

On symmetries of higher-order elastic constants

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In elastic crystals, a hyperelastic description is conventionally assumed, and the strain energy potential is idealized as a Taylor-series expansion in strain about an unstrained reference state. Coefficients of quadratic terms are second-order or linear elastic constants. Coefficients of higher-order terms are elastic constants of third order, fourth order, and so on. Recently published work by Telyatnik [*Acta Cryst.* (2024), **A80**, 394–404] extends prior knowledge of symmetry properties for anisotropic elastic constants of single crystals, as well as transversely isotropic and isotropic solids, to terms up to sixth order. Effective elastic constants for polycrystalline aggregates, with possible anisotropy, were reported by Telyatnik, in the same article, to the same order. A terse summary of nonlinear crystal elasticity and independent elastic constants of orders two and three are given in this commentary for context. Methods and results of Telyatnik, anticipated to be of great utility to crystal elasticity research, are then highlighted.

1. Nonlinear elasticity of crystals

Linear elasticity accurately describes the mechanical response of elastic solids when deformations are small and the stress–strain response is linear, meaning Hooke’s law applies. Linear elasticity theory (Voigt, 1910; Love, 1927; Hearmon, 1946) can be successfully applied to many, if not most, problems in structural mechanics. A nonlinear theory, on the other hand, is needed for accurate descriptions of mechanics of solids when deformations are large or when linearity breaks down.

All known solids are ultimately nonlinear. No finite volume of any real material can be compressed to a point of infinitesimal size: its bulk modulus must eventually increase with decreasing volume to prevent this. Nonlinear elasticity can describe wave propagation in pre-stressed crystals (Thurston & Brugger, 1964; Thurston *et al.*, 1966; Thurston, 1974) and short-range core effects from lattice defects (Teodosiu, 1982). At regimes departing more from linearity (Chang & Barsch, 1967), or in shock compression, elastic constants up to order four have been measured (Fowles, 1967; Graham, 1972). In strong crystals such as quartz, sapphire and diamond, large uniaxial compressive deformations can be reached before inelasticity from dislocation motion, deformation twinning or fracture ensues (Clayton, 2019). Chen *et al.* (2020) showed the importance of anisotropic constants up to fifth order on the stability of silicon.

Symmetries of second-order constants for anisotropic elasticity of crystals have been known for over a century (Voigt, 1910; Hearmon, 1946). Independent third-order constants have been known for all crystal classes since works by Fumi (1951) and Hearmon (1953), and those of fourth-order since the work of Brendel (1979). Measurements of third-order constants often rely on sound speeds in pre-

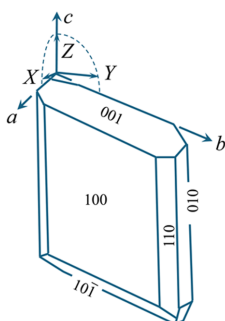


Table 1
Second-order elastic constants.

N, triclinic; M, monoclinic; O, orthorhombic; R, rhombohedral; T, tetragonal; H, hexagonal; C, cubic; iso, isotropic; I and II, classes of respective higher and lower symmetry. $A := \frac{1}{2}(C_{11} - C_{12})$. Bottom row: No. of independent constants. See Thurston (1974), Clayton (2011).

N	M	O	TII	TI	RII	RI	HII	HI	CII	CI	iso
11	11	11	11	11	11	11	11	11	11	11	11
12	12	12	12	12	12	12	12	12	12	12	12
13	13	13	13	13	13	13	13	13	12	12	12
14	0	0	0	0	14	14	0	0	0	0	0
15	15	0	0	0	15	0	0	0	0	0	0
16	0	0	16	0	0	0	0	0	0	0	0
22	22	22	11	11	11	11	11	11	11	11	11
23	23	23	13	13	13	13	13	12	12	12	12
24	0	0	0	0	-14	-14	0	0	0	0	0
25	25	0	0	0	-15	0	0	0	0	0	0
26	0	0	-16	0	0	0	0	0	0	0	0
33	33	33	33	33	33	33	33	11	11	11	11
34	0	0	0	0	0	0	0	0	0	0	0
35	35	0	0	0	0	0	0	0	0	0	0
36	0	0	0	0	0	0	0	0	0	0	0
44	44	44	44	44	44	44	44	44	44	44	A
45	0	0	0	0	0	0	0	0	0	0	0
46	46	0	0	0	-15	0	0	0	0	0	0
55	55	55	44	44	44	44	44	44	44	44	A
56	0	0	0	0	14	14	0	0	0	0	0
66	66	66	66	66	A	A	A	A	44	44	A
21	13	9	7	6	7	6	5	5	3	3	2

stressed crystals (Thurston & Brugger, 1964; Brugger, 1965; Thurston, 1974). Contemporary first-principles atomic simulations involving density functional theory (DFT) have been used to predict constants up to orders four and five (Chen *et al.*, 2020; Pandit & Bongiorno, 2023). Since elastic constants are ultimately related to interatomic forces (Born & Huang, 1954; Wallace, 1972), characteristics of elastic constants give insight into atomic-scale physics, and vice versa. Higher-order constants are associated with anharmonicity (Hiki & Granato, 1966; Hiki, 1981).

A brief primer is given here; theoretical presentations of nonlinear elasticity for anisotropic crystals are available in

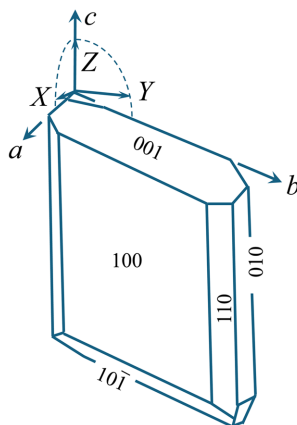


Figure 1
Standard coordinate axes $\{X_1, X_2, X_3\} \rightarrow \{X, Y, Z\}$ and natural lattice directions (a, b, c) for a triclinic class I crystal. Based on Brainerd *et al.* (1949) (redrawn by the author).

books on the subject (Thurston, 1974; Teodosiu, 1982; Clayton, 2011). Let $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$ be the spatial position vector of a material particle that occupied a reference position \mathbf{X} at some initial time $t = t_0$. Cartesian coordinates (x_k, X_K) with $k, K = 1, 2, 3$ are used for Euclidean 3-space, and repeated indices are summed. The deformation gradient $\mathbf{F}(\mathbf{X}, t)$ is the two-point tensor

$$\mathbf{F} = \partial \mathbf{x} / \partial \mathbf{X} \leftrightarrow F_{iJ} = \partial x_i / \partial X_J, \quad \det \mathbf{F} > 0. \quad (1)$$

Per the Cauchy–Born rule, primitive Bravais lattice vectors of a crystalline material at point (\mathbf{X}, t) deform affinely with $\mathbf{F}(\mathbf{X}, t)$ (Born & Huang, 1954; Clayton, 2011). The classical strain measure for nonlinear crystal elasticity is the Green–Lagrange strain (Wallace, 1972; Thurston, 1974; Clayton, 2011):

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T \mathbf{F} - \mathbf{1}) = \mathbf{E}^T \leftrightarrow E_{IJ} = \frac{1}{2}(F_{kI} F_{kJ} - \delta_{IJ}) = E_{JI}. \quad (2)$$

Strain energy per unit initial volume is $W(\mathbf{E}(\mathbf{F})) = \bar{W}(\mathbf{F})$. Isentropic or isothermal conditions are implied; elastic constants are isentropic or isothermal values. Cauchy (true) stress is

$$\boldsymbol{\sigma} = \frac{1}{\det \mathbf{F}} \mathbf{F} \frac{\partial W}{\partial \mathbf{E}} \mathbf{F}^T \leftrightarrow \sigma_{ij} = \frac{1}{\det F_{kK}} F_{iL} \frac{\partial W}{\partial E_{LM}} F_{jM}. \quad (3)$$

Using Greek indices $\alpha, \beta, \gamma, \dots = 1, 2, \dots, 6$ for Voigt notation (Thurston, 1974; Clayton, 2011), series expansion of W gives

$$W = W_0 + C_\alpha E_\alpha + \frac{1}{2} C_{\alpha\beta} E_\alpha E_\beta + \frac{1}{6} C_{\alpha\beta\gamma} E_\alpha E_\beta E_\gamma + \frac{1}{24} C_{\alpha\beta\gamma\delta} E_\alpha E_\beta E_\gamma E_\delta + \frac{1}{120} C_{\alpha\beta\gamma\delta\epsilon} E_\alpha E_\beta E_\gamma E_\delta E_\epsilon + \dots \quad (4)$$

The constant datum energy is W_0 , first-order $C_\alpha = 0$ for a stress-free reference state, second-order constants are $C_{\alpha\beta}$, third-order are $C_{\alpha\beta\gamma}$, and so on. Constants have implied symmetries:

$$C_{\alpha\beta} = C_{\beta\alpha}, \quad C_{\alpha\beta\gamma} = C_{\beta\alpha\gamma} = C_{\alpha\gamma\beta} = C_{\gamma\beta\alpha}, \quad \dots \quad (5)$$

For materials (*i.e.* crystal classes) of lowest (*i.e.* triclinic) symmetry, $C_{\alpha\beta}$ and $C_{\alpha\beta\gamma}$ have 21 and 56 independent components, respectively.

Denote by \mathbf{R} an orthogonal matrix ($\mathbf{R}^T \mathbf{R} = \mathbf{1}$) that belongs to the symmetry group of transformations for a given material (*e.g.* its Laue group or crystal class). Then $\bar{W}(\mathbf{R}\mathbf{F}) = \bar{W}(\mathbf{F})$ yields constraints among the elastic constants of each order dictated by that symmetry group. The greater the intrinsic symmetry, the more expansive the symmetry group, and heuristically the fewer independent elastic constants of a given order. For example, if a material is isotropic, \mathbf{R} can be any rotation, limiting the number of independent $C_{\alpha\beta}$ to two and $C_{\alpha\beta\gamma}$ to three.

For crystal structures, standard conventions are used to relate coordinate axes to directions in the lattice (Brainerd *et al.*, 1949); an example is shown in Fig. 1 for a triclinic crystal. Independent second- and third-order elastic constants (Fumi, 1951; Hearmon, 1953) for all 11 Laue groups and isotropic solids are reported for easy reference in Tables 1 and 2,

Table 2
Third-order elastic constants.

Notation in first row follows Table 1. $A := C_{111} + C_{112} - C_{222}$;
 $B := -\frac{1}{2}(C_{115} + 3C_{125})$; $C := \frac{1}{2}(C_{114} + 3C_{124})$; $D := -\frac{1}{4}(2C_{111} + C_{112} - 3C_{222})$;
 $E := -C_{114} - 2C_{124}$; $F := -C_{115} - 2C_{125}$; $G := -\frac{1}{2}(C_{115} - C_{125})$;
 $H := \frac{1}{2}(C_{114} - C_{124})$; $I := \frac{1}{4}(2C_{111} - C_{112} + C_{222})$; $J := \frac{1}{2}(C_{113} - C_{123})$;
 $K := -\frac{1}{2}(C_{144} - C_{155})$; $L := \frac{1}{2}(C_{112} - C_{123})$; $M := \frac{1}{4}(C_{111} - C_{112})$;
 $N := \frac{1}{8}(C_{111} - 3C_{112} + 2C_{123})$. Bottom row: No. of independent constants. See
 Thurston (1974), Clayton (2011).

N	M	O	TII	TI	RII	RI	HII	HI	CII	CI	iso
111	111	111	111	111	111	111	111	111	111	111	111
112	112	112	112	112	112	112	112	112	112	112	112
113	113	113	113	113	113	113	113	113	113	112	112
114	0	0	0	0	114	114	0	0	0	0	0
115	115	0	0	0	115	0	0	0	0	0	0
116	0	0	116	0	116	0	116	0	0	0	0
122	122	122	112	112	A	A	A	A	113	112	112
123	123	123	123	123	123	123	123	123	123	123	123
124	0	0	0	0	124	124	0	0	0	0	0
125	125	0	0	0	125	0	0	0	0	0	0
126	0	0	0	0	-116	0	-116	0	0	0	0
133	133	133	133	133	133	133	133	133	112	112	112
134	0	0	0	0	134	134	0	0	0	0	0
135	135	0	0	0	135	0	0	0	0	0	0
136	0	0	136	0	0	0	0	0	0	0	0
144	144	144	144	144	144	144	144	144	144	144	L
145	0	0	145	0	145	0	145	0	0	0	0
146	146	0	0	0	B	0	0	0	0	0	0
155	155	155	155	155	155	155	155	155	155	155	M
156	0	0	0	0	C	C	0	0	0	0	0
166	166	166	166	166	D	D	D	D	166	155	M
222	222	222	111	111	222	222	222	222	111	111	111
223	223	223	113	113	113	113	113	113	112	112	112
224	0	0	0	0	E	E	0	0	0	0	0
225	225	0	0	0	F	0	0	0	0	0	0
226	0	0	-116	0	116	0	116	0	0	0	0
233	233	233	133	133	133	133	133	133	113	112	112
234	0	0	0	0	-134	-134	0	0	0	0	0
235	235	0	0	0	-135	0	0	0	0	0	0
236	0	0	-136	0	0	0	0	0	0	0	0
244	244	244	155	155	155	155	155	155	166	155	M
245	0	0	-145	0	-145	0	-145	0	0	0	0
246	246	0	0	0	G	0	0	0	0	0	0
255	255	255	144	144	144	144	144	144	144	144	L
256	0	0	0	0	H	H	0	0	0	0	0
266	266	266	166	166	I	I	I	I	155	155	M
333	333	333	333	333	333	333	333	333	111	111	111
334	0	0	0	0	0	0	0	0	0	0	0
335	335	0	0	0	0	0	0	0	0	0	0
336	0	0	0	0	0	0	0	0	0	0	0
344	344	344	344	344	344	344	344	344	155	155	M
345	0	0	0	0	0	0	0	0	0	0	0
346	346	0	0	0	-135	0	0	0	0	0	0
355	355	355	344	344	344	344	344	344	166	155	M
356	0	0	0	0	134	134	0	0	0	0	0
366	366	366	366	366	J	J	J	J	144	144	L
444	0	0	0	0	444	444	0	0	0	0	0
445	445	0	0	0	445	0	0	0	0	0	0
446	0	0	446	0	145	0	145	0	0	0	0
455	0	0	0	0	-444	-444	0	0	0	0	0
456	456	456	456	456	K	K	K	K	456	456	N
466	0	0	0	0	124	124	0	0	0	0	0
555	555	0	0	0	-445	0	0	0	0	0	0
556	0	0	-446	0	-145	0	-145	0	0	0	0
566	566	0	0	0	125	0	0	0	0	0	0
666	0	0	0	0	-116	0	-116	0	0	0	0
56	32	20	16	12	20	14	12	10	8	6	3

following Brugger (1965), Thurston (1974) and Clayton (2011).

Also of theoretical interest are Cauchy symmetries arising if all interatomic forces are central, as from a pair potential (Love, 1927; Born & Huang, 1954). In tensor form, second-order constants then obey $C_{IJKL} = C_{IKJL} = C_{ILKJ}$; similar constraints arise at higher orders. In cubic classes of greatest symmetry, $C_{12} = C_{44}$, $C_{112} = C_{155}$ and $C_{123} = C_{144} = C_{456}$ in Voigt notation. In a Cauchy isotropic solid, $C_{\alpha\beta}$ and $C_{\alpha\beta\gamma}$ each contain but one independent constant, and Poisson's ratio $\nu = \frac{1}{4}$.

Symmetric second-order strain tensors differing from \mathbf{E} of (2) have been used in nonlinear elastic potentials akin to (4), with noted advantages for describing DFT (Nielsen, 1986) and shock (Clayton, 2019) data. Symmetries of elastic constant tensors of all orders are unchanged (e.g. Tables 1 and 2 remain valid) so long as the strain tensor has components referred to $\{X_K\}$; any such strain transforms the same under the action of \mathbf{R} . Values of $C_{\alpha\beta}$ are identical for all such strain measures, but values of $C_{\alpha\beta\gamma}$ and constants of successively higher orders generally differ, and (3) is transformed for strain different from \mathbf{E} . Another example is linear elasticity, for which the small strain tensor is $\boldsymbol{\epsilon} = \frac{1}{2}[\partial\mathbf{u}/\partial\mathbf{X} + (\partial\mathbf{u}/\partial\mathbf{X})^T]$ with displacement $\mathbf{u} = \mathbf{x} - \mathbf{X}$. To first order in $\partial\mathbf{u}/\partial\mathbf{X}$, $\boldsymbol{\epsilon} \approx \mathbf{E}$. Informally, when $|\mathbf{F} - \mathbf{1}| \ll 1$, $W_0 = 0$ and W is truncated at order two, (3) and (4) give Hooke's law:

$$\sigma_\alpha = \frac{\partial W}{\partial \epsilon_\alpha} = C_{\alpha\beta} \epsilon_\beta, \quad W = \frac{1}{2} C_{\alpha\beta} \epsilon_\alpha \epsilon_\beta. \quad (6)$$

The effective elastic constants of heterogeneous solids (e.g. polycrystalline aggregates) depend on the properties and orientations of constituents (Gnaupel-Herold, 2023). If an aggregate has a certain target symmetry, estimates or bounds on its effective 'averaged' constants can be obtained from theoretical averaging schemes. For second-order constants, well known estimates include upper and lower bounds of Voigt and Reuss, respectively, Hill's proposition (Hill, 1952) that interpolates between the two, and 'self-consistent' models (Kroner, 1958; De Wit, 1997). Such methods were extended to third-order constants for isotropic (Barsch, 1968; Lubarda, 1997) and textured (Johnson, 1985; Kube & Turner, 2016) polycrystals. Isotropic Voigt averages of fourth-order constants for aggregates of cubic crystals were derived by Krasilnikov & Vekilov (2019).

2. Nonlinear crystal elasticity to sixth order

Telyatnik (2024) recently developed numerically efficient algorithms for symbolic computations of effective elastic constants of orders two through six for polycrystalline aggregates having overall target symmetries of any crystal class, transverse isotropy or full isotropy. Constituent crystallites can have any anisotropy. Effective constants are defined as arithmetic averages over the minimal set of symmetry operations generating a given target symmetry. In cases of targeted transverse or full isotropy, continuous integrals replace discrete averages. For efficiency, nested calculations for higher symmetries apply precomputed averages from lower symmetries. Gauss-Jordan elimination is used to find algebraic

relationships among all elastic constants of a given order, for each target symmetry. Computations exceed capabilities of existing tools supplementing Vol. *D* of the *International Tables for Crystallography* (Authier & Zarembowitch, 2003).

Independent elastic constants and symmetry relationships for all crystal classes, transverse isotropy and full isotropy, for orders two through six, are provided in Appendix *A* of Telyatnik (2024) and Telyatnik (2021). Previously, such information (e.g. as in Tables 1 and 2) was available only for constants of all crystal classes and isotropy, to order four (Brendel, 1979). Averages for independent elastic constants, again up to sixth order, are given in Appendix *B* of Telyatnik (2024) and Telyatnik (2021). These include the target symmetries of all crystal classes, transverse isotropy and isotropy. Other appendices (Telyatnik, 2021; Telyatnik, 2024) list all components and rotation matrices. For anisotropic target symmetries, averages are defined as described in the preceding paragraph. These averages do not incorporate data on local crystal orientations (i.e. distribution functions) included in some prior definitions of effective third-order constants (Johnson, 1985; Kube & Turner, 2016). Therefore, anisotropic aggregate constants of Telyatnik (2024) cannot be expected to reproduce effective constants of textured polycrystalline metals, for example. However, these anisotropic aggregate values can serve as higher-symmetry approximations for constants of classes of lower true symmetry (Telyatnik, 2021).

For isotropic target symmetry, averaged constants (Telyatnik, 2024) are consistent with Voigt's postulate. Previous isotropic averages were usually limited to second and third orders, with the latter for constituents having cubic or hexagonal symmetry (Barsch, 1968; Lubarda, 1997; Kube & Turner, 2016). Previously, the highest known order of derived, isotropic Voigt-averaged constants was four, as reported in Appendix *A* of Krasilnikov & Vekilov (2019) for crystallites of general anisotropy (e.g. triclinic symmetry) and verified independently by Telyatnik (2024). Therefore, the isotropic Voigt-type averages for five independent fifth-order constants and seven independent sixth-order constants derived by Telyatnik (2024) appear to be a new and valuable contribution to nonlinear elasticity theory for solid crystals.

Finally, note that for some solids under extreme strain [e.g. rubbery polymers (Ogden, 1984) and biological tissues (Fung, 1993)] Taylor polynomials like (4) can be cumbersome so are often replaced with other functional forms (e.g. exponentials) needing fewer constants to fit data. These solids are often idealized as incompressible, for which (3) and (4) are inappropriate.

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