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Fourth-, Fifth- and Sixth-Order Elastic Constants in Crystals

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The fourth-order elastic constants (FOEC) of Laue groups *R*I, *R*II, *H*I, *C*II, and *I* have been calculated with the method of Hearmon. By use also of the results of Ghate for other Laue groups, the FOEC schemes for all crystal classes have been worked out. By the method of direct inspection the fifth- and sixth-order elastic constants have also been calculated for Laue groups *N*, *M*, *O*, *T*I, *T*II, *C*I, and *C*II. The number of independent constants for each Laue group agrees with the group-theoretical predictions.

Introduction

Recently there has been growing interest in the study of the higher-order elastic constants because of the experimental development in ultrasonic harmonic generation and wave interactions in solids (Lean & Tseng, 1970; Peters & Arnold, 1971; McMahon, 1968; Richardson, Thompson & Wilkinson, 1968). These rapid developments have been stimulated mainly by the possibility of utilization of the non-linear acoustical properties of solids for acoustic delay lines and similiar devices. Theoretical calculations of the effective higher-order elastic constants have been made in both piezoelectric and non-piezoelectric crystals (Mathus & Gupta, 1970). However, the analysis to orders higher than the third is still very incomplete. Birch (1947), Fumi (1951, 1952*a*, *b*, *c*, 1953) and Hearmon (1953) have derived the independent third-order constants for all crystal classes and Ghate (1964, 1965) has calculated the fourth-order constants for some crystal classes. Using a group-theoretical method, the number of independent elastic constants has been determined by Krishnamurty (1963) and Krishnamurty & Gopalakrishnamurty (1968) up to the fifth order, and by Chung (1972) to the sixth and seventh orders. Recently Barsch & Chang (1968) have discussed the effective elastic constants under hydrostatic pressure for cubic crystal symmetry. In principle, one should be able to express the effective constants of higher order in any other crystals if the higher-order constants at zero pressure are known.

It is the purpose of this paper to present the calculation and results for the fourth-order elastic constants (FOEC) for Laue groups *R*I, *R*II, *H*I, *H*II, *T*II, *C*II, and *I*, and the fifth-order elastic constants (FFOEC) and sixth-order elastic constants (SOEC) for Laue groups *N*, *M*, *O*, *T*I, *T*II, *C*I, and *C*II. The results are presented in the form of tables. The number of independent constants of the different orders agrees with the group-theoretical predictions of Krishnamurty (1963), Krishnamurty & Gopalakrishnamurty (1968) and Chung (1972) in all cases.

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The scheme of elastic constants

The elastic energy ϕ can be written as a Taylor expansion of the Lagrangian strain components η:

$$\phi=\phi_1+\phi_2+\phi_3+\phi_4+\phi_5+\phi_6+\dots .$$

For a body with no initial stresses ϕ_0 and ϕ_1 can be set equal to zero, and ϕ_2, ϕ_3, ϕ_4, ϕ_5, ϕ_6 can be expressed as:

$$\phi_2=\frac{1}{2!}C_{ijkl}\eta_{ij}\eta_{kl}$$

$$\phi_3=\frac{1}{3!}C_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn}$$

$$\phi_4=\frac{1}{4!}C_{ijklmnop}\eta_{ij}\eta_{kl}\eta_{mn}\eta_{op}$$

$$\phi_5=\frac{1}{5!}C_{ijklmnopqr}\eta_{ij}\eta_{kl}\eta_{mn}\eta_{op}\eta_{qr}$$

$$\phi_6=\frac{1}{6!}C_{ijklmnopqrst}\eta_{ij}\eta_{kl}\eta_{mn}\eta_{op}\eta_{qr}\eta_{st}$$

and the subscripts $i, j, k, l, \dots$ take values 1, 2, and 3 and the $C_{ijk}\dots$ are elastic constants of different orders. In the classical theory of elasticity, the strains η are assumed to be small, and the terms of higher order than the second are neglected. If the strains are not infinitesimal, then the higher-order strain terms enter into the strain-energy function.

The standard Voigt notation may be used for simplification. Each pair of indices *ij* may be abbreviated as a single index with:

$$11\rightarrow1;\ 22\rightarrow2;\ 33\rightarrow3;\ 23,\ 32\rightarrow4;\ 13,\ 31\rightarrow5;\ 12,\ 21\rightarrow6\,.$$

The 21 second-order elastic constants C_{jk} may be written as C_{11}, C_{22}, C_{66}, ... in this notation. Similiarly this rule is extended to higher-order elastic constants. In all the tables presented in this paper, for simplicity the letter C is omitted, *e.g.* 11111, 122234, ... *etc.* represent C_{11111}, C_{122234}, ... *etc.*, respectively.

While the method of direct inspection can be applied for groups *N*, *M*, *O*, *T*I, *T*II, *C*I, and *C*II, the same cannot easily be applied to *R*I, *R*II, *H*I, and *H*II. A method similiar to that of Hearmon (1953) will be used.

Calculations of FOEC (for *R*I, *R*II, *H*I, and *H*II)

Owing to the invariance property of the strain energy with respect to transformation of axes, some of the elastic constants can be set to zero if the transformation is one corresponding to the symmetry operation of the crystal.

For the trigonal and hexagonal crystals, the coordinates transform under rotation by an angle θ about the x_3 axis

$$\left.\begin{aligned} x_1' &= mx_1+nx_2 \\ x_2' &= -nx_1+mx_2 \\ x_3' &= x_3 \end{aligned}\right\} \qquad (1)$$

where $m=\cos\theta$, $n=\sin\theta$. The strains transform according to the equations

$$\eta_{kl}'=a_{ik}a_{jl}\eta_{ij} \qquad (2)$$

where a_{ik}, a_{jl} are direction cosines and $i, j, k, l=1, 2$ or 3. The summation over repeated indices is implied. Equation (2) can be written out as:

$$\left.\begin{aligned} \eta_1' &= m^2\eta_1+n^2\eta_2+2mn\eta_6 \\ \eta_2' &= n^2\eta_1+m^2\eta_2-2mn\eta_6 \\ \eta_3' &= \eta_3 \\ \eta_4' &= m\eta_4-n\eta_5 \\ \eta_5' &= n\eta_4+m\eta_5 \\ \eta_6' &= -mn\eta_1+mn\eta_2+(m^2-n^2)\eta_6 . \end{aligned}\right\} \qquad (3)$$

Table 1. *Fourth-order elastic constants* (*FOEC*) (Contn. from p. 3)

R (1)	N (2)	RII (3)	RI (4)	HII (5)	HI (6)	TII (7)	CTI (8)	I (9)
96	2346	1235-2.1135	0	0	0	0	0	0
48	2355	1344	1344	1344	1344	1344	1244	2.1122-1123
96	2356	2.1134-1234	2.1134-1234	0	0	0	0	0
48	2366	6.1113-1123 -3.2223	6.1113-1123 -3.2223	6.1113-1123 -3.2223	6.1113-1123 -3.2223	1366	1255	3.1112-1123
32	2444	-(1444+1455)/2	-(1444+1455)/2	0	0	0	0	0
96	2445	-(3.1555-1445)/2	0	0	0	0	0	0
96	2446	(2.1145-1245)/2	0	(2.1145-1245)/2	0	-1556	0	0
96	2455	(1455-3.1555)/2	0	0	0	0	0	0
192	2456	-2.1144+2.1155 +1244-1255	-2.1144+2.1155 +1244-1255	-2.1144+2.1155 +1244-1255	-2.1144+2.1155 +1244-1255	1456	1456	1456
96	2466	-(5.1114-1156 -3.1124)/3	-(5.1114-1156 -3.1124)/3	0	0	0	0	0
32	2555	-(1555+1245)/2	0	0	0	0	0	0
96	2556	-(2.1145-1245)/2	0	-(2.1145-1245)/2	0	-1446	0	0
96	2566	-(10.1115+3.1146 -6.1125)/6	0	0	0	0	0	0
32	2666	-(4.1116)/3	0	-(4.1116)/3	0	-1666	0	0
1	3333	---	---	---	---	--	1111	1111
8	3334	0	0	0	0	0	0	0
8	3335	0	0	0	0	0	0	0
8	3336	0	0	0	0	0	0	0
24	3344	---	---	---	---	--	1155	4.1111-1112
48	3345	0	0	0	0	0	0	0
48	3346	-2.1335	0	0	0	0	0	0
24	3355	3344	3344	3344	3344	3344	1166	4.1111-1112
48	3356	2.1334	2.1334	0	0	0	0	0
24	3366	2.1133-1233	2.1133-1233	2.1133-1233	2.1133-1233	---	1144	2.1122-1123
32	3444	---	---	0	0	0	0	0
96	3445	---	0	0	0	0	0	0
96	3446	1345	0	1345	0	---	0	0
96	3455	3.3444	3.3444	0	0	0	0	0
192	3456	2(1355-1344)	2(1355-1344)	2(1355-1344)	2(1355-1344)	---	1456	-2.1144+2.1155 -3.1244+3.1255
96	3466	2.1234	2.1234	0	0	0	0	0
32	3555	-3445/3	0	0	0	0	0	0
96	3556	-1345	0	-1345	0	-3446	0	0
96	3566	2.1235	0	0	0	0	0	0
32	3666	-(4.1136)/3	0	-(4.1136)/3	0	0	0	0
16	4444	---	---	---	---	---	---	2.1111+1122 -2.1112
64	4445	0	0	0	0	---	0	0
64	4446	-(3.1555+1445)/2	0	0	0	0	0	0
96	4455	2.4444	2.4444	2.4444	2.4444	---	---	4.1111+2.1122 -4.1112
192	4456	(3.1444+1445)/2	(3.1444+1445)/2	0	0	0	0	0
96	4466	1144+1155+(1244 -1255)/2	1144+1155+(1244 -1255)/2	1144+1155+(1244 -1255)/2	1144+1155+(1244 -1255)/2	---	4455	4.1111+2.1122 -4.1112
64	4555	0	0	0	0	-4445	0	0
192	4556	-(3.1555+1445)/2	0	0	0	0	0	0
192	4566	2.1245	0	2.1245	0	0	0	0
64	4666	-(4.1115-12.1124 -4.1146)/6	0	0	0	0	0	0
16	5555	4444	4444	4444	4444	4444	4444	2.1111+1122 -2.1112
64	5563	(3.1444+1445)/2	(3.1444+1445)/2	0	0	0	0	0
96	5566	1144+1155-(3.1244 -1255)/2	1144+1155-(3.1244 -1255)/2	1144+1155-(3.1244 -1255)/2	1144+1155-(3.1244 -1255)/2	4466	4455	4.1111+2.1122 -4.1112
64	5666	(4.1114-12.1124 +2.1156)/6	(4.1114-12.1124 +2.1156)/6	0	0	0	0	0
16	6666	(2.1111-5.1112 +3.1122+1166)/3	(2.1111-5.1112 +3.1122+1166)/3	(2.1111-5.1112 +3.1122+1166)/3	(2.1111-5.1112 +3.1122+1166)/3	---	4444	2.1111+1122 -2.1112