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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.

The scheme of elastic constants

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

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

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 $i, j, k, l, \ldots$ take values 1, 2, and 3 and the $C_{ijk}\ldots$ 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:

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

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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, TI, TII, CI, and CII, the same cannot easily be applied to RI, RII, HI, and HII. 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*)

R (1)	N (2)	RII (3)	RI (4)	HII (5)	HI (6)	TII (7)	CII (8)	I (9)
36	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	-(4.1125-12.1124 -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

Table 1 (*cont.*)

R	N	RII	RI	HII	HI	TII	CII	I
	Triclinic	Trigonal		Hexagonal		Tetragonal	Cubic	Isotropic
	$1(C_1)$ $\bar{1}(S_2)$	$3(C_3)$, $\bar{3}(C_{3i})$	$3m(C_{3v})$, $32(D_3)$, $\bar{3}\frac{2}{m}(D_{3d})$	$6(C_6)$, $\bar{6}(C_{3h})$, $\frac{6}{m}(C_{6h})$	$6m2(D_{3h})$, $6mm$ (C_{6v}), $622(D_6)$ $\frac{622}{mmm}(D_{6h})$	$4(C_4)$ $\bar{4}(S_4)$ $\frac{4}{m}(C_{4h})$	$23(T)$ $\frac{2}{m}\bar{3}(T_h)$	
	126	42	28	24	19	36	14	4
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)
1	1111	---	---	---	---	--	--	---
4	1112	---	---	---	---	--	--	---
4	1113	---	---	---	---	--	--	1112
8	1114	---	---	0	0	0	0	0
8	1115	---	0	0	0	0	0	0
8	1116	---	0	---	0	--	0	0
6	1122	---	---	---	---	--	--	---
12	1123	---	---	---	---	--	--	---
24	1124	---	---	0	0	0	0	0
24	1125	---	0	0	0	0	0	0
24	1126	-1116	0	-1116	0	--	0	0
6	1133	---	---	---	---	--	1122	1122
24	1134	---	---	0	0	0	0	0
24	1135	---	0	0	0	0	0	0
24	1136	---	0	---	0	--	0	0
24	1144	---	---	---	---	--	--	2.1122-1123
48	1145	---	0	---	0	--	0	0
48	1146	---	0	0	0	0	0	0
24	1155	---	---	---	---	--	--	4.1111-1123
48	1156	---	---	0	0	0	0	0
24	1166	---	---	---	---	--	--	4.1111-1112
4	1222	(8.1111+7.1112 -2.1166)/9	(8.1111+7.1112 -2.1166)/9	(8.1111+7.1112 -2.1166)/9	(8.1111+7.1112 -2.1166)/9	1112	1112	1112
12	1223	3.1113+1123 -3.2223	3.1113+1123 -3.2223	3.1113+1123 -3.2223	3.1113+1123 -3.2223	1123	1123	1123
24	1224	-(2.1114+3.1124 -1156)/3	-(2.1114+3.1124 -1156)/3	0	0	0	0	0
24	1225	-(2.1115+3.1125 +1146)/3	0	0	0	0	0	0
24	1226	-1116	0	-1116	0	-1126	0	0
12	1233	---	---	---	---	--	1123	1123
48	1234	---	---	0	0	0	0	0
48	1235	---	0	0	0	0	0	0
48	1236	-2.1136	0	-2.1136	0	0	0	0
48	1244	---	---	---	---	--	--	3.1112-1123
96	1245	---	0	---	0	0	0	0
96	1246	-2(1115+1125)	0	0	0	0	0	0
48	1255	---	---	---	---	1244	--	3.1112-1123
96	1256	2(1114+1124)	2(1114+1124)	0	0	0	0	0
48	1266	4.1111+2.1112 -2.1122	4.1111+2.1112 -2.1122	4.1111+2.1112 -2.1122	4.1111+2.1112 -2.1122	--	--	4.1111+2.1112 -2.1122
4	1333	---	---	---	---	--	1112	1112
24	1334	---	---	0	0	0	0	0
24	1335	---	0	0	0	0	0	0
24	1336	0	0	0	0	--	0	0
48	1344	---	---	---	---	--	1255	3.1112-1123
96	1345	---	0	---	0	--	0	0
96	1346	-2.1135-3.1235	0	0	0	0	0	0
48	1355	---	---	---	---	--	1266	1126
96	1356	2.1134	2.1134	0	0	0	0	0
48	1366	-6.1113-1123 +9.2223	6.1113-1123 +9.2223	6.1113-1123 +9.2223	6.1113-1123 +9.2223	--	1244	3.1112-1123
32	1444	---	---	0	0	0	0	0
96	1445	---	0	0	0	0	0	0
96	1446	(2.1145+3.1245)/2	0	(2.1145+3.1245)/2	0	--	0	0
96	1455	---	---	0	0	0	0	0
192	1456	-2.1144+2.1155 -3.1244+3.1255	-2.1144+2.1155 -3.1244+3.1255	-2.1144+2.1155 -3.1244+3.1255	-2.1144+2.1155 -3.1244+3.1255	--	--	-2.1144+2.1155 -3.1244+3.1255
96	1466	-1114-1124 +1156	-1114-1124 +1156	0	0	0	0	0
32	1555	---	0	0	0	0	0	0
96	1556	-(2.1145+3.1245)/2	0	-(2.1145+3.1245)/2	0	--	0	0
96	1566	-1115-1125 -1146	0	0	0	0	0	0
32	1666	-4.1116/3	0	0	0	--	0	0
1	2222	(5.1111+1112 +1166)/9	0	(5.1111+1112 +1166)/9	0	1111	1111	1111
4	2223	---	---	---	---	1113	1112	1112
8	2224	-(1114+1156)/3	-(1114+1156)/3	0	0	0	0	0
8	2225	-(1115-1146)/3	0	0	0	0	0	0
8	2226	1116	0	1116	0	-1116	0	0
6	2233	1133	1133	1133	1133	1133	1122	1122
24	2234	-1134-1234	-1134-1234	0	0	0	0	0
24	2235	-1135-1235	0	0	0	0	0	0
20	2236	1136	0	1136	0	-1136	0	0
24	2244	(2.1155-1244 +1255)/2	(2.1155-1244 +1255)/2	(2.1155-1244 +1255)/2	(2.1155-1244 +1255)/2	1155	1166	4.1111-1112
48	2245	-1145-1245	0	-1145-1245	0	-1145	0	0
48	2246	-(8.1115+1146)/3	0	0	0	0	0	0
24	2255	(2.1144+1244 -1255)/2	(2.1144+1244 -1255)/2	(2.1144+1244 -1255)/2	(2.1144+1244 -1255)/2	1144	1144	2.1122-1123
48	2256	(8.1114-1156)/3	(8.1114-1156)/3	0	0	0	0	0
24	2266	(16.1111-4.1112 -1166)/3	(16.1111-4.1112 -1166)/3	(16.1111-4.1112 -1166)/3	(16.1111-4.1112 -1166)/3	1166	1155	4.1111
4	2333	1333	1333	1333	1333	1333	1113	1113
24	2334	-1334	-1334	0	0	0	0	0
24	2335	-1335	0	0	0	0	0	0
24	2336	0	0	0	0	-1336	0	0
48	2344	1355	1355	1355	1355	1355	1266	4.1111+2.1112 -2.1122
96	2345	-1345	0	-1345	0	-1345	0	0

The invariance property of the strain energy thus leads to a system of equations with the values of m and n given by:

$$\text{Trigonal: } m=-\tfrac{1}{2},\ n=\frac{\sqrt{3}}{2} \quad \text{or} \quad m=\tfrac{1}{2},\ n=-\frac{\sqrt{3}}{2}$$

$$\text{Hexagonal: } m=\tfrac{1}{2},\ n=\frac{\sqrt{3}}{2} \quad \text{or} \quad m=-\tfrac{1}{2},\ n=-\frac{\sqrt{3}}{2}.$$

Because of the invariance of η_3 in equations (3), all the FOEC with an added index '3' satisfy the equations (A1)–(A10) for TOEC given by Hearmon (1953). Therefore, only five additional sets of equations are needed for the remaining FOEC not containing the index '3'. These equations (B1)–(B5) are given in the Appendix. For the hexagonal system, all the terms in equations (B2) and (B4) are set to zero owing to the symmetry operations.

The final results for FOEC calculated in this way for *R*I, *R*II, *H*I, and *H*II are given in Table 1. The column headings, reading from top to bottom, are (1) name of system (and its short form), (2) the Hermann–Mauguin and Schönflies symbols of the classes, (3) the number of independent constants and (4) column number. While the numerals in column (2) represent the FOEC in a triclinic system, they also serve as a list of all constants for other crystals whether they are independent or not. The independent ones in other crystal classes will be indicated by a bar and the dependent ones are expressed in terms of them. In this way, the independent number of FOEC for a Laue group is just the number of bars in that column. With the Table given by Ghate (1965) for Laue groups *N*, *M*, *O*, *C*I, and *T*I, the scheme for FOEC is now complete. The ratio R is defined as $R=C_{pqrs}/C_{ijklmnot}$ (for FOEC), where $pqrs$ and $ijklmnot$ are single and double indices respectively. The sum of all values of R for nth order elastic constants should be 3^{2n}. This can be used as a double check in preparing the Tables 1–3.

The FOEC for an isotropic system can be obtained by combining the cubic system (*C*II) with hexagonal system (*H*II). The result gives the four independent constants as 1111, 1112, 1122, and 1123. The equations relating the different constants for an isotropic system agree with those given by Krishnamurty (1963).

Calculations for FFOEC and SOEC

The direct-inspection method employed here is the same as that used for second-, third-, and fourth-order constants (Fumi, 1951, 1952*a*, *b*, *c*, 1953; Hearmon, 1953; Ghate, 1964, 1965). The results of FFOEC and SOEC are presented in Tables 2 and 3. These Tables are presented in the similar manner to Table 1.

In principle the FFOEC and SOEC could be worked out for the other Laue groups as we did for FOEC in the previous section except for the formidable algebra involved. A computer should be ultilized for this lengthy calculation.

To illustrate the use of this kind of table, we can write the terms of the elastic energy ϕ_5 for a cubic crystal. To do this, we first list the resulting 18 independent FFOEC and the equivalent coefficients in Table 4. From Table 4 the elastic energy ϕ_5 for a cubic crystal can then be written. The result is the sum of all the terms given in Table 5 divided by 5!. This expression has many more terms than of the lower order. The terms in ϕ_4 and ϕ_6 of other crystals can be worked out in the same way.

Applications

With the continuing improvement of the experimental accuracy in velocity measurement and the development of the method of shock waves (Graham, 1972), the determination of higher-order elastic constants becomes possible for all types of crystals. The contribution of higher-order terms in the experiments involv-

Table 2. *Fifth-order elastic constants* (*FFOEC*)

R	N Tri-clinic		M Mono-clinic		O Ortho-rhombic	TI Tetragonal	TII	CI Cubic	CII
	1 $\bar{1}$		2 2/m m		222 mmm	4mm $\bar{4}$2m 422 4/mmm	4 $\bar{4}$ 4/m	$\bar{4}$3m 432 m3m	23 $\frac{2}{m}\bar{3}$
		$m=x_2x_3$ $C_2=x_1$	$m=x_3x_1$ $C_2=x_2$	$m=x_1x_2$ $C_2=x_3$					
	252	136	136	136	78	44	68	18	26
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)
1	11111	---	---	---	---	---	---	---	---
5	11112	---	---	---	---	---	---	---	---
5	11113	---	---	---	---	---	---	11112	---
10	11114	---	0	0	0	0	0	0	0
10	11115	0	---	0	0	0	0	0	0
10	11116	0	0	---	0	0	---	0	0
10	11122	---	---	---	---	---	---	---	---
20	11123	---	---	---	---	---	---	---	---
40	11124	---	0	0	0	0	0	0	0
40	11125	0	---	0	0	0	0	0	0
40	11126	0	0	---	0	0	---	0	0
10	11133	---	---	---	---	---	---	11122	---
40	11134	---	0	0	0	0	0	0	0
40	11135	0	---	0	0	0	0	0	0
40	11136	0	0	---	0	0	---	0	0
40	11144	---	---	---	---	---	---	---	---
80	11145	0	0	---	0	0	---	0	0
80	11146	0	---	0	0	0	0	0	0
40	11155	---	---	---	---	---	---	---	---
80	11156	---	0	0	0	0	0	0	0
40	11166	---	---	---	---	---	---	11155	---
10	11222	---	---	---	---	11122	11122	11122	11122

Table 2 (*cont.*)

R (1)	N (2)	(3)	M (4)	(5)	O (6)	TI (7)	TII (8)	CI (9)	CII (10)
30	11223	---	---	---	---	---	---	---	---
60	11224	---	0	0	0	0	0	0	0
60	11225	0	---	0	0	0	0	0	0
60	11226	0	0	---	0	0	0	0	0
30	11233	---	---	---	---	---	---	11223	11223
120	11234	---	0	0	0	0	0	0	0
120	11235	0	---	0	0	0	0	0	0
120	11236	0	0	---	0	0	---	0	0
120	11244	---	---	---	---	---	---	---	---
240	11245	0	0	---	0	0	---	0	0
240	11246	0	---	0	0	0	0	0	0
120	11255	---	---	---	---	---	---	---	---
240	11256	---	0	0	0	0	0	0	0
120	11266	---	---	---	---	---	---	---	---
10	11333	---	---	---	---	---	---	11122	11122
60	11334	---	0	0	0	0	0	0	0
60	11335	0	---	0	0	0	0	0	0
60	11336	0	0	---	0	0	---	0	0
120	11344	---	---	---	---	---	---	11244	---
240	11345	0	0	---	0	0	---	0	0
240	11346	0	---	0	0	0	0	0	0
120	11355	---	---	---	---	---	---	11266	---
240	11356	---	0	0	0	0	0	0	0
120	11366	---	---	---	---	---	---	11255	---
80	11444	---	0	0	0	0	0	0	0
240	11445	0	---	0	0	0	0	0	0
240	11446	0	0	---	0	0	---	0	0
240	11455	---	0	0	0	0	0	0	0
480	11456	---	---	---	---	---	---	---	---
240	11466	---	0	0	0	0	0	0	0
80	11555	0	---	0	0	0	0	0	0
240	11556	0	0	---	0	0	---	0	0
240	11566	0	---	0	0	0	0	0	0
80	11666	0	0	---	0	0	---	0	0
5	12222	---	---	---	---	11112	11112	11112	11112
20	12223	---	---	---	---	11123	11123	11123	11123
40	12224	---	0	0	0	0	0	0	0
40	12225	0	---	0	0	0	0	0	0
40	12226	0	0	---	0	0	-11126	0	0
30	12233	---	---	---	---	11233	11233	11223	11223
120	12234	---	0	0	0	0	0	0	0
120	12235	0	---	0	0	0	0	0	0
120	12236	0	0	---	0	0	-11236	0	0
120	11224	---	---	---	---	11255	11255	11255	11366
240	12245	0	0	---	0	0	-11245	0	0
240	12246	0	---	0	0	0	0	0	0
120	12255	---	---	---	---	11244	11244	11244	11344
240	12256	---	0	0	0	0	0	0	0
120	12266	---	---	---	---	11266	11266	11266	11244
20	12333	---	---	---	---	---	---	11123	11123
120	12334	---	0	0	0	0	0	0	0
120	12335	0	---	0	0	0	0	0	0
120	12336	0	0	---	0	0	0	0	0
240	12344	---	---	---	---	---	---	---	---
480	12345	0	0	---	0	0	0	0	0
480	12346	0	---	0	0	0	0	0	0
240	12355	---	---	---	---	12344	12344	12344	12344
480	12356	---	0	0	0	0	0	0	0
240	12366	---	---	---	---	---	---	12344	12344
160	12444	---	0	0	0	0	0	0	0
480	12445	0	---	0	0	[illegible]		0	0
480	12446	0	0	---	0	0	---	0	0
480	12455	---	0	0	0	0	0	0	0
960	12456	---	---	---	---	---	---	---	---
480	12466	---	0	0	0	0	0	0	0
160	12555	0	---	0	0	0	0	0	0
480	12556	0	0	---	0	0	-12446	0	0
480	12566	0	---	0	0	0	0	0	0
160	12666	0	0	---	0	0	0	0	0
5	13333	---	---	---	---	---	---	11112	11112
40	13334	---	0	0	0	0	0	0	0
40	13335	0	---	0	0	0	0	0	0
40	13336	0	0	---	0	0	---	0	0
120	13344	---	---	---	---	---	---	11255	11255
240	13345	0	0	---	0	0	---	0	0
240	13346	0	---	0	0	0	0	0	0
120	13355	---	---	---	---	---	---	11266	11266
240	13356	---	0	0	0	0	0	0	0
120	13366	---	---	---	---	---	---	11244	11244
160	13444	---	0	0	0	0	0	0	0
480	13445	0	---	0	0	0	0	0	0
480	13446	0	0	---	0	0	---	0	0
480	13455	---	0	0	0	0	0	0	0
960	13456	---	---	---	---	---	---	12456	12456
480	13466	---	0	0	0	0	0	0	0
160	13555	0	---	0	0	0	0	0	0
480	13556	0	0	---	0	0	---	0	0
480	13566	0	---	0	0	0	0	0	0
160	13666	0	0	---	0	0	---	0	0
80	14444	---	---	---	---	---	---	---	---
320	14445	0	0	---	0	0	---	0	0
320	14446	0	---	0	0	0	0	0	0
480	14455	---	---	---	---	---	---	---	---
960	14456	---	0	0	0	0	0	0	0
480	14466	---	---	---	---	---	---	14455	---
320	14555	0	0	---	0	0	---	0	0
960	14556	0	---	0	0	0	0	0	0
960	14566	0	0	---	0	0	---	0	0
320	14666	0	---	0	0	0	0	0	0
80	15555	---	---	---	---	---	---	---	---
320	15556	---	0	0	0	0	0	0	0

Table 2 (*cont.*)

R (1)	N (2)	(3)	M (4)	(5)	O (6)	TI (7)	TII (8)	CI (9)	CII (10)
480	15566	---	---	---	---	---	---	---	---
320	15666	---	0	0	0	0	0	0	0
80	16666	---	---	---	---	---	---	15555	---
1	22222	---	---	---	---	11111	11111	11111	11111
5	22223	---	---	---	---	11113	11113	11112	11113
10	22224	---	0	0	0	0	0	0	0
10	22225	0	---	0	0	0	0	0	0
10	22226	0	0	---	0	0	-11116	0	0
10	22233	---	---	---	---	11133	11133	11122	11122
40	22234	---	0	0	0	0	0	0	0
40	22235	0	---	0	0	0	0	0	0
40	22236	0	0	---	0	0	-11136	0	0
40	22244	---	---	---	---	11155	11155	11155	11166
80	22245	0	0	---	0	0	-11145	0	0
80	22246	0	---	0	0	0	0	0	0
40	22255	---	---	---	---	11144	11144	11144	11144
80	22256	---	0	0	0	0	0	0	0
40	22266	---	---	---	---	11166	11166	11155	11155
10	22333	---	---	---	---	11133	11333	11122	11133
60	22334	---	0	0	0	0	0	0	0
60	22335	0	---	0	0	0	0	0	0
60	22336	0	0	---	0	0	-11336	0	0
120	22344	---	---	---	---	11355	11355	11266	11266
240	22345	0	0	---	0	0	-11345	0	0
240	22346	0	---	0	0	0	0	0	0
120	22355	---	---	---	---	11344	11244	11244	11244
240	22356	---	0	0	0	0	0	0	0
120	22366	---	---	---	---	11366	11366	11255	11255
80	22444	---	0	0	0	0	0	0	0
240	22445	0	---	0	0	0	0	0	0
240	22446	0	0	---	0	0	-11556	0	0
240	22455	---	0	0	0	0	0	0	0
480	22456	---	---	---	---	11456	11456	11456	11456
240	22466	---	0	0	0	0	0	0	0
80	22555	0	---	0	0	0	0	0	0
240	22556	0	0	---	0	0	-11446	0	0
240	22566	0	---	0	0	0	0	0	0
80	22666	0	0	---	0	0	-11666	0	0
5	23333	---	---	---	---	13333	13333	11112	11113
40	23334	---	0	0	0	0	0	0	0
40	23335	0	---	0	0	0	0	0	0
40	23336	0	0	---	0	0	-13336	0	0
120	23344	---	---	---	---	13355	13355	11266	11355
240	23345	0	0	---	0	0	-13345	0	0
240	23346	0	---	0	0	0	0	0	0
120	23355	---	---	---	---	13344	13344	11255	11366
240	23356	---	0	0	0	0	0	0	0
120	23366	---	---	---	---	13366	13366	11244	11344
160	23444	---	0	0	0	0	0	0	0
480	23445	0	---	0	0	0	0	0	0
480	23446	0	0	---	0	0	-13556	0	0
480	23455	---	0	0	0	0	0	0	0
960	23456	---	---	---	---	13456	13456	12456	12456
480	23466	---	0	0	0	0	0	0	0
160	23555	0	---	0	0	0	0	0	0
480	23556	0	0	---	0	0	-13446	0	0
480	23566	0	---	0	0	0	0	0	0
160	23666	0	0	---	0	0	-13666	0	0
80	24444	---	---	---	---	15555	15555	15555	16666
320	24445	0	0	---	0	0	-14555	0	0
320	24446	0	---	0	0	0	0	0	0
480	24455	---	---	---	---	14455	14455	14455	14466
960	24456	---	0	0	0	0	0	0	0
480	24466	---	---	---	---	15566	15566	15566	15566
320	24555	0	0	---	0	0	-14445	0	0
960	24556	0	---	0	0	0	0	0	0
960	24566	0	0	---	0	0	-14566	0	0
320	24666	0	---	0	0	0	0	0	0
80	25555	---	---	---	---	14444	14444	14444	14444
320	25556	---	0	0	0	0	0	0	0
480	25566	---	---	---	---	14466	14466	14455	14455
330	25666	---	0	0	0	0	0	0	0
80	26666	---	---	---	---	16666	16666	15555	15555
1	33333	---	---	---	---	---	---	11111	11111
10	33334	---	0	0	0	0	0	0	0
10	33335	0	---	0	0	0	0	0	0
10	33336	0	0	---	0	0	0	0	0
40	33344	---	---	---	---	---	---	11155	11155
80	33345	0	0	---	0	0	0	0	0
80	33346	0	---	0	0	0	0	0	0
40	33355	---	---	---	---	33344	33344	11155	11166
80	33356	---	0	0	0	0	0	0	0
40	33366	---	---	---	---	---	---	11144	11144
80	33444	---	0	0	0	0	0	0	0
240	33445	0	---	0	0	0	0	0	0
240	33446	0	0	---	0	0	---	0	0
240	33455	---	0	0	0	0	0	0	0
480	33456	---	---	---	---	---	---	11456	11456
240	33466	---	0	0	0	0	0	0	0
80	33555	0	---	0	0	0	0	0	0
240	33556	0	0	---	0	0	33446	0	0
240	33566	0	---	0	0	0	0	0	0
80	33666	0	0	---	0	0	0	0	0
80	34444	---	---	---	---	---	---	15555	15555
320	34445	0	0	---	0	0	---	0	0
320	34446	0	---	0	0	0	0	0	0
480	34455	---	---	---	---	---	---	15566	15566
960	34456	---	0	0	0	0	0	0	0
480	34466	---	---	---	---	---	---	14455	14455
320	34555	0	0	---	0	0	-34445	0	0
960	34556	0	---	0	0	0	0	0	0
960	34566	0	0	---	0	0	0	0	0
320	34666	0	---	0	0	0	0	0	0

Table 2 (*cont.*)

R (1)	N (2)	(3)	M (4)	(5)	O (6)	TI (7)	TII (8)	CI (9)	CII (10)
80	35555	---	---	---	---	34444	34444	15555	16666
320	35556	---	0	0	0	0	0	0	0
480	35566	---	---	---	---	34466	34466	14455	14466
320	35666	---	0	0	0	0	0	0	0
80	36666	---	---	---	---	---	---	14444	14444
32	44444	---	0	0	0	0	0	0	0
160	44445	0	---	0	0	0	0	0	0
160	44446	0	0	---	0	0	---	0	0
320	44455	---	0	0	0	0	0	0	0
640	44456	---	---	---	---	---	---	---	---
320	44466	---	0	0	0	0	0	0	0
320	44555	0	---	0	0	0	0	0	0
960	44556	0	0	---	0	0	0	0	0
960	44566	0	---	0	0	0	0	0	0
320	44666	0	0	---	0	0	---	0	0
160	45555	---	0	0	0	0	0	0	0
640	45556	---	---	---	---	44456	44456	44456	44456
960	45566	---	0	0	0	0	0	0	0
640	45666	---	---	---	---	---	---	44456	44456
160	46666	---	0	0	0	0	0	0	0
32	55555	0	---	0	0	0	0	0	0
160	55556	0	0	---	0	0	-44446	0	0
320	55566	0	---	0	0	0	0	0	0
320	55666	0	0	---	0	0	-44666	0	0
160	56666	0	---	0	0	0	0	0	0
32	66666	0	0	---	0	0	0	0	0

Table 3. *Sixth-order elastic constants* (*SOEC*)

R	N Tri- clinic 1 1̄		M Mono- clinic 2 2/m m		O Ortho- rhombic 222 mmm	TI Tetragonal 4mm 4̄2m 4/mmm	TII 4 4̄ 4/m	CI Cubic 4̄3m 432 m3m	CII 23 2/m 3̄
		$m=x_2x_3$ $C_2=x_1$	$m=x_3x_1$ $C_2=x_2$	$m=x_1x_2$ $C_2=x_3$					
(1)	462 (2)	246 (3)	246 (4)	246 (5)	138 (6)	79 (7)	124 (8)	32 (9)	48 (10)
1	111111	---	---	---	---	---	---	---	---
6	111112	---	---	---	---	---	---	---	---
6	111113	---	---	---	---	---	---	111112	---
12	111114	---	0	0	0	0	0	0	0
12	111115	0	---	0	0	0	0	0	0
12	111116	0	0	---	0	0	---	0	0
15	111122	---	---	---	---	---	---	---	---
30	111123	---	---	---	---	---	---	---	---
60	111124	---	0	0	0	0	0	0	0
60	111125	0	---	0	0	0	0	0	0
60	111126	0	0	---	0	0	---	0	0
15	111133	---	---	---	---	---	---	111122	---
60	111134	---	0	0	0	0	0	0	0
60	111135	0	---	0	0	0	0	0	0
60	111136	0	0	---	0	0	---	0	0
60	111144	---	---	---	---	---	---	---	---
120	111145	0	0	---	0	0	---	0	0
120	111146	0	---	0	0	0	0	0	0
60	111155	---	---	---	---	---	---	---	---
120	111156	---	0	0	0	0	0	0	0
60	111166	---	---	---	---	---	---	111155	---
20	111222	---	---	---	---	---	---	---	---
60	111223	---	---	---	---	---	---	---	---
120	111224	---	0	0	0	0	0	0	0
120	111225	0	---	0	0	0	0	0	0
120	111226	0	0	---	0	0	---	0	0
60	111233	---	---	---	---	---	---	111223	111223
240	111234	---	0	0	0	0	0	0	0
240	111235	0	---	0	0	0	0	0	0
240	111236	0	0	---	0	0	---	0	0
240	111244	---	---	---	---	---	---	---	---
480	111245	0	0	---	0	0	---	0	0
480	111246	0	---	0	0	0	0	0	0
240	111255	---	---	---	---	---	---	---	---
480	111256	---	0	0	0	0	0	0	0
240	111266	---	---	---	---	---	---	---	---
20	111333	---	---	---	---	---	---	111222	111222
120	111334	---	0	0	0	0	0	0	0
120	111335	0	---	0	0	0	0	0	0
120	111336	0	0	---	0	0	---	0	0
240	111344	---	---	---	---	---	---	111244	---
480	111345	0	0	---	0	0	---	0	0
480	111346	0	---	0	0	0	0	0	0
240	111355	---	---	---	---	---	---	111266	---
480	111356	---	0	0	0	0	0	0	0
240	111366	---	---	---	---	---	---	111255	---
160	111444	---	0	0	0	0	0	0	0
480	111445	0	---	0	0	0	0	0	0
480	111446	0	0	---	0	0	---	0	0
480	111455	---	0	0	0	0	0	0	0
960	111456	---	---	---	---	---	---	---	---
480	111466	---	0	0	0	0	0	0	0
160	111555	0	---	0	0	0	0	0	0
480	111556	0	0	---	0	0	---	0	0
480	111566	0	---	0	0	0	0	0	0
160	111666	0	0	---	0	0	---	0	0
15	112222	---	---	---	---	111122	111122	111122	111122
60	112223	---	---	---	---	111223	111223	111223	111223
120	112224	---	0	0	0	0	0	0	0

Table 3 (*cont.*)

R (1)	N (2)	(3)	M (4)	(5)	O (6)	TI (7)	TII (8)	CI (9)	CII (10)
120	112225	0	---	0	0	0	0	0	0
120	112226	0	0	---	0	0	-111226	0	0
90	112233	---	---	---	---	---	---	---	---
360	112234	---	0	0	0	0	0	0	0
360	112235	0	---	0	0	0	0	0	0
360	112236	0	0	---	0	0	0	0	0
360	112244	---	---	---	---	---	---	---	---
720	112245	0	0	---	0	0	0	0	0
720	112246	0	---	0	0	0	0	0	0
360	112255	---	---	---	---	112244	112244	112244	113344
720	112256	---	0	0	0	0	0	0	0
360	112266	---	---	---	---	---	---	---	---
60	112333	---	---	---	---	---	---	111223	111223
360	112334	---	0	0	0	0	0	0	0
360	112335	0	---	0	0	0	0	0	0
360	112336	0	0	---	0	0	---	0	0
720	112344	---	---	---	---	---	---	---	---
1440	112345	0	0	---	0	0	---	0	0
1440	112346	0	---	0	0	0	0	0	0
720	112355	---	---	---	---	---	---	---	---
1440	112356	---	0	0	0	0	0	0	0
720	112366	---	---	---	---	---	---	112355	---
480	112444	---	0	0	0	0	0	0	0
1440	112445	0	---	0	0	0	0	0	0
1440	112446	0	0	---	0	0	---	0	0
1440	112455	---	0	0	0	0	0	0	0
2880	112456	---	---	---	---	---	---	---	---
1440	112466	---	0	0	0	0	0	0	0
480	112555	0	---	0	0	0	0	0	0
1440	112556	0	0	---	0	0	---	0	0
1440	112566	0	---	0	0	0	0	0	0
480	112666	0	0	---	0	0	---	0	0
15	113333	---	---	---	---	---	---	111122	111122
120	113334	---	0	0	0	0	0	0	0
120	113335	0	---	0	0	0	0	0	0
120	113336	0	0	---	0	0	---	0	0
360	113344	---	---	---	---	---	---	112244	112255
720	113345	0	0	---	0	0	---	0	0
720	113346	0	---	0	0	0	0	0	0
360	113355	---	---	---	---	---	---	112266	112266
720	113356	---	0	0	0	0	0	0	0
360	113366	---	---	---	---	---	---	112244	112244
480	113444	---	0	0	0	0	0	0	0
1440	113445	0	---	0	0	0	0	0	0
1440	113446	0	0	---	0	0	---	0	0
1440	113455	---	0	0	0	0	0	0	0
2880	113456	---	---	---	---	---	---	112456	---
1440	113466	---	0	0	0	0	0	0	0
480	113555	0	---	0	0	0	0	0	0
1440	113556	0	0	---	0	0	---	0	0
1440	113566	0	---	0	0	0	0	0	0
480	113666	0	0	---	0	0	---	0	0
240	114444	---	---	---	---	---	---	---	---
960	114445	0	0	---	0	0	---	0	0
960	114446	0	---	0	0	0	0	0	0
1440	114455	---	---	---	---	---	---	---	---
2880	114456	---	0	0	0	0	0	0	0
1440	114466	---	---	---	---	---	---	114455	---
960	114555	0	0	---	0	0	---	0	0
2880	114556	0	---	0	0	0	0	0	0
2880	114556	0	0	---	0	0	---	0	0
960	114666	0	---	0	0	0	0	0	0
240	115555	---	---	---	---	---	---	---	---
960	115556	---	0	0	0	0	0	0	0
1440	115566	---	---	---	---	---	---	---	---
960	115666	---	0	0	0	0	0	0	0
240	116666	---	---	---	---	---	---	115555	---
6	122222	---	---	---	---	111112	111112	111113	111112
30	122223	---	---	---	---	111123	111123	111123	111123
60	122224	---	0	0	0	0	0	0	0
60	122225	0	---	0	0	0	0	0	0
60	122226	0	0	---	0	0	-111126	0	0
60	122233	---	---	---	---	111233	111233	111223	111223
240	122234	---	0	0	0	0	0	0	0
240	122235	0	---	0	0	0	0	0	0
240	122236	0	0	---	0	0	-111236	0	0
240	122244	---	---	---	---	111255	111255	111255	111366
480	122245	0	0	---	0	0	-111245	0	0
480	122246	0	---	0	0	0	0	0	0
240	122255	---	---	---	---	111244	111244	111244	111344
480	122256	---	0	0	0	0	0	0	0
240	122266	---	---	---	---	111266	111266	111266	111355
60	122333	---	---	---	---	112333	112333	111223	111233
360	122334	---	0	0	0	0	0	0	0
360	122335	0	---	0	0	0	0	0	0
360	122336	0	0	---	0	0	-112336	0	0
720	122344	---	---	---	---	112355	112355	112355	112355
1440	122345	0	0	---	0	0	-112345	0	0
1440	122346	0	---	0	0	0	0	0	0
720	122355	---	---	---	---	112344	112344	112344	112344
1440	122356	---	0	0	0	0	0	0	0
720	122366	---	---	---	---	112366	112366	112355	112355
480	122444	---	0	0	0	0	0	0	0
1440	122445	0	---	0	0	0	0	0	0
1440	122446	0	0	---	0	0	-112556	0	0
1440	122455	---	0	0	0	0	0	0	0
2880	122456	---	---	---	---	112456	112456	112456	113456
1440	122466	---	0	0	0	0	0	0	0
480	122555	0	---	0	0	0	0	0	0

Table 3 (*cont.*)

R (1)	N (2)	(3)	M (4)	(5)	O (6)	TI (7)	TII (8)	CI (9)	CII (10)
1440	122556	0	0	---	0	0	-112446	0	0
1440	122566	0	---	0	0	0	0	0	0
480	122666	0	0	---	0	0	-112666	0	0
30	123333	---	---	---	---	---	---	111123	111123
240	123334	---	0	0	0	0	0	0	0
240	123335	0	---	0	0	0	0	0	0
240	123336	0	0	---	0	0	0	0	0
720	123344	---	---	---	---	---	---	112355	112355
1440	123345	0	0	---	0	0	0	0	0
1440	123346	0	---	0	0	0	0	0	0
720	123355	---	---	---	---	123344	123344	112355	112366
1440	123356	---	0	0	0	0	0	0	0
720	123366	---	---	---	---	---	---	112344	112344
960	123444	---	0	0	0	0	0	0	0
2880	123445	0	---	0	0	0	0	0	0
2880	123446	0	0	---	0	0	---	0	0
2880	123455	---	0	0	0	0	0	0	0
5760	123456	---	---	---	---	---	---	---	---
2880	123466	---	0	0	0	0	0	0	0
960	123555	0	---	0	0	0	0	0	0
2880	123556	0	0	---	0	0	-123446	0	0
2880	123566	0	---	0	0	0	0	0	0
960	123666	0	0	---	0	0	0	0	0
480	124444	---	---	---	---	---	---	---	---
1920	124445	0	0	---	0	0	---	0	0
1920	124446	0	---	0	0	0	0	0	0
2880	124455	---	---	---	---	---	---	---	---
5760	124456	---	0	0	0	0	0	0	0
2880	124466	---	---	---	---	---	---	---	---
1920	124555	0	0	---	0	0	-124445	0	0
5760	124556	0	---	0	0	0	0	0	0
5760	124566	0	0	---	0	0	0	0	0
1920	124666	0	---	0	0	0	0	0	0
480	125555	---	---	---	---	124444	124444	124444	---
1920	125556	---	0	0	0	0	0	0	0
2880	125566	---	---	---	---	124466	124466	124466	---
1920	125666	---	0	0	0	0	0	0	0
480	126666	---	---	---	---	---	---	---	---
6	133333	---	---	---	---	---	---	111112	111112
60	133334	---	0	0	0	0	0	0	0
60	133335	0	---	0	0	0	0	0	0
60	133336	0	0	---	0	0	---	0	0
240	133344	---	---	---	---	---	---	111255	111255
480	133345	0	0	---	0	0	---	0	0
480	133346	0	---	0	0	0	0	0	0
240	133355	---	---	---	---	---	---	111266	111266
480	133356	---	0	0	0	0	0	0	0
240	133366	---	---	---	---	---	---	111244	111244
480	133444	---	0	0	0	0	0	0	0
1440	133445	0	---	0	0	0	0	0	0
1440	133446	0	0	---	0	0	---	0	0
1440	133455	---	0	0	0	0	0	0	0
2880	133456	---	---	---	---	---	---	112456	112456
1440	133466	---	0	0	0	0	0	0	0
480	133555	0	---	0	0	0	0	0	0
1440	133556	0	0	---	0	0	---	0	0
1440	133566	0	---	0	0	0	0	0	0
480	133666	0	0	---	0	0	0	0	0
480	134444	---	---	---	---	---	---	124444	125555
1920	134445	0	0	---	0	0	---	0	0
1920	134446	0	---	0	0	0	0	0	0
2880	134455	---	---	---	---	---	---	124466	125566
5760	134456	---	0	0	0	0	0	0	0
2880	134466	---	---	---	---	---	---	124455	124455
1920	134555	0	0	---	0	0	---	0	0
5760	134556	0	---	0	0	0	0	0	0
5760	134566	0	0	---	0	0	---	0	0
1920	134666	0	---	0	0	0	0	0	0
480	135555	---	---	---	---	---	---	126666	126666
1920	135556	---	0	0	0	0	0	0	0
2880	135566	---	---	---	---	---	---	124466	124466
1920	135666	---	0	0	0	0	0	0	0
480	136666	---	---	---	---	---	---	124444	124444
192	144444	---	0	0	0	0	0	0	0
960	144445	0	---	0	0	0	0	0	0
960	144446	0	0	---	0	0	---	0	0
1920	144455	---	0	0	0	0	0	0	0
3840	144456	---	---	---	---	---	---	---	---
1920	144466	---	0	0	0	0	0	0	0
1920	144555	0	---	0	0	0	0	0	0
5760	144556	0	0	---	0	0	---	0	0
5760	144566	0	---	0	0	0	0	0	0
1920	144666	0	0	---	0	0	---	0	0
960	145555	---	0	0	0	0	0	0	0
3840	145556	---	---	---	---	---	---	---	---
5760	145566	---	0	0	0	0	0	0	0
3840	145666	---	---	---	---	---	---	145556	---
960	146666	---	0	0	0	0	0	0	0
192	155555	0	---	0	0	0	0	0	0
960	155556	0	0	---	0	0	---	0	0
1920	155566	0	---	0	0	0	0	0	0
1920	155666	0	0	---	0	0	---	0	0
960	156666	0	---	0	0	0	0	0	0
192	166666	0	0	---	0	0	---	0	0
1	222222	---	---	---	---	111111	111111	111111	111111
6	222223	---	---	---	---	111113	111113	111112	111113
12	222224	---	0	0	0	0	0	0	0
12	222225	0	---	0	0	0	0	0	0
12	222226	0	0	---	0	0	-111116	0	0
15	222233	---	---	---	---	111133	111133	111122	111122
60	222234	---	0	0	0	0	0	0	0

Table 3 (*cont.*)

R (1)	N (2)	(3)	M (4)	(5)	O (6)	TI (7)	TII (8)	CI (9)	CII (10)
60	222235	0	---	0	0	0	0	0	0
60	222236	0	0	---	0	0	-111136	0	0
60	222244	---	---	---	---	111155	111155	111155	111166
120	222245	0	0	---	0	0	-111145	0	0
120	222246	0	---	0	0	0	0	0	0
60	222255	---	---	---	---	111144	111144	111144	111144
120	222256	---	0	0	0	0	0	0	0
60	222266	---	---	---	---	111166	111166	111155	111155
20	222333	---	---	---	---	111333	111333	111222	111333
120	222334	---	0	0	0	0	0	0	0
120	222335	0	---	0	0	0	0	0	0
120	222336	0	0	---	0	0	-111336	0	0
240	222344	---	---	---	---	111355	111355	111266	111266
480	222345	0	0	---	0	0	-111345	0	0
480	222346	0	---	0	0	0	0	0	0
240	222355	---	---	---	---	111344	111344	111244	111244
480	222356	---	0	0	0	0	0	0	0
240	222366	---	---	---	---	111366	111366	111255	111255
160	222444	---	0	0	0	0	0	0	0
480	222445	0	---	0	0	0	0	0	0
480	222446	0	0	---	0	0	-111556	0	0
480	222455	---	0	0	0	0	0	0	0
960	222456	---	---	---	---	111456	111456	111456	111456
480	222466	---	0	0	0	0	0	0	0
160	222555	0	---	0	0	0	0	0	0
480	222556	0	0	---	0	0	-111446	0	0
480	222566	0	---	0	0	0	0	0	0
160	222666	0	0	---	0	0	-111666	0	0
15	223333	---	---	---	---	113333	111133	111122	111133
120	223334	---	0	0	0	0	0	0	0
120	223335	0	---	0	0	0	0	0	0
120	223336	0	0	---	0	0	-113336	0	0
360	223344	---	---	---	---	113355	113355	112266	113355
720	223345	0	0	---	0	0	-113345	0	0
720	223346	0	---	0	0	0	0	0	0
360	223355	---	---	---	---	113344	113344	112244	113366
720	223356	---	0	0	0	0	0	0	0
360	223366	---	---	---	---	113366	113366	112244	113344
480	223444	---	0	0	0	0	0	0	0
1440	223445	0	---	0	0	0	0	0	0
1440	223446	0	0	---	0	0	-113556	0	0
1440	223455	---	0	0	0	0	0	0	0
2880	223456	---	---	---	---	113456	113456	112456	112456
1440	223466	---	0	0	0	0	0	0	0
480	223555	0	---	0	0	0	0	0	0
1440	223556	0	0	---	0	0	-113446	0	0
1440	223566	0	---	0	0	0	0	0	0
480	223666	0	0	---	0	0	-113666	0	0
240	224444	---	---	---	---	115555	115555	115555	116666
960	224445	0	0	---	0	0	-114555	0	0
960	224446	0	---	0	0	0	0	0	0
1440	224455	---	---	---	---	114455	114455	114455	114466
2880	224456	---	0	0	0	0	0	0	0
1440	224466	---	---	---	---	115566	115566	115566	115566
960	224555	0	0	---	0	0	-114445	0	0
2880	224556	0	---	0	0	0	0	0	0
2880	224566	0	0	---	0	0	-114566	0	0
960	224666	0	---	0	0	0	0	0	0
240	225555	---	---	---	---	114444	114444	114444	114444
960	225556	---	0	0	0	0	0	0	0
1440	225566	---	---	---	---	114466	114466	114455	114455
960	225666	---	0	0	0	0	0	0	0
240	226666	---	---	---	---	116666	116666	115555	115555
6	233333	----	----	----	----	133333	133333	111112	111113
60	233334	---	0	0	0	0	0	0	0
60	233335	0	---	0	0	0	0	0	0
60	233336	0	0	---	0	0	-133336	0	0
240	233344	---	---	---	---	133355	133355	111266	111355
480	233345	0	0	---	0	0	-133345	0	0
480	233346	0	---	0	0	0	0	0	0
240	233355	---	---	---	---	133344	133344	111255	111366
480	233356	---	0	0	0	0	0	0	0
240	233366	---	---	---	---	133366	133366	111244	111344
480	233444	---	0	0	0	0	0	0	0
1440	233445	0	---	0	0	0	0	0	0
1440	233446	0	0	---	0	0	-133556	0	0
1440	233455	---	0	0	0	0	0	0	0
2880	233456	---	---	---	---	133456	133456	112456	133456
1440	233466	---	0	0	0	0	0	0	0
480	233555	0	---	0	0	0	0	0	0
1440	233556	0	0	---	0	0	-133446	0	0
1440	233566	0	---	0	0	0	0	0	0
480	233666	0	0	---	0	0	-133666	0	0
480	234444	---	---	---	---	135555	135555	126666	135555
1920	234445	0	0	---	0	0	134555	0	0
1920	234446	0	---	0	0	0	0	0	0
2880	234455	---	---	---	---	134455	134455	124466	135566
5760	234456	---	0	0	0	0	0	0	0
2880	234466	---	---	---	---	135566	135566	124466	134455
1920	234555	0	0	---	0	0	-134445	0	0
5760	234556	0	---	0	0	0	0	0	0
5760	234566	0	0	---	0	0	-134566	0	0
1920	234666	0	---	0	0	0	0	0	0
480	235555	---	---	---	---	134444	134444	124444	136666
1920	235556	---	0	0	0	0	0	0	0
2880	235566	---	---	---	---	134466	134466	124455	134466
1920	235666	---	0	0	0	0	0	0	0
480	236666	---	---	---	---	136666	136666	124444	134444
192	244444	---	0	0	0	0	0	0	0
960	244445	0	---	0	0	0	0	0	0
960	244446	0	0	---	0	0	-155556	0	0
1920	244455	---	0	0	0	0	0	0	0
3840	244456	---	---	---	---	145556	145556	145556	145666

Table 3 (*cont.*)

R (1)	N (2)	(3)	M (4)	(5)	O (6)	TI (7)	TII (8)	CI (9)	CII (10)
1920	244466	---	0	0	0	0	0	0	0
1920	244555	0	---	0	0	0	0	0	0
5760	244556	0	0	---	0	0	-144556	0	0
5760	244566	0	---	0	0	0	0	0	0
1920	244666	0	0	---	0	0	-155666	0	0
960	245555	---	0	0	0	0	0	0	0
3840	245556	---	---	---	---	144456	144456	144456	144456
5760	245566	---	0	0	0	0	0	0	0
3840	245666	---	---	---	---	145666	145666	145556	145556
960	246666	---	0	0	0	0	0	0	0
192	255555	0	---	0	0	0	0	0	0
960	255556	0	0	---	0	0	-144446	0	0
1920	255566	0	---	0	0	0	0	0	0
1920	255666	0	0	---	0	0	-144666	0	0
960	256666	0	---	0	0	0	0	0	0
192	266666	0	0	---	0	0	-166666	0	0
1	333333	---	---	---	---	---	---	111111	111111
12	333334	---	0	0	0	0	0	0	0
12	333335	0	---	0	0	0	0	0	0
12	333336	0	0	---	0	0	0	0	0
60	333344	---	---	---	---	---	---	111155	111155
120	333345	0	0	---	0	0	0	0	0
120	333346	0	---	0	0	0	0	0	0
60	333355	---	---	---	---	333344	333344	111155	111166
120	333356	---	0	0	0	0	0	0	0
60	333366	---	---	---	---	---	---	111144	111144
160	333444	---	0	0	0	0	0	0	0
480	333445	0	---	0	0	0	0	0	0
480	333446	0	0	---	0	0	---	0	0
480	333455	---	0	0	0	0	0	0	0
960	333456	---	---	---	---	---	---	111456	111456
480	333466	---	0	0	0	0	0	0	0
160	333555	0	---	0	0	0	0	0	0
480	333556	0	0	---	0	0	-333446	0	0
480	333566	0	---	0	0	0	0	0	0
160	333666	0	0	---	0	0	0	0	0
240	334444	---	---	---	---	---	---	115555	115555
960	334445	0	0	---	0	0	---	0	0
960	334446	0	---	0	0	0	0	0	0
1440	334455	---	---	---	---	---	---	115566	115566
2880	334456	---	0	0	0	0	0	0	0
1440	334466	---	---	---	---	---	---	114455	114455
960	334555	0	0	---	0	0	-334445	0	0
2880	334556	0	---	0	0	0	0	0	0
2880	334566	0	0	---	0	0	0	0	0
960	334666	0	---	0	0	0	0	0	0
240	335555	---	---	---	---	334444	334444	115555	116666
960	335556	---	0	0	0	0	0	0	0
1440	335566	---	---	---	---	334466	334466	114455	114466
960	335666	---	0	0	0	0	0	0	0
240	336666	---	---	---	---	---	---	114444	114444
192	344444	---	0	0	0	0	0	0	0
960	344445	0	---	0	0	0	0	0	0
960	344446	0	0	---	0	0	---	0	0
1920	344455	---	0	0	0	0	0	0	0
3840	344456	---	---	---	---	---	---	145556	145556
1920	344466	---	0	0	0	0	0	0	0
1920	344555	0	---	0	0	0	0	0	0
5760	344556	0	0	---	0	0	0	0	0
5760	344566	0	---	0	0	0	0	0	0
1920	344666	0	0	---	0	0	---	0	0
960	345555	---	0	0	0	0	0	0	0
3840	345556	---	---	---	---	344456	344456	145556	145666
5760	345566	---	0	0	0	0	0	0	0
3840	345666	---	---	---	---	---	---	144456	144456
960	346666	---	0	0	0	0	0	0	0
192	355555	0	---	0	0	0	0	0	0
960	355556	0	0	---	0	0	-344446	0	0
1920	355566	0	---	0	0	0	0	0	0
1920	355666	0	0	---	0	0	-344666	0	0
960	356666	0	---	0	0	0	0	0	0
192	366666	0	0	---	0	0	0	0	0
64	444444	---	---	---	---	---	---	---	---
384	444445	0	0	---	0	0	---	0	0
384	444446	0	---	0	0	0	0	0	0
960	444455	---	---	---	---	---	---	---	---
1920	444456	---	0	0	0	0	0	0	0
960	444466	---	---	---	---	---	---	444455	---
1280	444555	0	0	---	0	0	0	0	0
3840	444556	0	---	0	0	0	0	0	0
3840	444566	0	0	---	0	0	---	0	0
1280	444666	0	---	0	0	0	0	0	0
960	445555	---	---	---	---	444455	444455	444455	444466
3840	445556	---	0	0	0	0	0	0	0
5760	445566	---	---	---	---	---	---	---	---
3840	445666	---	0	0	0	0	0	0	0
960	446666	---	---	---	---	---	---	444455	---
384	455555	0	0	---	0	0	-444445	0	0
1920	455556	0	---	0	0	0	0	0	0
3840	455566	0	0	---	0	0	-444566	0	0
3840	455666	0	---	0	0	0	0	0	0
1920	456666	0	0	---	0	0	0	0	0
384	466666	0	---	0	0	0	0	0	0
64	555555	---	---	---	---	444444	444444	444444	444444
384	555556	---	0	0	0	0	0	0	0
960	555566	---	---	---	---	444466	444466	444455	444455
1280	555666	---	0	0	0	0	0	0	0
960	556666	---	---	---	---	446666	446666	444455	444466
384	566666	---	0	0	0	0	0	0	0
64	666666	---	---	---	---	---	---	444444	444444

Table 4. *The 18 independent fifth-order elastic constants and their equivalence for a cubic crystal*

11111 = 22222 = 33333
11112 = 11113 = 12222 = 13333 = 22223 = 23333
11122 = 11133 = 11222 = 11333 = 22233 = 22333
11123 = 12223 = 12333
11144 = 22255 = 33366
11155 = 11166 = 22244 = 22266 = 33344 = 33355
11223 = 11233 = 12233
11244 = 11344 = 12255 = 13366 = 22355 = 23366
11255 = 11366 = 12244 = 13344 = 22366 = 23355
11266 = 11355 = 12266 = 13355 = 22344 = 23344
11456 = 22456 = 33456
12344 = 12355 = 12366
12456 = 13456 = 23456
14444 = 25555 = 36666
14455 = 14466 = 24455 = 25566 = 34466 = 35566
15555 = 16666 = 24444 = 26666 = 34444 = 35555
15566 = 24466 = 34455
44456 = 45556 = 45666

Table 5. *Elastic energy ϕ_5 for a cubic crystal*

$$C_{11111}(\eta_1^5+\eta_2^5+\eta_3^5)$$
$$C_{11112}[\eta_1^4(\eta_2+\eta_3)+\eta_2^4(\eta_1+\eta_3)+\eta_3^4(\eta_1+\eta_2)]$$
$$C_{11122}[\eta_1^3(\eta_2^3+\eta_3^2)+\eta_2^3(\eta_1^2+\eta_3^2)+\eta_3^3(\eta_1^2+\eta_2^2)]$$
$$C_{11123}(\eta_1^3\eta_2\eta_3+\eta_1\eta_2^3\eta_3+\eta_1\eta_2\eta_3^3)$$
$$C_{11144}(\eta_1^3\eta_4^3+\eta_2^3\eta_5^2+\eta_3^3\eta_6^2)$$
$$C_{11155}[\eta_1^3(\eta_5^2+\eta_6^2)+\eta_2^3(\eta_4^2+\eta_6^2)+\eta_3^3(\eta_4^2+\eta_5^2)]$$
$$C_{11223}(\eta_1^2\eta_2^2\eta_3+\eta_1^2\eta_2^3\eta_2+\eta_2^2\eta_3^2\eta_1)$$
$$C_{11244}[\eta_1^2\eta_4^2(\eta_2+\eta_3)+\eta_2^2\eta_5^2(\eta_1+\eta_3)+\eta_3^2\eta_6^2(\eta_1+\eta_2)]$$
$$C_{11255}[\eta_1^2\eta(\eta_2\eta_5^2+\eta_3\eta_6^2)+\eta_2^2(\eta_1\eta_4^2+\eta_3\eta_6^2)+\eta_3^2(\eta_1\eta_4^2+\eta_2\eta_5^2)]$$
$$C_{11266}[\eta_1\eta_2\eta_6^2(\eta_1+\eta_2)+\eta_1\eta_3\eta_5^2(\eta_1+\eta_3)+\eta_2\eta_3\eta_4^2(\eta_2+\eta_3)]$$
$$C_{11456}[\eta_4\eta_5\eta_6(\eta_1^2+\eta_2^2+\eta_3^2)]$$
$$C_{12344}[\eta_1\eta_2\eta_3(\eta_2^4+\eta_5^2+\eta_6^2)]$$
$$C_{12456}[\eta_4\eta_5\eta_6(\eta_1\eta_2+\eta_1\eta_3+\eta_2\eta_3)]$$
$$C_{14444}(\eta_1\eta_4^4+\eta_2\eta_5^4+\eta_3\eta_6^4)$$
$$C_{14455}[\eta_4^2\eta_5^2(\eta_1+\eta_2)+\eta_4^2\eta_6^2(\eta_1+\eta_3)+\eta_4^2\eta_5^2(\eta_2+\eta_3)]$$
$$C_{15555}[\eta_5^4(\eta_1+\eta_3)+\eta_4^4(\eta_2+\eta_3)+\eta_6^4(\eta_1+\eta_2)]$$
$$C_{15566}(\eta_1\eta_5^2\eta_6^2+\eta_2\eta_4^2\eta_6^2+\eta_3\eta_4^2\eta_5^2)$$
$$C_{44456}[\eta_4\eta_5\eta_6(\eta_4^2+\eta_5^2+\eta_6^2)]$$

ing non-linear effects is appreciable, which is consistent with the point made by Chang & Barcsh (1967) that the convergence of the series expansion for the strain energy is fairly slow. The recently developed theory (Ljamov, 1972; Ljamov, Hsu & White, 1972) for the calculation of the non-linear effects in the sound velocity, can also be extended to include higher-order terms. Recent measurements in quartz (Lean & Tseng, 1970) make the inclusion of higher-order terms in calculating the amplitude of the harmonic generations pertinent.

Summary

By the use of the symmetry properties of different crystal classes, the schemes of elastic constants have been worked out to higher orders. The number of these constants agree very well with the group-theoretical predictions. These tables can provide the basis for the investigation of non-linear effects of higher orders in different solids.

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APPENDIX

Equations relating the different FOEC for trigonal and hexagonal systems

Equations (B1)

4444 independent
4445 = 4555 = 0
4455 = 2 . 4444
5555 = 4444

Equations (B2)

1444, 1445, 1455, 1555 independent
2444 = $-\frac{1}{2}$(1444 + 1455)   2445 = $-\frac{1}{2}$(3 . 1555 − 1445)
2455 = $-\frac{1}{2}$(3 . 1444 − 1455)   2555 = $-\frac{1}{2}$(1555 + 1445)
4446 = $-\frac{1}{2}$(3 . 1555 + 1445)   4456 = $\frac{1}{2}$(3 . 1444 + 1445)
4556 = $-\frac{1}{2}$(3 . 1555 + 1445)   5556 = $\frac{1}{2}$(3 . 1444 + 1445)

Equations (B3)

1144, 1145, 1155, 1244, 1245, 1255 independent
1446 = $\frac{1}{2}$(2 . 1145 + 3 . 1245)   1556 = $-\frac{1}{2}$(2 . 1145 + 3 . 1245)
1456 = −2 . 1144 + 2 . 1155 − 3 . 1244 + 3 . 1255
2244 = $\frac{1}{2}$(2 . 1155 − 1244 + 1255)
2255 = $\frac{1}{2}$(2 1144 + 1244 − 1255)
2446 = $\frac{1}{2}$(2 . 1145 − 1245)   2556 = $-\frac{1}{2}$(2 . 1145 − 1245)
2245 = −(1145 + 1245)   4566 = 2 . 1245
2456 = −2 . 1144 + 2 . 1155 + 1244 − 1255
4466 = $\frac{1}{2}$(2 . 1144 + 2 . 1155 + 1244 − 3 . 1255)
5566 = $\frac{1}{2}$(2 . 1144 + 2 . 1155 − 3 . 1244 + 1255)

Equations (B4)

1114, 1115, 1124, 1125, 1146, 1156 independent
1224 = −(2 . 1114 + 3 . 1124 − 1156)/3
1225 = −(2 . 1115 + 3 . 1125 + 1146)/3
1246 = −2(1115 + 1125)   1256 = 2(1114 + 1124)
1466 = −(1114 + 1124 − 1156)   1566 = −(1115 + 1125 + 1146)
2224 = −(1114 + 1156)/3   2225 = −(1115 − 1146)/3
2246 = −(8 . 1115 + 1146)/3   2256 = (8 . 1114 − 1156)/3
2466 = −(5 . 1114 − 1156 − 3 . 1124)/3
2566 = −(5 . 1115 + 1146 − 3 . 1125)/3
4666 = −2(1115 − 3 . 1124 − 1146)/3
5666 = 2(1114 − 3 . 1125 + 1156)/3

Equations (B5)

1111, 1112, 1116, 1122, 1166 independent
1126 = −1116   1226 = −1116
1222 = (8 . 1111 + 7 . 1112 − 2 . 1166)/9
1266 = 2(2 . 1111 + 1112 − 1122)
166 = −4 . 1116/3   2222 = (5 . 1111 + 1112 + 1166)/9
2226 = 1116   2266 = (16 . 1111 − 4 . 1112 − 1166)/9
2666 = −4 . 1116/3
6666 = (2 . 1111 − 5 . 1112 + 3 . 1122 + 1166)/3

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The Crystal-Structural Transformation NaCl-type → CsCl-type: Analysis by Martensite Theory

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Orientation relations, interface (habit plane) orientations, and shape changes have been computed by martensite theory for the crystal-structural transformation NaCl-type (f.c.c.) → CsCl-type (primitive cubic), especially in alkali halides. The lattice correspondence used involves contraction along the three-fold axis of a primitive rhombohedron of f.c.c. For the matrix analysis a computer program was written in FORTRAN. Mathematical solutions were obtained using two lattice-invariant shears based on slip and one based on transformation twinning. There are three types of solution. Within each of the three types multiplicity due to symmetry leads to 24 variants. Possible habit planes are near to $\{\bar{1}11\}_I$, $\{210\}_I$ and $\{310\}_I$. Shape changes are large. Predictions agree with observations within experimental error. As the principles applied need not exclude some changes of stoichiometry, they may be relevant to topotaxy.

1. Introduction

Transformation between the NaCl and CsCl structures provides a test of the magnitude of structure change that can proceed martensitically in ionic crystals. Elucidation of the mechanism may also be relevant to topotactic reactions between compounds structurally related to these. Transformations between these structures in the alkali halides at normal or high pressure are also of some technological interest. The transformation of the NaCl to the CsCl structure involves a change of first coordination, from 6 to 8, associated in all known examples with a large volume change, $\Delta V/V_{CsCl} = 17\%$. Martensite theory, which has mainly been applied to alloys, should facilitate description of many structural changes in macroscopic non-metallic crystals, and have special value when there is a large change of lattice. Recent experiments by Fraser & Kennedy (1972) and Livshitz, Ryabinin, Larionov & Zverev (1969) indicate that, under some circumstances, the transformation NaCl-type ⇄ CsCl-type is indeed martensitic. Such experiments provide some data against which to compare predictions, which themselves can serve as a guide to the interpretation of observations.

The present work uses martensite theory to predict orientation relations, interface orientations and shape changes in martensitic transformation from the NaCl structure to the CsCl structure. The analysis is similar for a series of salts because the ratios of the lattice parameters are similar. Results are presented for CsCl, NH_4Cl, NH_4Br and NH_4I, and also for a sufficient range of ratio of lattice parameters to include KCl and other alkali halides which transform under pressure. All these compounds have the NaCl structure in phase I and the CsCl structure in phase II.

2. Theory

2.1 *General principles*

An introduction to martensite theory is given by Kelly & Groves (1970) and by Owen & Shoen (1971). Wayman (1964) and Christian (1965) provide more detailed accounts. Numerous reviews include a recent one by Bowles & Wayman (1972). Original statements of the theory are by Bowles & Mackenzie (1954), and Wechsler, Lieberman & Read (1953). These treatments were applied to metallic alloys. As a different lattice deformation has been used for this transformation, the mathematical analysis has been correspondingly mod-