Acta Cryst. (1979). A**35**, 525–533

Independent Fourth-Order Elastic Coefficients for All Crystal Classes

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(*Received* 29 *June* 1978; *accepted* 16 *January* 1979)

Abstract

Numerical methods can be used to obtain the dependence relations between components of an nth-rank tensor for the particular symmetries of each crystal class. The program has been used successfully to calculate the fourth-order elastic coefficients, corresponding to a tensor of eighth rank for all crystal classes and the isotropic case.

1. Introduction

Higher-order non-linear coefficients have an important place in the behaviour of acoustical devices. In fact, they induce the dependence between the velocity and the amplitude of an elastic wave which causes variations of the time delay and harmonic generation in delay lines and filters. In resonators, they introduce an amplitude–frequency effect as shown by Gagnepain & Besson (1975). Also, the non-linear coefficients are involved in the sensitivity of these devices when subjected to external perturbations such as temperature fluctuations, pressure, accelerations, vibrations, forces, *etc*. These phenomena are the cause of instabilities in devices which need to be stable (particularly in the case of oscillators). Conversely, the non-linearities sometimes can be used, for instance for sensor applications.

The major part of these phenomena can be explained in terms of third-order coefficients. However, the increasing precision of measurement systems reveals phenomena which can be justified only with the introduction of fourth-order coefficients. Moreover, the dependence between the amplitude and the velocity of an elastic wave cannot be explained completely without taking into account the fourth-order coefficients (Tiersten, 1974, 1975).

In order to obtain the equations describing the behaviour of acoustical devices, it is necessary to know the interdependence relations between non-linear coefficients which are components of tensors, for instance, the third- and fourth-order elastic coefficients are components of sixth- and eighth-rank tensors respectively.

The interdependence relations depend on the particular symmetries of each crystal class (see for example Nye, 1957). Zero coefficients, independent coefficients and interdependence relations are well known for tensors up to sixth rank. They are listed by Thurston (1974) and Bechmann & Hearmon (1969). Some particular cases of eighth-rank tensors were studied by Krishnamurty (1963) and Markenscoff (1976) but no systematic investigations have been performed because of the very large number of calculations required.

The method used here to obtain interdependence relations between tensor components is based on the fundamental transformation law for tensors; the tensor components must be unchanged when the transformation corresponds to a symmetry of the crystal.

For instance, for a second rank tensor σ_{ij}, this law is written $\sigma'_{ij} = \alpha_{ik}\alpha_{jl}\sigma_{kl}$, where the α_{ij}'s represent the matrix elements of a particular considered rotation; if this rotation corresponds to a symmetry of the crystal, the tensor σ_{ij} remains unchanged and the transformation law becomes $\sigma_{ij} = \alpha_{ik}\alpha_{jl}\sigma_{kl}$. When all the equations are developed it appears they can be grouped into systems which, when solved, give the interdependence relations.

In the most general case this method needs 3^{2n} terms for an nth-rank tensor, *e.g.* 81 for $n = 2$ but more than 500 000 for $n = 6$ and more than 4×10^7 for $n = 8$. Although this method cannot be used manually, the tensor formulation is particularly suitable for numerical methods.

2. Crystal symmetries

Suppose that a particular physical property of a crystal can be described by a tensor of nth rank ($n = 8$, for example). In a transformation of axes, the components of this tensor $C_{efghijkl}$ become:

$$C'_{mnpqrstx} = \alpha_{me}\alpha_{nf}\alpha_{pg}\alpha_{qh}\alpha_{ri}\,\alpha_{sj}\alpha_{tk}\alpha_{xl}\,C_{efghijkl} \qquad (1)$$

where α_{ij} is the transformation matrix.

If the transformation corresponds to a symmetry of the crystal, relation (1) is an identity and we have:

$$C'_{mnpqrstx} = C_{mnpqrstx}.$$

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Table 1. *Symmetries of the different crystal classes*

Crystal system	Laue group		Generators	Fourth-order independent coefficients	Crystal classes (point groups)		Generators
(*a*)	(*b*)	(*c*)	(*d*)	(*e*)	(*f*)	(*g*)	(*h*)
Triclinic	N	I	R^1	126/126	1 $\bar{1}$	C_1 C_i	R^1 $-R^1$
Monoclinic	M	II	R_z^2	70/70	2 $\bar{2}$ $2/m$	C_2 C_s C_{2h}	R_z^2 $-R_z^2$ $-R^1, R_z^2$
Orthorhombic	O	III	R_x^2, R_z^2	42/42	222 $mm2$ mmm	D_2 C_{2v} D_{2h}	R_x^2, R_z^2 $-R_x^2, R_z^2$ $-R^1, R_x^2, R_z^2$
Tetragonal	TII	IV*a*	R_z^4	64/36	4 $\bar{4}$ $4/m$	C_4 S_4 C_{4h}	R_z^4 $-R_z^4$ $-R^1, R_z^4$
	TI	IV*b*	R_z^4, R_x^2	42/25	422 $4mm$ $\bar{4}2m$ $4/mmm$	D_4 C_{4v} D_{2d} D_{4h}	R_x^2, R_z^4 $-R_x^2, R_z^4$ $R_x^2, -R_z^4$ $-R^1, R_x^2, R_z^4$
Rhombohedral (trigonal)	RII	V*a*	R_z^3	118/42	3 $\bar{3}$	C_3 C_{3i}	R_z^3 $-R^1, R_z^3$
	RI	V*b*	R_x^2, R_z^3	69/28	32 $3m$ $\bar{3}m$	D_3 C_{3v} D_{3d}	R_x^2, R_z^3 $-R_x^2, R_z^3$ $-R^1, R_x^2, R_z^3$
Hexagonal	HII	VI*a*	R_z^6	64/24	6 $\bar{6}$ $6/m$	C_6 C_{3h} C_{6h}	R_z^6 $-R_z^6$ $-R^1, R_z^6$
	HI	VI*b*	R_x^2, R_z^6	42/19	622 $6mm$ $\bar{6}m2$ $6/mmm$	D_6 C_{6v} D_{3h} D_{6h}	R_x^2, R_z^6 $-R_x^2, R_z^6$ $R_x^2, -R_z^6$ $-R^1, R_x^2, R_z^6$
Cubic (isometric)	CII	VII*a*	R_x^2, R_y^2, R_p^3	42/14	23 $m3$	T T_h	R_z^2, R_p^3 $-R^1, R_z^2, R_p^3$
	CI	VII*b*	R_x^4, R_y^4, R_z^4	42/11	432 $\bar{4}3m$ $m3m$	O T_d O_h	R_z^4, R_p^3 $-R_z^4, R_p^3$ $-R^1, R_z^4, R_p^3$
Isotropic	I		All	42/4			All

(*a*) Usual name of the crystal system.
(*b*) Laue groups after Thurston (1974).
(*c*) Laue groups after Bechmann & Hearmon (1969).
(*d*) Generators for even-rank tensors after Thurston (1974). R_z^n means a rotation of $2\pi/n$ about the z axis. p axis corresponds to the direction ⟨111⟩.
(*e*) Number of non-zero coefficients and number of independent fourth-order coefficients.
(*f*) Hermann–Mauguin symbols for the point groups.
(*g*) Schoenflies symbols.
(*h*) Generators for odd-rank tensors after Birss (1963). $-R^1$ means the transformation matrix $-\delta_{ij}$.

Table 1 summarizes the symmetries corresponding to the 11 Laue groups and to the 32 crystal classes.

3. Numerical method

3.1. *Principle of the method*

The best way of presenting the principle of the numerical calculation is to give a typical example. In the rhombohedral system class 3, a second-rank tensor σ_{ij} representing some physical property of the crystal remains unchanged by a $2\pi/3$ rotation about the z axis. In the tensor transformation law, the a_{ij}'s are the elements of the matrix

$$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

In such a case, the nine equations $\sigma_{ij} = a_{ik}a_{jl}\sigma_{kl}$ become:

$$\sigma_{11} = \frac{1}{4}\sigma_{11} - \frac{\sqrt{3}}{4}\sigma_{12} - \frac{\sqrt{3}}{4}\sigma_{21} + \frac{3}{4}\sigma_{22},$$

$$\sigma_{12} = \frac{\sqrt{3}}{4}\sigma_{11} + \frac{1}{4}\sigma_{12} - \frac{3}{4}\sigma_{21} - \frac{\sqrt{3}}{4}\sigma_{22},$$

$$\sigma_{13} = -\frac{1}{2}\sigma_{13} + \frac{\sqrt{3}}{2}\sigma_{23},$$

$$\sigma_{21} = \frac{\sqrt{3}}{4}\sigma_{11} - \frac{3}{4}\sigma_{12} + \frac{1}{4}\sigma_{21} - \frac{\sqrt{3}}{4}\sigma_{22},$$

$$\sigma_{22} = \frac{3}{4}\sigma_{11} + \frac{\sqrt{3}}{4}\sigma_{12} + \frac{\sqrt{3}}{4}\sigma_{21} + \frac{1}{4}\sigma_{22},$$

$$\sigma_{23} = -\frac{\sqrt{3}}{2}\sigma_{13} - \frac{1}{3}\sigma_{23},$$

$$\sigma_{31} = -\frac{1}{2}\sigma_{31} + \frac{\sqrt{3}}{2}\sigma_{32},$$

$$\sigma_{32} = -\frac{\sqrt{3}}{2}\sigma_{31} - \frac{1}{2}\sigma_{32},$$

$$\sigma_{33} = \sigma_{33}.$$

It is obvious that these equations are divided into four systems: one of four equations with four variables, two of two equations with two variables and one of one equation with one variable.

They can be easily transformed into a homogeneous system and reduced into the following systems:

$$\begin{cases} 3\sigma_{11} + \sqrt{3}\sigma_{12} + \sqrt{3}\sigma_{21} - 3\sigma_{22} = 0 \\ \sigma_{11} - \sqrt{3}\sigma_{12} - \sqrt{3}\sigma_{21} - \sigma_{22} = 0\ , \end{cases}$$

$$\begin{cases} -3\sigma_{13} + \sqrt{3}\sigma_{23} = 0 \\ \sigma_{13} + \sqrt{3}\sigma_{23} = 0\ , \end{cases}$$

$$\begin{cases} -3\sigma_{31} + \sqrt{3}\sigma_{32} = 0 \\ \sigma_{31} + \sqrt{3}\sigma_{32} = 0\ , \end{cases}$$

σ_{33} being independent.

When solved, the first system gives $\sigma_{11} = \sigma_{22}$ and $\sigma_{21} = -\sigma_{12}$, the second and third systems give $\sigma_{13} = \sigma_{23} = 0$ and $\sigma_{31} = \sigma_{32} = 0$ respectively. Hence for class 3, a second-rank non-symmetrical tensor takes the form:

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & 0 \\ -\sigma_{12} & \sigma_{11} & 0 \\ 0 & 0 & \sigma_{33} \end{pmatrix},$$

and therefore there are three independent coefficients (as given by Thurston, 1974).

3.2. *Homogeneous systems*

The program used here to obtain the homogeneous systems for the fourth-order elastic coefficients follows almost exactly the preceding principle. These coefficients are components of an eighth-rank symmetrical tensor which enables one to write them in the form C_{IJKL}, where the four subscripts vary from 1 to 6 following the notation of Voigt (1928): 11 = 1, 22 = 2, 33 = 3, 23 = 32 = 4, 31 = 13 = 5, 12 = 21 = 6. The order of the subscripts has no importance. Thus there exist at most 126 fourth-order elastic coefficients.

Fig. 1 shows the flow chart of the program used and Fig. 2 is an extract showing the form in which the homogeneous equations are obtained. For any generator, these equations involve at most 20 variables. For a given generator, when all the 126 equations are obtained, it appears they can be grouped into systems

Table 2. *Systems of equations for the group R*II

Number of systems	1	1	1	2	1	1	2	1	1	2	1	1
Number of equations	20	18	15	12	10	9	6	5	4	3	2	1

containing at most 20 equations. The number of systems and the number of equations in each system depends on the considered generator. For example, one obtains 15 systems of n equations in n variables for the trigonal system (RII group, generator R_k^3) as shown in Table 2.

There is a total of 126 equations corresponding to the 126 possible fourth-order elastic coefficients.

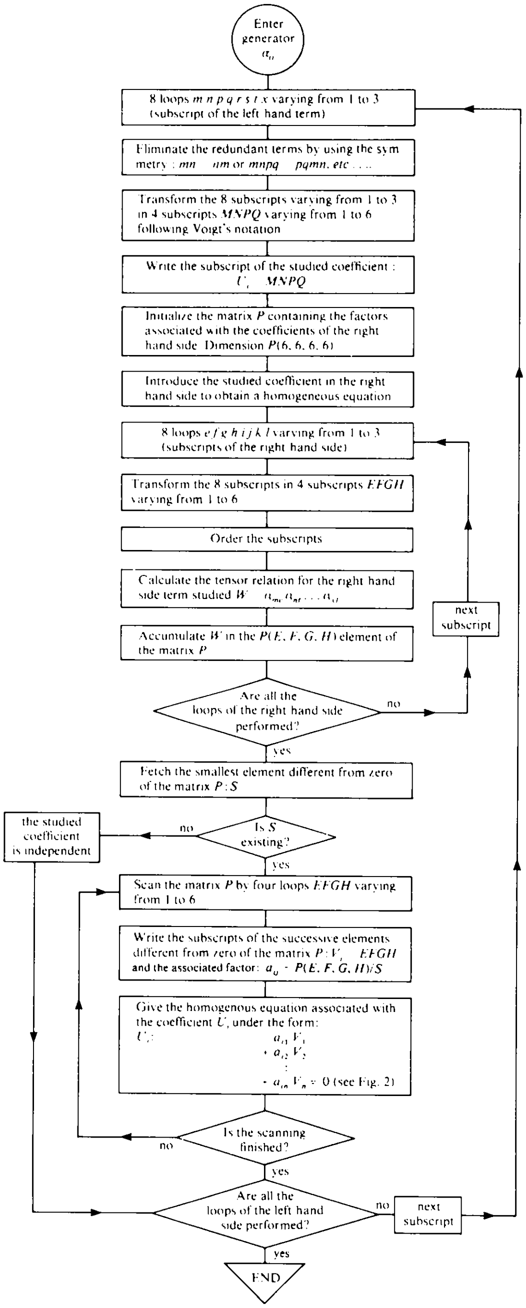
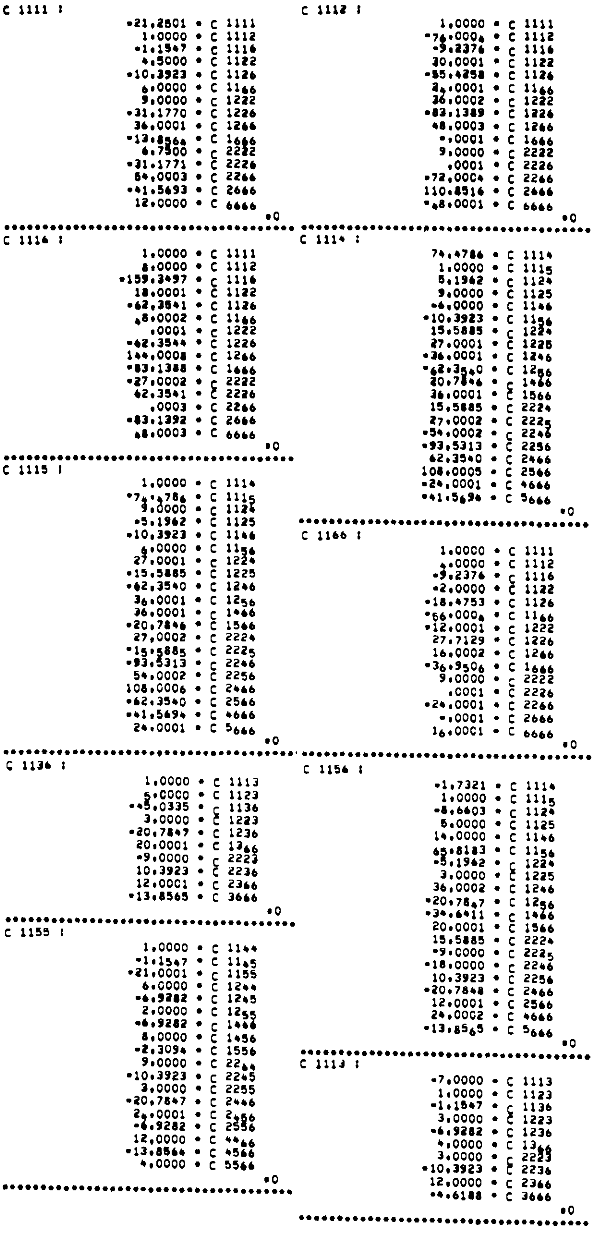


Fig. 1. Flow chart of the program giving the homogeneous equations.

3.3. *Resolution of the homogeneous systems*

When all the homogeneous equations corresponding to the studied generator are obtained from the first program, it is possible by simple examination to group them into systems as can be shown by the example given in § 3.1 or by the extract given in Fig. 2. They are homogeneous systems of n equations in m unknowns (generally $n = m$).

The problem is to calculate the rank of these systems and to obtain the dependence relations between



```
C 1111 :
           •21,2801 • C 1111
             1,0000 • C 1112
            •1,1547 • C 1116
             4,5000 • C 1122
           •10,3923 • C 1126
             6,0000 • C 1166
             9,0000 • C 1222
           •31,1770 • C 1226
            36,0001 • C 1266
           •13,8564 • C 1666
             6,7500 • C 2222
           •31,1771 • C 2226
            54,0003 • C 2266
           •41,5693 • C 2666
            12,0000 • C 6666
                                •0
••••••••••••••••••••••••••••••••••••••
C 1116 :
             1,0000 • C 1111
             8,0000 • C 1112
          •159,3497 • C 1116
            18,0001 • C 1122
           •62,3541 • C 1126
            48,0002 • C 1166
              ,0001 • C 1222
           •62,3544 • C 1226
           144,0008 • C 1266
           •83,1388 • C 1666
           •27,0002 • C 2222
            62,3541 • C 2226
              ,0003 • C 2266
           •83,1392 • C 2666
            48,0003 • C 6666
                                •0
••••••••••••••••••••••••••••••••••••••
C 1115 :
             1,0000 • C 1114
           •74,4786 • C 1115
             9,0000 • C 1124
            •5,1962 • C 1125
           •10,3923 • C 1146
             6,0000 • C 1156
            27,0001 • C 1224
           •15,5885 • C 1225
           •62,3540 • C 1246
            36,0001 • C 1256
            36,0001 • C 1466
           •20,7846 • C 1566
            27,0002 • C 2224
           •15,5885 • C 2225
           •93,5313 • C 2246
            54,0002 • C 2256
           108,0006 • C 2466
           •62,3540 • C 2566
           •41,5694 • C 4666
            24,0001 • C 5666
                                •0
••••••••••••••••••••••••••••••••••••••
C 1136 :
             1,0000 • C 1113
             5,0000 • C 1123
           •45,0335 • C 1136
             3,0000 • C 1223
           •20,7847 • C 1236
            20,0001 • C 1366
            •9,0000 • C 2223
            10,3923 • C 2236
            12,0001 • C 2366
           •13,8565 • C 3666
                                •0
••••••••••••••••••••••••••••••••••••••
C 1155 :
             1,0000 • C 1144
            •1,1547 • C 1145
           •21,0001 • C 1155
             6,0000 • C 1244
            •6,9282 • C 1245
             2,0000 • C 1255
            •6,9282 • C 1466
             8,0000 • C 1456
            •2,3094 • C 1556
             9,0000 • C 2244
           •10,3923 • C 2245
             3,0000 • C 2255
           •20,7847 • C 2446
            24,0001 • C 2456
            •6,9282 • C 2556
            12,0000 • C 4466
           •13,8564 • C 4566
             4,0000 • C 5566
                                •0
••••••••••••••••••••••••••••••••••••••
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C 1112 :
             1,0000 • C 1111
           •76,0006 • C 1112
            •9,2376 • C 1116
            30,0001 • C 1122
           •55,4258 • C 1126
            24,0001 • C 1166
            36,0002 • C 1222
           •83,1389 • C 1226
            48,0003 • C 1266
             •,0001 • C 1666
             9,0000 • C 2222
              ,0001 • C 2226
           •72,0004 • C 2266
           110,8516 • C 2666
           •48,0001 • C 6666
                                •0
••••••••••••••••••••••••••••••••••••••
C 1114 :
            74,4786 • C 1114
             1,0000 • C 1115
             5,1962 • C 1124
             9,0000 • C 1125
            •6,0000 • C 1146
           •10,3923 • C 1156
            15,5885 • C 1224
            27,0001 • C 1225
           •36,0001 • C 1246
           •62,3540 • C 1256
            20,7846 • C 1466
            36,0001 • C 1566
            15,5885 • C 2224
            27,0002 • C 2225
           •54,0002 • C 2246
           •93,5313 • C 2256
            62,3540 • C 2466
           108,0005 • C 2566
           •24,0001 • C 4666
           •41,5694 • C 5666
                                •0
••••••••••••••••••••••••••••••••••••••
C 1166 :
             1,0000 • C 1111
             4,0000 • C 1112
            •9,2376 • C 1116
            •2,0000 • C 1122
           •18,4753 • C 1126
           •66,0006 • C 1166
           •12,0001 • C 1222
            27,7129 • C 1226
            16,0002 • C 1266
           •36,9506 • C 1666
             9,0000 • C 2222
              ,0001 • C 2226
           •24,0001 • C 2266
             •,0001 • C 2666
            16,0001 • C 6666
                                •0
••••••••••••••••••••••••••••••••••••••
C 1156 :
            •1,7321 • C 1114
             1,0000 • C 1115
            •8,6603 • C 1124
             5,0000 • C 1125
            14,0000 • C 1146
            65,8183 • C 1156
            •5,1962 • C 1224
             3,0000 • C 1225
            36,0002 • C 1246
           •20,7847 • C 1256
           •34,6411 • C 1466
            20,0001 • C 1566
            15,5885 • C 2224
            •9,0000 • C 2225
           •18,0000 • C 2246
            10,3923 • C 2256
           •20,7848 • C 2466
            12,0001 • C 2566
            24,0002 • C 4666
           •13,8565 • C 5666
                                •0
••••••••••••••••••••••••••••••••••••••
C 1113 :
            •7,0000 • C 1113
             1,0000 • C 1123
            •1,1547 • C 1136
             3,0000 • C 1223
            •6,9282 • C 1236
             4,0000 • C 1366
             3,0000 • C 2223
           •10,3923 • C 2236
            12,0000 • C 2366
            •4,6188 • C 3666
                                •0
••••••••••••••••••••••••••••••••••••••
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Fig. 2. Facsimile showing the form under which the homogeneous equations are obtained.

coefficients. One obtains at the same time the zero and independent coefficients.

Although program libraries probably include algorithms able to solve this problem, the particular form of the systems to be reduced makes the work simpler so that the program has been conceived in Basic language and used with a desk-top computer. The simplification comes from the a_{ij}'s which can always be reduced to integers or integers multiplied by $\sqrt{3}$, whatever the generator is. This fact is easy to understand by examining the matrices of the possible generators, the elements of which are always rational or rational numbers multiplied by $\sqrt{3}$ as shown by Birss (1963).

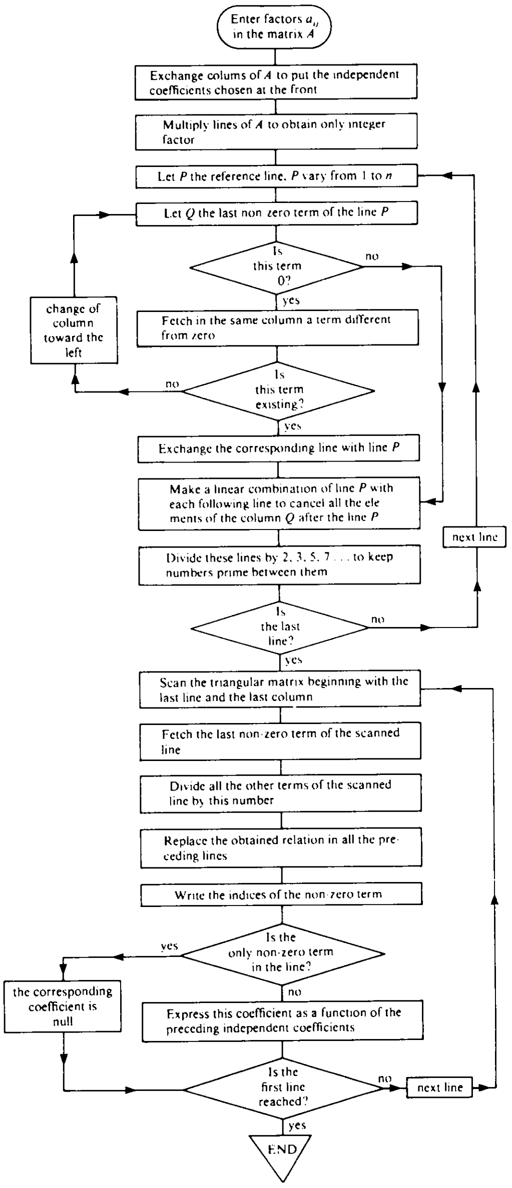

Fig. 3. Flow chart of the program used to obtain dependence relations between coefficients.

Fig. 3 shows the flow chart of the program used. The matrix of the coefficient factors is set in triangular form by expressing one of the coefficients as a function of all the others and carrying the relation obtained over the $n-1$ remaining equations and so on. Eventually one obtains k relations between the n coefficients ($k \leq n$). Some equations give zero coefficients, others express dependent coefficients as functions of independent coefficients. The arbitrary choice of these independent coefficients was made by taking into account the degree of symmetry between subscripts; that is, in order of preference the coefficients are taken as C_{IIII}, C_{IIJJ}, C_{IIIJ}, C_{IIJK}, C_{IJKL}. For equal symmetry, the lower numerical value is chosen. Use of another choice is, of course, a matter of personal preference and the modification presents no difficulty.

3.4. *Remark*

For groups having several generators, results are obtained by means of the resolution program, systems corresponding to the different generators being considered simultaneously. The isotropic case is treated by applying the resolution program to all generators of the Laue groups and then using all the resulting dependence relations simultaneously.

4. Results and verifications

The coefficients obtained by this method are given according to the notations and definitions of Brugger (1965). The two programs have been checked on the second- and third-order elastic coefficients for all the Laue groups as well as the second- and third-order piezoelectric coefficients for the point group 32. One obtains, in this way, the classical results compiled by Thurston (1974) and Bechmann & Hearmon (1969). By changing the choice of the independent coefficients, the fourth-order elastic coefficients given by Markenscoff (1976) for the Laue group *R*I were checked.† The fourth-order elastic coefficients for group *C*1 given by Krishnamurty (1963) are correct but the relations he obtains manually for the isotropic case, although using the proper coefficients, are erroneous.

The number of independent coefficients obtained for each Laue group corresponds to that calculated by group theory and given by Krishnamurty (1963) and Krishnamurty & Gopalakrishnamurty (1968).

Table 3 summarizes the results obtained for the eleven Laue groups and the isotropic case. Only the subscripts are specified. The asterisk (*) indicates an independent coefficient and the numbers in brackets refer to the footnotes.

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† Except for an error of sign in the coefficient C_{1122}.

Table 3. *Independent fourth-order elastic coefficients for the* 32 *crystal classes*

	M												
N	*X*	*Y*	*Z*	*O*	*T*II	*T*I	*R*II	*R*I	*H*II	*H*I	*C*II	*C*I	*I*
1111	*	*	*	*	*	*	*	*	*	*	*	*	*
1112	*	*	*	*	*	*	(1)	(1)	(1)	(1)	*	*	(57)
1113	*	*	*	*	*	*	*	*	*	*	*	1112	1112
1114	*	0	0	0	0	0	*	*	0	0	0	0	0
1115	0	*	0	0	0	0	*	0	0	0	0	0	0
1116	0	0	*	0	*	0	*	0	*	0	0	0	0
1122	*	*	*	*	*	*	*	*	*	*	*	*	*
1123	*	*	*	*	*	*	*	*	*	*	*	*	(58)
1124	*	0	0	0	0	0	(2)	(2)	0	0	0	0	0
1125	0	*	0	0	0	0	(3)	0	0	0	0	0	0
1126	0	0	*	0	*	0	(4)	0	(4)	0	0	0	0
1133	*	*	*	*	*	*	*	*	*	*	1122	1122	1122
1134	*	0	0	0	0	0	*	*	0	0	0	0	0
1135	0	*	0	0	0	0	*	0	0	0	0	0	0
1136	0	0	*	0	*	0	−3666	0	−3666	0	0	0	0
1144	*	*	*	*	*	*	*	*	*	*	*	*	*
1145	0	0	*	0	*	0	*	0	*	0	0	0	0
1146	0	*	0	0	0	0	(5)	0	0	0	0	0	0
1155	*	*	*	*	*	*	*	*	*	*	*	*	(59)
1156	*	0	0	0	0	0	(6)	(6)	0	0	0	0	0
1166	*	*	*	*	*	*	(7)	(7)	(7)	(7)	*	1155	1155
1222	*	*	*	*	1112	1112	(8)	(8)	(8)	(8)	1113	1112	1112
1223	*	*	*	*	1123	1123	(9)	(9)	(9)	(9)	1123	1123	1123
1224	*	0	0	0	0	0	(10)	(10)	0	0	0	0	0
1225	0	*	0	0	0	0	(11)	0	0	0	0	0	0
1226	0	0	*	0	−1126	0	(12)	0	(12)	0	0	0	0
1233	*	*	*	*	*	*	(13)	(13)	(13)	(13)	1123	1123	1123
1234	*	0	0	0	0	0	(14)	(14)	0	0	0	0	0
1235	0	*	0	0	0	0	(15)	0	0	0	0	0	0
1236	0	0	*	0	0	0	3666	0	3666	0	0	0	0
1244	*	*	*	*	*	*	(16)	(16)	(16)	(16)	*	*	(60)
1245	0	0	*	0	0	0	(17)	0	(17)	0	0	0	0
1246	0	*	0	0	0	0	(18)	0	0	0	0	0	0
1255	*	*	*	*	1244	1244	(19)	(19)	(19)	(19)	*	1244	1244
1256	*	0	0	0	0	0	(20)	(20)	0	0	0	0	0
1266	*	*	*	*	*	*	(21)	(21)	(21)	(21)	*	*	(61)
1333	*	*	*	*	*	*	*	*	*	*	1112	1112	1112
1334	*	0	0	0	0	0	*	*	0	0	0	0	0
1335	0	*	0	0	0	0	*	0	0	0	0	0	0
1336	0	0	*	0	*	0	0	0	0	0	0	0	0
1344	*	*	*	*	*	*	*	*	*	*	1255	1244	1244
1345	0	0	*	0	*	0	3446	0	3446	0	0	0	0
1346	0	*	0	0	0	0	(22)	0	0	0	0	0	0
1355	*	*	*	*	*	*	*	*	*	*	1266	1266	1266
1356	*	0	0	0	0	0	(23)	(23)	0	0	0	0	0
1366	*	*	*	*	*	*	(24)	(24)	(24)	(24)	1244	1244	1244

(1) $C_{1112} = -\frac{1}{8}C_{1111} + \frac{3}{8}C_{2222} - 2C_{6666} + \frac{3}{4}C_{1122}.$

(2) $C_{1124} = -\frac{1}{3}C_{2224} - \frac{4}{3}C_{5666}.$

(3) $C_{1125} = -\frac{1}{3}C_{2225} + \frac{4}{3}C_{4666}.$

(4) $C_{1126} = -\frac{1}{3}C_{1116}.$

(5) $C_{1146} = \frac{1}{6}C_{1115} + \frac{1}{2}C_{2225}.$

(6) $C_{1156} = -\frac{1}{6}C_{1114} - \frac{1}{2}C_{2224}.$

(7) $C_{1166} = -\frac{3}{16}C_{1111} + \frac{5}{16}C_{2222} + \frac{1}{3}C_{6666} - \frac{1}{8}C_{1122}.$

(8) $C_{1222} = \frac{3}{8}C_{1111} - \frac{1}{8}C_{2222} - 2C_{6666} + \frac{3}{4}C_{1122}.$

(9) $C_{1223} = C_{1113} - C_{2223} + C_{1123}.$

(10) $C_{1224} = -\frac{1}{3}C_{1114} + \frac{4}{3}C_{5666}.$

(11) $C_{1225} = -\frac{1}{3}C_{1115} - \frac{4}{3}C_{4666}.$

(12) $C_{1226} = -\frac{1}{3}C_{1116}.$

(13) $C_{1233} = C_{1133} - 2C_{3366}.$

(14) $C_{1234} = -\frac{1}{2}C_{1134} - \frac{1}{2}C_{2234}.$

(15) $C_{1235} = -\frac{1}{2}C_{1135} - \frac{1}{2}C_{2235}.$

(16) $C_{1244} = \frac{1}{2}C_{1144} + 2C_{1155} - \frac{3}{2}C_{2244} - 2C_{4466}$

(17) $C_{1245} = -\frac{1}{3}C_{1145} + \frac{2}{3}C_{1446}.$

(18) $C_{1246} = -\frac{1}{6}C_{1115} + \frac{1}{6}C_{2225} - \frac{2}{3}C_{4666}.$

(19) $C_{1255} = \frac{1}{2}C_{1144} + C_{1155} - \frac{1}{2}C_{2244} - 2C_{4466}.$

(20) $C_{1256} = \frac{1}{6}C_{1114} - \frac{1}{6}C_{2224} - \frac{2}{3}C_{5666}.$

(21) $C_{1266} = \frac{1}{16}C_{1111} + \frac{1}{16}C_{2222} - \frac{1}{3}C_{6666} - \frac{1}{8}C_{1122}.$

(22) $C_{1346} = \frac{1}{4}C_{1135} + \frac{3}{4}C_{2235}$

(23) $C_{1356} = -\frac{1}{4}C_{1134} - \frac{3}{4}C_{2234}.$

(24) $C_{1366} = -\frac{1}{2}C_{1113} + \frac{3}{4}C_{2223} - \frac{1}{4}C_{1123}.$

(57) $C_{1112} = \frac{1}{4}C_{1111} - 2C_{4444} + \frac{3}{4}C_{1122}.$

(58) $C_{1123} = C_{1122} - 2C_{1144}.$

(59) $C_{1155} = \frac{1}{8}C_{1111} + \frac{1}{3}C_{4444} - \frac{1}{8}C_{1122}.$

(60) $C_{1244} = \frac{1}{16}C_{1111} - \frac{1}{2}C_{4444} - \frac{1}{16}C_{1122} + \frac{1}{2}C_{1144}.$

(61) $C_{1266} = \frac{1}{8}C_{1111} - \frac{1}{3}C_{4444} - \frac{1}{8}C_{1122}.$

Table 3 (*cont.*)

N	*M*			*O*	*T*II	*T*I	*R*II	*R*I	*H*II	*H*I	*C*II	*C*I	*I*
	X	*Y*	*Z*										
1444	*	0	0	0	0	0	*	*	0	0	0	0	0
1445	0	*	0	0	0	0	(25)	0	0	0	0	0	0
1446	0	0	*	0	*	0	*	0	*	0	0	0	0
1455	*	0	0	0	0	0	(26)	(26)	0	0	0	0	0
1456	*	*	*	*	*	*	(27)	(27)	(27)	(27)	*	*	(62)
1466	*	0	0	0	0	0	(28)	(28)	0	0	0	0	0
1555	0	*	0	0	0	0	*	0	0	0	0	0	0
1556	0	0	*	0	*	0	−1446	0	−1446	0	0	0	0
1566	0	*	0	0	0	0	(29)	0	0	0	0	0	0
1666	0	0	*	0	*	0	(30)	0	(30)	0	0	0	0
2222	*	*	*	*	1111	1111	*	*	*	*	1111	1111	1111
2223	*	*	*	*	1113	1113	*	*	*	*	1112	1112	1112
2224	*	0	0	0	0	0	*	*	0	0	0	0	0
2225	0	*	0	0	0	0	*	0	0	0	0	0	0
2226	0	0	*	0	−1116	0	1116	0	1116	0	0	0	0
2233	*	*	*	*	1133	1133	1133	1133	1133	1133	1122	1122	1122
2234	*	0	0	0	0	0	*	*	0	0	0	0	0
2235	0	*	0	0	0	0	*	0	0	0	0	0	0
2236	0	0	*	0	−1136	0	−3666	0	−3666	0	0	0	0
2244	*	*	*	*	1155	1155	*	*	*	*	1166	1155	1155
2245	0	0	*	0	−1145	0	(31)	0	(31)	0	0	0	0
2246	0	*	0	0	0	0	(32)	0	0	0	0	0	0
2255	*	*	*	*	1144	1144	(33)	(33)	(33)	(33)	1144	1144	1144
2256	*	0	0	0	0	0	(34)	(34)	0	0	0	0	0
2266	*	*	*	*	1166	1166	(35)	(35)	(35)	(35)	1155	1155	1155
2333	*	*	*	*	1333	1333	1333	1333	1333	1333	1113	1112	1112
2334	*	0	0	0	0	0	−1334	−1334	0	0	0	0	0
2335	0	*	0	0	0	0	−1335	0	0	0	0	0	0
2336	0	0	*	0	−1336	0	0	0	0	0	0	0	0
2344	*	*	*	*	1355	1355	1355	1355	1355	1355	1266	1266	1266
2345	0	0	*	0	−1345	0	−3446	0	−3446	0	0	0	0
2346	0	*	0	0	0	0	(36)	0	0	0	0	0	0
2355	*	*	*	*	1344	1344	1344	1344	1344	1344	1244	1244	1244
2356	*	0	0	0	0	0	(37)	(37)	0	0	0	0	0
2366	*	*	*	*	1366	1366	(38)	(38)	(38)	(38)	1255	1244	1244
2444	*	0	0	0	0	0	*	*	0	0	0	0	0
2445	0	*	0	0	0	0	(39)	0	0	0	0	0	0
2446	0	0	*	0	−1556	0	(40)	0	(40)	0	0	0	0
2455	*	0	0	0	0	0	(41)	(41)	0	0	0	0	0
2456	*	*	*	*	1456	1456	(42)	(42)	(42)	(42)	1456	1456	1456
2466	*	0	0	0	0	0	(43)	(43)	0	0	0	0	0
2555	0	*	0	0	0	0	*	0	0	0	0	0	0
2556	0	0	*	0	−1446	0	(44)	0	(44)	0	0	0	0
2566	0	*	0	0	0	0	(45)	0	0	0	0	0	0
2666	0	0	*	0	−1666	0	(46)	0	(46)	0	0	0	0

(25) $C_{1445} = -\frac{1}{3}C_{1555} - \frac{2}{3}C_{2555}.$
(26) $C_{1455} = -\frac{1}{3}C_{1444} - \frac{2}{3}C_{2444}.$
(27) $C_{1456} = -\frac{1}{4}C_{1144} - \frac{1}{2}C_{1155} + \frac{3}{4}C_{2244}.$
(28) $C_{1466} = -\frac{1}{6}C_{1114} - \frac{1}{6}C_{2224} + \frac{1}{3}C_{5666}.$
(29) $C_{1566} = -\frac{1}{6}C_{1115} - \frac{1}{6}C_{2225} - \frac{1}{3}C_{4666}.$
(30) $C_{1666} = -\frac{1}{3}C_{1116}.$
(31) $C_{2245} = -\frac{1}{3}C_{1145} - \frac{4}{3}C_{1446}.$
(32) $C_{2246} = -\frac{1}{2}C_{1115} - \frac{1}{6}C_{2225}.$
(33) $C_{2255} = C_{1144} + C_{1155} - C_{2244}.$
(34) $C_{2256} = \frac{1}{2}C_{1114} + \frac{1}{6}C_{2224}.$
(35) $C_{2266} = \frac{5}{16}C_{1111} - \frac{3}{16}C_{2222} + \frac{1}{3}C_{6666} - \frac{1}{8}C_{1122}.$
(36) $C_{2346} = -\frac{3}{4}C_{1135} - \frac{1}{4}C_{2235}.$

(37) $C_{2356} = \frac{3}{4}C_{1134} + \frac{1}{4}C_{2234}.$
(38) $C_{2366} = \frac{1}{2}C_{1113} - \frac{1}{4}C_{2223} - \frac{1}{4}C_{1123}.$
(39) $C_{2445} = -\frac{2}{3}C_{1555} - \frac{1}{3}C_{2555}.$
(40) $C_{2446} = \frac{2}{3}C_{1145} - \frac{1}{3}C_{1446}.$
(41) $C_{2455} = -\frac{2}{3}C_{1444} - \frac{1}{3}C_{2444}.$
(42) $C_{2456} = -\frac{1}{4}C_{1144} + \frac{1}{2}C_{1155} - \frac{1}{4}C_{2244}.$
(43) $C_{2466} = -\frac{1}{6}C_{1114} - \frac{1}{6}C_{2224} - \frac{1}{3}C_{5666}.$
(44) $C_{2556} = -\frac{2}{3}C_{1145} + \frac{1}{3}C_{1446}.$
(45) $C_{2566} = -\frac{1}{6}C_{1115} - \frac{1}{6}C_{2225} + \frac{1}{3}C_{4666}.$
(46) $C_{2666} = -\frac{1}{3}C_{1116}.$
(62) $C_{1456} = \frac{1}{32}C_{1111} + \frac{1}{12}C_{4444} - \frac{1}{32}C_{1122} - \frac{1}{4}C_{1144}.$

Table 3 (*cont.*)

	M												
N	*X*	*Y*	*Z*	*O*	*T*II	*T*I	*R*II	*R*I	*H*II	*H*I	*C*II	*C*I	*I*
3333	*	*	*	*	*	*	*	*	*	*	1111	1111	1111
3334	*	0	0	0	0	0	0	0	0	0	0	0	0
3335	0	*	0	0	0	0	0	0	0	0	0	0	0
3336	0	0	*	0	0	0	0	0	0	0	0	0	0
3344	*	*	*	*	*	*	*	*	*	*	1155	1155	1155
3345	0	0	*	0	0	0	0	0	0	0	0	0	0
3346	0	*	0	0	0	0	−1335	0	0	0	0	0	0
3355	*	*	*	*	3344	3344	3344	3344	3344	3344	1166	1155	1155
3356	*	0	0	0	0	0	1334	1334	0	0	0	0	0
3366	*	*	*	*	*	*	*	*	*	*	1144	1144	1144
3444	*	0	0	0	0	0	*	*	0	0	0	0	0
3445	0	*	0	0	0	0	−3555	0	0	0	0	0	0
3446	0	0	*	0	*	0	*	0	*	0	0	0	0
3455	*	0	0	0	0	0	−3444	−3444	0	0	0	0	0
3456	*	*	*	*	*	*	(47)	(47)	(47)	(47)	1456	1456	1456
3466	*	0	0	0	0	0	(48)	(48)	0	0	0	0	0
3555	0	*	0	0	0	0	*	0	0	0	0	0	0
3556	0	0	*	0	−3446	0	−3446	0	−3446	0	0	0	0
3566	0	*	0	0	0	0	(49)	0	0	0	0	0	0
3666	0	0	*	0	0	0	*	0	*	0	0	0	0
4444	*	*	*	*	*	*	*	*	*	*	*	*	*
4445	0	0	*	0	*	0	0	0	0	0	0	0	0
4446	0	*	0	0	0	0	(50)	0	0	0	0	0	0
4455	*	*	*	*	*	*	(51)	(51)	(51)	(51)	*	*	(51)
4456	*	0	0	0	0	0	(52)	(52)	0	0	0	0	0
4466	*	*	*	*	*	*	*	*	*	*	4455	4455	4455
4555	0	0	*	0	−4445	0	0	0	0	0	0	0	0
4556	0	*	0	0	0	0	(53)	0	0	0	0	0	0
4566	0	0	*	0	0	0	(54)	0	(54)	0	0	0	0
4666	0	*	0	0	0	0	*	0	0	0	0	0	0
5555	*	*	*	*	4444	4444	4444	4444	4444	4444	4444	4444	4444
5556	*	0	0	0	0	0	(55)	(55)	0	0	0	0	0
5566	*	*	*	*	4466	4466	(56)	(56)	(56)	(56)	4455	4455	4455
5666	*	0	0	0	0	0	*	*	0	0	0	0	0
6666	*	*	*	*	*	*	*	*	*	*	4444	4444	4444

(47) $C_{3456} = -\frac{1}{2}C_{1344} + \frac{1}{2}C_{1355}$.
(48) $C_{3466} = -\frac{1}{2}C_{1134} - \frac{1}{2}C_{2234}$.
(49) $C_{3566} = -\frac{1}{2}C_{1135} - \frac{1}{2}C_{2235}$.
(50) $C_{4446} = -\frac{1}{2}C_{1555} + \frac{1}{2}C_{2555}$.
(51) $C_{4455} = \frac{1}{3}C_{4444}$.
(52) $C_{4456} = \frac{1}{6}C_{1444} - \frac{1}{6}C_{2444}$.
(53) $C_{4556} = -\frac{1}{6}C_{1555} + \frac{1}{6}C_{2555}$.
(54) $C_{4566} = -\frac{1}{3}C_{1145} + \frac{2}{3}C_{1446}$.
(55) $C_{5556} = \frac{1}{2}C_{1444} - \frac{1}{2}C_{2444}$.
(56) $C_{5566} = -C_{1155} + C_{2244} + C_{4466}$.

Except for the monoclinic system, where three orientations have been studied, the reference is always the z axis, as shown in column (d) of Table 1.

5. Conclusion

The program used for the fourth-order elastic coefficients can be adapted without difficulty to the calculation of coefficients of all kinds and all orders (permittivity, piezoelectricity, *etc.*), as long as they are components of a tensor for which equation (1) holds. In practice, the time of calculation is an exponential function of the rank of the tensor, thus a practical upper limit is reached for tenth-rank tensors.

There is no difficulty in applying the program to the calculation of the relations between coefficients for any rotation for which the matrix is known.

The author wishes to thank Dr J.-J. Gagnepain for his interest and support and Dr B. A. Auld for revising this manuscript.

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Acta Cryst. (1979). A**35**, 533–536

Magnetic Structure of $PrCo_2Ge_2$, a Neutron Diffraction Study

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(*Received* 31 *January* 1978; *accepted* 25 *January* 1979)

Abstract

The crystallographic structure of the compound $PrCo_2Ge_2$ is of the $BaAl_4$ type. The space group is $I4/mmm$ and the lattice constants are $a = 4{\cdot}048$ and $c = 10{\cdot}178$ Å. A neutron diffraction study revealed a transition to a magnetically ordered state at $T_N \sim 27$ K and six superlattice lines below T_N. It is possible to index these lines according to a sinusoidal magnetic structure with a period $\tau^{-1} = 13{\cdot}94$ Å along **c**. Observed intensities are consistent with ordering of the Pr sublattice with the magnetic axis along **c**.

I. Introduction

The compound $PrCo_2Ge_2$ belongs (McCall, Narasimhan & Butera, 1973*a*) to the series of compounds AB_2X_2 (A = U, Th, rare-earth; B = Mn, Fe, Co; X = Si, Ge). These compounds crystallize with the $BaAl_4$-type structure, which belongs to the tetragonal space group $I4/mmm$ (D^{17}_{4h}). The lattice constants of $PrCo_2Ge_2$ as determined by X-rays (McCall *et al.*, 1973*a*) are $a = 4{\cdot}048$ and $c = 10{\cdot}178$ Å. Magnetic-susceptibility measurements (McCall, Narasimhan & Butera, 1973*b*) exhibit a peak at 28 K with the susceptibility rising with decreasing temperature down to 4·2 K. It was suggested that this behaviour is due to the antiferromagnetic ordering of the Pr ion. In the present paper we report the results of a neutron diffraction study of a powder sample of $PrCo_2Ge_2$, undertaken in order to determine the magnetic structure of this compound.

II. Experimental

The powder sample was synthesized by arc melting under an atmosphere of argon gas. Neutron diffraction patterns were taken at room temperature (RT) and liquid-helium temperature (LT). The RT and LT patterns are shown in Fig. 1. All the reflections observed in the RT pattern are in agreement with the reported lattice constants (McCall *et al.*, 1973*a*). Six superlattice lines are observed in the LT pattern. The remaining lines can be indexed according to the unit cell with lattice constants $a = b = 4{\cdot}037$ and $c = 10{\cdot}173$ Å.

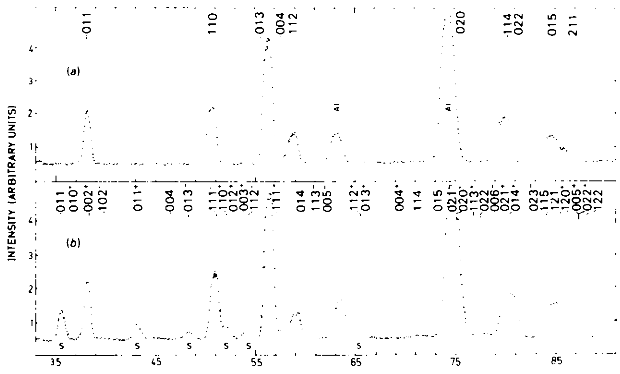

Fig. 1. Neutron ($\lambda = 2{\cdot}45$ Å) diffraction patterns of $PrCo_2Ge_2$ at (*a*) RT and (*b*) LT. No reflection was observed in the range $5° < 2\theta < 33°$ (not shown). The subscripts S in the LT pattern are for superlattice lines. The RT and the LT patterns were indexed according to $a = 4{\cdot}048$, $c = 10{\cdot}178$ Å and $a' = 4{\cdot}037$, $c' = 10{\cdot}173$ Å and $\tau^{-1} = 13{\cdot}94$ Å respectively.

0567-7394/79/040533-04$01.00