equaled 1.73 instead of 1.83. Concerning U (four-atom orthorhombic unit cell), as Donohue pointed out,³⁰ the 12 closest-neighbor atoms form a polyhedron that resembles a cph arrangement; thus, in U we expect a relatively low-moderate elastic anisotropy.

V. CONCLUSIONS

One can define a general elastic-anisotropy index A^* that includes all crystal symmetries, cubic through triclinic. For cubic symmetry, this index agrees with Zener's index: $A = 2C_{44}/(C_{11} - C_{12})$.

Close-packed-hexagonal elements group fairly tightly at a low-moderate elastic anisotropy: $A^* = 1.3 \pm 0.3$ (excluding three outliers). This contrasts with the fcc average of 2.8 ± 0.8 .

Low cph anisotropy can be confirmed by considering measurements on allotropes, homologous elements, Mendeleev-table-adjacent fcc-cph elements, and lanthanides-actinides.

For the close-packed-hexagonal case, a central-force first-neighbor-only model predicts $A^* = 1.40$, which agrees closely with observation.

Concepts developed here may apply usefully to lanthanides and higher actinides, which show many hexagonal-crystal-structure phases together with many lower-symmetry phases. The relevant concept here is that higher crystal symmetry may relate to higher elastic anisotropy.

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APPENDIX: ALTERNATIVE EQ. (9) DERIVATION

We can derive Eq. (9) more simply in a way that shows clearly the fcc-cph elastic-coefficient relationship. We start with a result from Born's equation of state for fcc lattices. For the fcc counterpart to Eq. (9), Born found the following elastic-coefficient matrix:³¹

$$c_{ij} = \frac{f}{\sqrt{2}d} \begin{pmatrix} 2 & 1 & 1 & 0 & 0 & 0 \\ & 2 & 1 & 0 & 0 & 0 \\ & & 2 & 0 & 0 & 0 \\ & & & 1 & 0 & 0 \\ & & & & 1 & 0 \\ & & & & & 1 \end{pmatrix} \quad (\text{A1})$$

Here, we use c_{ij} to denote cubic symmetry and C_{ij} to denote hexagonal symmetry. To convert to the cph case, we equate the two bulk moduli,

$$(2C_{11} + C_{22} + 2C_{12} + 4C_{13})/9 = (c_{11} + 2c_{12})/3. \quad (\text{A2})$$

We equate the elastic stiffnesses in the close-packed directions, $[-1100]$ and $[110]$,

$$C_{11} = (c_{11} + c_{12} + 2c_{44})/2. \quad (\text{A3})$$

And we equate the elastic stiffnesses in directions perpendicular to the close-packed planes, $[0001]$ and $[111]$,

$$C_{33} = (c_{11} + 2c_{12} + 4c_{44})/3. \quad (\text{A4})$$

Combining all these with the two Cauchy relationships $C_{12} = C_{66}$ and $C_{13} = C_{44}$ yields the following approximation to Eq. (9):

$$C_{ij} = \frac{f}{12\sqrt{2}d} \begin{pmatrix} 30 & 10 & 8 & 0 & 0 & 0 \\ & 30 & 8 & 0 & 0 & 0 \\ & & 28 & 0 & 0 & 0 \\ & & & 8 & 0 & 0 \\ & & & & 8 & 0 \\ & & & & & 10 \end{pmatrix}. \quad (\text{A5})$$

Computing the anisotropy, we get $A^* = 1.31$, lower by 6% than the more accurate, but more difficult to derive, value of 1.40. A principal failure of this approximation is the prediction that $C_{11} > C_{33}$, opposite observation for most materials.

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