Appendix 5

Coordinate transformations and crystal symmetries

A5.1 ROTATIONS OF THE COORDINATE SYSTEM

In Appendix 2 it was shown that the general form of the transformation relating the coordinates x_k, x'_k of a point P in two rectangular cartesian coordinate systems Ox_k and Ox_k, with a common origin O is

$$x_k = a_{km}x'_m \tag{A5.1}$$

where

$$a_{km}a_{kn} = \delta_{mn} \tag{A5.2}$$

and the inverse of Eqn (A5.1) is

$$x'_k = a_{mk}x_m \tag{A5.3}$$

It was also stated in Appendix 2 that these equations describe either a rotation of the coordinate system, or a rotation accompanied by an inversion. In the first case, the determinant $\det\{a_{km}\} = +1$, in the second $\det\{a_{km}\} = -1$. In the rest of this Appendix, only rotations are considered, so always $\det\{a_{km}\} = +1$.

An alternative description of a rotation of the coordinate system can be given by specifying the axis about which the rotation is to take place along with the magnitude of the rotation. Clearly, for any point on the axis of the rotation, the coordinates x_k and x'_k will be identical, so that from Eqns (A5.1) and (A5.4)

$$x_k = a_{km}x_m, \qquad x_k = a_{mk}x_m \tag{A5.4}$$

In particular, for a rotation about the original coordinate axis Ox_1, the unit vector with components (1,0,0) is invariant, leading to the special form for the matrix A with elements a_{km}

$$\begin{pmatrix} 1 & & 0 \\ 0 & a_{22} & a_{23} \\ 0 & a_{32} & a_{33} \end{pmatrix}$$

Us[illegible] ations Eqn (A5.2) and the condition on the deter-
mi[illegible] rther reduces to

$$\begin{pmatrix} 1 & & 0 \\ 0 & & -s \\ 0 & & c \end{pmatrix} \qquad \text{(A5.5)}$$

wh[illegible] $= \sin(\theta)$ for an angle θ which corresponds to the amount by which the original Ox_2 axis is rotated towards Ox_3, as illustrated in Fig. A5.1.

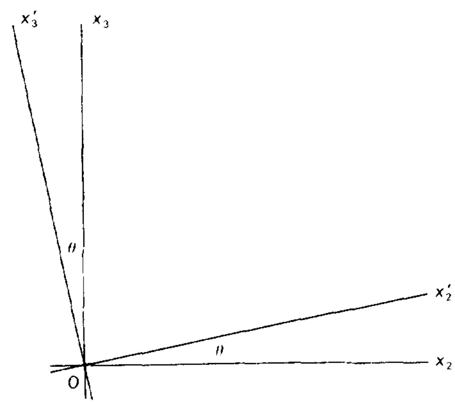

Fig. A5.1 Rotation about Ox_1.

The corresponding matrices for rotations about the other two axes are

$$\begin{pmatrix} c & 0 & -s \\ 0 & 1 & 0 \\ s & 0 & c \end{pmatrix} \qquad \text{(A5.6)}$$

for rotation about Ox_2 and

$$\begin{pmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \text{(A5.7)}$$

for rotation about Ox_3.

Rotations about some axis other than one of the coordinate axes are

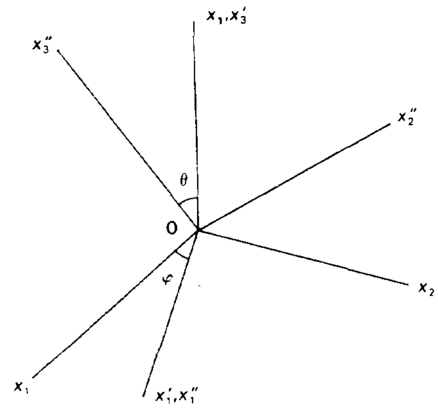

Fig. A5.2 Coordinate system for a doubly rotated plate.

usually regarded as composite transformations, built up of a succession of simple rotations. In the present context it is sufficient to consider two successive rotations, as used to describe the ***double rotated*** crystal plates. As shown in Fig. A5.2, the coordinate system Ox_k'' associated with a double rotated plate can be thought of as being obtained from the crystallographic system by a composition of, first, a rotation ϕ about the Z or Ox_3 axis to form an intermediate system Ox_k', followed by a second rotation θ about the Ox_1' axis. If x_k, x_k' and x_k'' are the coordinates of a point in the three systems, and if a'_{km} and a''_{km} are the first and second transformations, then

$$x_k = a'_{km}x'_m$$
$$x'_m = a''_{mn}x''_n$$

so that combining the two

$$x_k = a'_{km}a''_{mn}x''_n = a^*_{kn}x''_n \tag{A5.8}$$

Thus the matrix of the composite rotation, say A^*, is just the matrix product of the matrices A' and A'' of the component transformations

$$\begin{pmatrix} c_\phi & -s_\phi & 0 \\ s_\phi & c_\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_\theta & -s_\theta \\ 0 & s_\theta & c_\theta \end{pmatrix}$$

with the obvious notation $c_\phi = \cos(\phi)$ etc. Multiplying out the matrices gives A^* as

$$\begin{pmatrix} \cos(\phi) & -\sin(\phi)\cos(\theta) & \sin(\phi)\sin(\theta) \\ \sin(\phi) & \cos(\phi)\cos(\theta) & -\cos(\phi)\sin(\theta) \\ 0 & \sin(\theta) & \cos(\theta) \end{pmatrix}$$

In the plate coordinate system the plate normal has components δ_{2k} and therefore the components of the plate normal in the original system of the crystal axes are $n_k = a^*_{km}\delta_{2m} = a^*_{k2}$. Thus

$$\begin{aligned} n_1 &= -\sin(\phi)\cos(\theta) \\ n_2 &= \cos(\phi)\cos(\theta) \\ n_3 &= \sin(\theta) \end{aligned} \tag{A5.9}$$

For the rotated Y-cuts, the angle $\phi = 0$ and then n_k reduces to

$$\begin{aligned} n_1 &= 0 \\ n_2 &= \cos(\theta) \\ n_3 &= \sin(\theta) \end{aligned} \tag{A5.10}$$

A5.2 CRYSTAL SYMMETRIES

The optic or Z axis of quartz is a trigonal or threefold axis. The electric or X axis is a digonal or twofold axis. Because of the presence of the trigonal axis perpendicular to the X axis, the latter is repeated in the plane normal to Z at intervals of 120°, so consequently there are three electric axes, all equivalent. The trigonal axis is not repeated by the twofold axis, since a 180° rotation about any of the X axes transforms the trigonal axis into itself. The twofold symmetry does however ensure that the trigonal axis is not polar. The single trigonal and three digonal axes completely describe the symmetry of quartz.

The presence of these symmetry elements means that the material properties of quartz, as described by the arrays of dielectric, piezoelectric and elastic constants introduced in Appendix 4, must satisfy certain conditions. Consider, for example a rotation of the crystal through 120° about the optic axis. This is a symmetry operation and hence the material constants for the rotated material should be identical to those of the unrotated material. But a rotation of the material relative to a fixed coordinate system is exactly equivalent to an opposite rotation of the coordinate system keeping the crystal fixed, and then the consequence of symmetry is that the material constants in the rotated coordinate system should be identical to those in the original system. If the rotation of the coordinate system is represented by Eqn (A5.1), and if a particular material property is represented by a tensor with components $t_{kmp..}$, then using the tensor transformation law given in Section A2.2, symmetry requires

$$t_{kmp..} = a_{kl}a_{mn}a_{pq}..t_{lnq..} \tag{A5.11}$$

A5.3 SECOND-RANK TENSOR PROPERTIES

The dielectric constants and the thermal expansion coefficients are examples of material properties represented by second-rank tensors. The symmetry conditions for these quantities take the form

$$t_{km} = a_{kl} a_{mn} t_{ln} \tag{A5.12}$$

Suppose first that the a_{km} correspond to a 180° rotation about the X or Ox_1 axis. From Eqn (5.5) the corresponding matrix A_X is

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{A5.13}$$

Writing Eqn (A5.12) in matrix form, with T the matrix with elements t_{km} and $\tilde{A}$ denoting the transpose of A, gives

$$T = AT\tilde{A} \tag{A5.14}$$

Carrying out the multiplications leads to the matrix identity

$$\begin{pmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix} = \begin{pmatrix} t_{11} & -t_{12} & -t_{13} \\ -t_{21} & t_{22} & t_{23} \\ -t_{31} & t_{32} & t_{33} \end{pmatrix}$$

and thus T reduces to

$$\begin{pmatrix} t_{11} & 0 & 0 \\ 0 & t_{22} & t_{23} \\ 0 & t_{32} & t_{33} \end{pmatrix} \tag{A5.15}$$

If now the symmetry operation of a 120° rotation about Z or Ox_3, with matrix A given by Eqn (A5.7), is considered, Eqn (A5.14) leads to

$$T = \begin{pmatrix} t_{11}c^2 + t_{22}s^2 & (t_{11} - t_{22})cs & -st_{23} \\ (t_{11} - t_{22})cs & t_{11}s^2 + t_{22}c^2 & ct_{23} \\ -st_{32} & ct_{32} & t_{33} \end{pmatrix}$$

Since $c = \cos(120)$ and $s = \sin(120)$ are both non-zero it follows that finally T has the form

$$\begin{pmatrix} t_{11} & 0 & 0 \\ 0 & t_{11} & 0 \\ 0 & 0 & t_{33} \end{pmatrix} \tag{A5.16}$$

Hence any second-rank tensor property in a material of symmetry type 32 is, when referred to the crystallographic axes, represented by a diagonal matrix with just two independent components.

A5.4 THIRD- AND FOURTH-RANK TENSOR PROPERTIES: MATRIX NOTATION

The application of the symmetry conditions to second-rank tensors is straightforward, but the situation is complicated with higher-rank tensors because of the large number of components and the fact that matrix methods cannot be applied directly. Both difficulties can be removed by making use of the symmetries of the higher-rank tensors representing the piezoelectric and elastic properties of a material to reduce the number of indices. These symmetries were discussed in Section A4.2. Taking the elastic constants c_{klmn} as an example, the symmetry of the stress and strain tensors results in symmetry in the pairs of indices kl and mn, while the definition of the cs as second derivatives of a function of state results in symmetry between the pairs. Thus $c_{klmn} = c_{lkmn} = c_{mnkl}$. These symmetries reduce the number of independent cs from $3^4 = 81$ to 21.

The reduced notation consists in replacing pairs of indices km, with k, m running from 1 to 3, with single indices K, M . . running from 1 to 6 according to the following rules

K:	1	2	3	4	5	6
km:	11	22	33	23 or 32	31 or 13	12 or 21

The rule is applied directly to the stress t_{kl}, the elastic constants c_{klmn} and the piezoelectric constants e_{klm}, to give the reduced stresses t_K, elastic constants c_{KL} and piezoelectric constants e_{kL}. (Note only the second and third indices of the e_{klm} are reduced.) In their reduced form, the stresses can be represented by a 6×1 column matrix T, the elastic constants by a 6×6 square matrix c and the piezoelectric constants by a 3×6 rectangular matrix e.

For the strains S_{kl}, the elastic compliances s_{klmn} and the piezoelectric constants d_{klm}, the rule is modified by introducing factors of 2 when the index pair to be replaced has unequal elements. Thus for the strains, $S_K = S_{kl}$ when $k = l$ but otherwise $S_K = 2S_{kl}$. For the compliances, $s_{KM} = s_{klmn}$ when both $k = l$ and $m = n$; if only one of these conditions hold, then $s_{KM} = 2s_{klmn}$, while if neither holds $s_{KM} = 4s_{klmn}$. Finally, for the piezoelectric constants, $d_{kL} = d_{klm}$ if $l = m$, and if $l <> m$ then $d_{kL} = 2d_{klm}$. The matrices corresponding to the strain, compliances, and piezoelectric constants can then be denoted S, s and d, respectively. The factors of 2 in the above definitions are introduced in order that the matrix forms of the linear constitutive relations should be free from such factors. The tensor forms of the constitutive equations are

$$t_{kl} = c_{klmn}S_{mn} - e_{jkl}E_j$$
$$D_k = e_{klm}S_{lm} + \epsilon_{kl}E_l$$

or alternatively

$$S_{kl} = s_{klmn}t_{mn} + d_{jkl}E_j$$
$$D_k = d_{klm}t_{lm} + \epsilon_{kl}E_l$$

and in matrix form with the above definitions the corresponding equations are

$$\begin{aligned} T &= cS - \tilde{e}E \\ D &= eS + \epsilon E \end{aligned} \tag{A5.17}$$

and

$$\begin{aligned} S &= sT + \tilde{d}E \\ D &= dT + \epsilon E \end{aligned} \tag{A5.18}$$

where it should be noted that ϵ has been used to denote the matrix of dielectric constants in both 'clamped' and 'free' cases. The numerical values of the matrix elements are of course different in the two cases.

Having established the reduced notation, it remains to determine how the matrix representations of the third- and fourth-order tensor properties transform under changes of the coordinate system. Under the coordinate transformation Eqn (A5.1), the tensor stresses transform according to

$$t'_{km} = a_{jk} a_{lm} t_{jl} \tag{A5.19}$$

By writing this and the corresponding expression for the transformation of the tensor strains out in full, and replacing the tensor components by matrix components throughout, the transformations for the matrix stresses and strains can be obtained by inspection in the form

$$T' = \tilde{M}T \qquad S' = \tilde{N}S \tag{A5.20}$$

where M and N are 6×6 matrices whose elements are formed from the elements of the transformation matrix A. Their explicit representations are given in Figs. 5.3 and 5.4. The inverse transformations are obtained in the same way from the inverse of A, but since A^{-1} is just the transpose of A, the inverses of M and N can be obtained by simply reversing all pairs of indices for the elements of A in Figs. A5.3 and A5.4. It then follows by inspection that

$$\tilde{N}^{-1} = M \tag{A5.21}$$

so that Eqns (A5.20) can be replaced by

$$T' = \tilde{M}T \qquad S = MS' \tag{A5.22}$$

With the transformation laws for the electric field and displacement E and D in the matrix form

$$E = AE' \qquad D' = \tilde{A}D$$

the constitutive relations Eqn (A5.17) can then be manipulated into the form

$$\begin{aligned} T' &= (\tilde{M}cM)S' - (\tilde{M}\tilde{e}A)E' \\ D' &= (\tilde{A}eM)S' + (\tilde{A}\epsilon A)E' \end{aligned}$$

a_{11}^2	a_{12}^2	a_{13}^2	$a_{12}a_{13}$	$a_{13}a_{11}$	$a_{11}a_{12}$
a_{21}^2	a_{22}^2	a_{23}^2	$a_{22}a_{23}$	$a_{23}a_{21}$	$a_{21}a_{22}$
a_{31}^2	a_{32}^2	a_{33}^2	$a_{32}a_{33}$	$a_{33}a_{31}$	$a_{31}a_{32}$
$2a_{21}a_{31}$	$2a_{22}a_{32}$	$2a_{23}a_{33}$	$a_{22}a_{33}+a_{32}a_{23}$	$a_{23}a_{31}+a_{33}a_{21}$	$a_{21}a_{32}+a_{31}a_{22}$
$2a_{31}a_{11}$	$2a_{32}a_{12}$	$2a_{33}a_{13}$	$a_{32}a_{13}+a_{12}a_{33}$	$a_{33}a_{11}+a_{13}a_{31}$	$a_{31}a_{12}+a_{11}a_{32}$
$2a_{11}a_{21}$	$2a_{12}a_{22}$	$2a_{13}a_{23}$	$a_{12}a_{23}+a_{22}a_{13}$	$a_{13}a_{21}+a_{23}a_{11}$	$a_{11}a_{22}+a_{21}a_{12}$

Fig. A5.3 Matrix *M*.

a_{11}^2	a_{12}^2	a_{13}^2	$2a_{12}a_{13}$	$2a_{13}a_{11}$	$2a_{11}a_{12}$
a_{21}^2	a_{22}^2	a_{23}^2	$2a_{22}a_{23}$	$2a_{23}a_{21}$	$2a_{21}a_{22}$
a_{31}^2	a_{32}^2	a_{33}^2	$2a_{32}a_{33}$	$2a_{33}a_{31}$	$2a_{31}a_{32}$
$a_{21}a_{31}$	$a_{22}a_{32}$	$a_{23}a_{33}$	$a_{22}a_{33}+a_{32}a_{23}$	$a_{23}a_{31}+a_{33}a_{21}$	$a_{21}a_{32}+a_{31}a_{22}$
$a_{31}a_{11}$	$a_{32}a_{12}$	$a_{33}a_{13}$	$a_{32}a_{13}+a_{12}a_{33}$	$a_{33}a_{11}+a_{13}a_{31}$	$a_{31}a_{12}+a_{11}a_{32}$
$a_{11}a_{21}$	$a_{12}a_{22}$	$a_{13}a_{23}$	$a_{12}a_{23}+a_{22}a_{13}$	$a_{13}a_{21}+a_{23}a_{11}$	$a_{11}a_{22}+a_{21}a_{12}$

Fig. A5.4 Matrix *N*.

It then follows that the desired transformation laws are

$$c' = \tilde{M}cM \qquad e' = \tilde{A}eM \tag{A5.23}$$

Similar expressions can be derived for the compliances s and the d piezoelectric constants if desired.

When the transformation matrix A corresponds to a symmetry operation of the material, then the Eqns (A5.23) become identities that have to be satisfied by the material constants

$$c = \tilde{M}cM \qquad e = \tilde{A}eM \tag{A5.24}$$

These are exactly analogous to the identities (Eqn (A5.14)) already discussed in detail for the second-rank tensor case, differing only in being more tedious to apply. Consequently, only the results of applying the symmetry operations of quartz to the arrays of elastic and piezoelectric constants are given here. It is found that the number of independent constants reduces to two piezoelectric and six elastic constants, with the matrices having the following forms.

Piezoelectric constants

$$\begin{pmatrix} e_{11} & -e_{11} & & e_{14} & & 0 \\ 0 & & & & -e_{14} & -e_{11} \\ 0 & & & & & 0 \end{pmatrix}$$

Ela

where

$$c_{66} = (c_{11} - c_{12})/2$$

A5.5 TRANSFORMATION EQUATIONS FOR ROTATED Y-CUTS

The plate coordinate system for a rotated Y-cut (Chapter 2) is obtained from the crystallographic axes by rotation about Ox_1 through an angle θ. Hence the A matrix has the form of Eqn (A5.5). The corresponding M matrix is shown in Fig. A5.5. Using these matrices in the transformations of Eqn (A5.12) and

1	0	0	0	0	0
0	c^2	s^2	$-cs$	0	0
0	s^2	c^2	cs	0	0
0	$2cs$	$-2cs$	c^2-s^2	0	0
0	0	0	0	c	s
0	0	0	0	$-s$	c

Fig. A5.5 Matrix M for rotated Y-cuts.

(A5.23), along with the matrices for the material constants obtained by applying the symmetry identities, leads to expressions for the material constants in the plate coordinate system. Once again, the algebra is tedious but straightforward, so only the results are given.

Dielectric constants

$$\epsilon'_{11} = \epsilon_{11}$$
$$\epsilon'_{22} = c^2\epsilon_{11} + s^2\epsilon_{33}$$
$$\epsilon'_{33} = s^2\epsilon_{11} + c^2\epsilon_{33}$$
$$\epsilon'_{23} = cs(\epsilon_{33} - \epsilon_{11})$$

Piezoelectric constants

$$e'_{11} = e_{11}$$
$$e'_{12} = -c^2e_{11} + 2cse_{14}$$
$$e'_{13} = -s^2e_{11} - 2cse_{14}$$
$$e'_{14} = cse_{11} + (c^2 - s^2)e_{14}$$
$$e'_{25} = -c^2e_{14} + sce_{11}$$

$$e'_{26} = -cse_{14} - c^2e_{11}$$
$$e'_{35} = sce_{14} - s^2e_{11}$$
$$e'_{36} = s^2e_{14} + sce_{11}$$

Elastic constants

$$c'_{11} = c_{11}$$
$$c'_{22} = c^4c_{11} + s^4c_{33} + 2s^2c^2(2c_{44} + c_{13}) - 4sc^3c_{14}$$
$$c'_{33} = s^4c_{11} + c^4c_{33} + 2s^2c^2(2c_{44} + c_{13}) + 4cs^3c_{14}$$
$$c'_{44} = c_{44} + s^2c^2(c_{11} + c_{33} - 2c_{13} - 4c_{44}) + 2cs(c^2 - s^2)c_{14}$$
$$c'_{55} = c^2c_{44} - 2scc_{14} + s^2c_{66}$$
$$c'_{66} = s^2s_{44} + 2scc_{14} + c^2c_{66}$$
$$c'_{12} = c^2c_{12} + s^2c_{13} + 2csc_{14}$$
$$c'_{13} = s^2c_{12} + c^2c_{13} - 2csc_{14}$$
$$c'_{14} = (c^2 - s^2)c_{14} - cs(c_{12} - c_{13})$$
$$c'_{23} = (c^4 + s^4)c_{13} + c^2s^2(c_{11} + c_{33} - 4c_{44}) + 2cs(c^2 - s^2)c_{14}$$
$$c'_{24} = c^2(4s^2 - 1)c_{14} + sc[s^2c_{33} - c^2c_{11} + (2c_{44} + c_{13})(c^2 - s^2)]$$
$$c'_{34} = -s^2(4c^2 - 1)c_{14} + sc[c^2c_{33} - s^2c_{11} - (2c_{44} + c_{13})(c^2 - s^2)]$$
$$c'_{56} = (c^2 - s^2)c_{14} - sc(c_{66} - c_{44})$$

In all the above, $c = \cos(\theta)$ and $s = \sin(\theta)$, and all constants not explicitly listed are either determined by the symmetry of the arrays or else are zero.