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THE PIEZOELECTRIC EFFECT

INTRODUCTION

Piezoelectric crystals, particularly quartz, are used to control and manage the frequencies of the carrier signals used in electric communications. No other method of frequency control has been devised which competes with the vibrating quartz piezoid in accuracy, convenience, cost, and reliability. The quartz crystal unit provides coupling between the mechanical resonance frequency of the piezoid and the electric circuit, i.e., it is an electromechanical transducer. In doing so an extremely small amount of power is dissipated, with the result that the resonant frequency is very precisely determined. Finally, the resonant frequency is dependent on the dimensions of the piezoid and the mechanical and physical properties of quartz, which are highly stable.

THEORY OF PIEZOELECTRICITY

The coupling between the mechanical properties of the quartz and the electric circuit is through the piezoelectric effect. Although the piezoelectric effect was discovered in 1880 and the mathematical theory of the effect is completely established, little has been written about the origin of the effect. The latest books on the physics of solids seldom devote more than a paragraph to the subject and, if mentioned at all in textbooks on general physics, the treatment is usually superficial and/or confused with electrostriction.

To understand the origin of the piezoelectric effect, we first consider an electric dipole. A dipole is two charges of the same magnitude and opposite sign separated by a fixed distance. A dipole consisting of the charges $+q$ and $-q$ separated by a distance d is shown in Fig. 4.1. The dipole moment is defined as the product of the charge and the separation. The dipole moment of the dipole of Fig. 4.1 is therefore qd. The dipole moment is a vector quantity having the direction of the line joining the negative charge to the positive charge.

We will now compute the electric-field intensity at a point P at a distance r from the point midway between the charges along a line joining the two. We assume that $r \gg d$.

The electric field may be computed by application of Coulomb's law, but it is easier to compute first the electrostatic potential at point P and then to compute the field (intensity) by using $-E=\partial V/\partial r$. The potential due to a charge q at a point situated a distance r from the charge is very simply given by

$$V_p = \frac{4\pi\epsilon_0 q}{r} = \frac{kq}{r} \qquad k = 4\pi\epsilon_0$$

The potential at a point due to several charges is the algebraic sum of the contributions of the several charges.

The potential of P, Fig. 4.1, is

$$V = k\left(\frac{+q}{r-a} + \frac{-q}{r+a}\right) = kq\,\frac{2a}{r^2-a^2}$$

and if a^2 is negligible compared with r,

$$V = \frac{2kqa}{r^2}$$

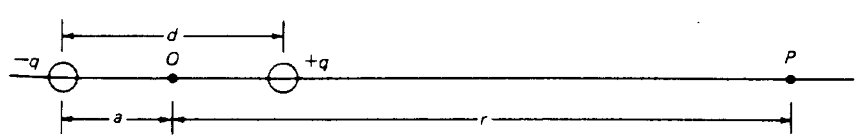

Fig. 4.1. An electric dipole.

The electric-field intensity is then

$$E = -\frac{\partial V}{\partial r} = \frac{4kqa}{r^3} = \frac{2kqd}{r^3} \tag{14}$$

Equation (14) shows that the electric-field intensity of a dipole, at a distant point along the axis of the dipole, is proportional to the dipole moment. Any change in the dipole must, therefore, cause a corresponding change in the electric field. This is the origin of the piezoelectric effect.

It is interesting and instructive to consider a slightly more complicated two-dimensional model. Suppose that six charges are located at the corners of a regular hexagon, as shown in Fig. 4.2. We take the X axis to be parallel to the line joining opposite charges and let a be the distance between the charges along this line.

We compute the potential V at a point P at a distance $OP = r$, where we assume $r \gg a$. The contribution to the potential due to charge q_1 is $kq/(r-a/2)$. The contributions from q_2 and q_3 are each given by $kq/(r+a/4)$ if $OP = r$ is so large compared with a that a line from q_2 to P can be considered practically parallel to OP.

The potential at P due to the three positive charges is therefore

$$V_+ = k\left(\frac{q}{(r-a/2)} + \frac{2q}{(r+a/4)}\right)$$

$$= +\frac{3kq}{r}$$

after neglecting a term $a^2/8$.

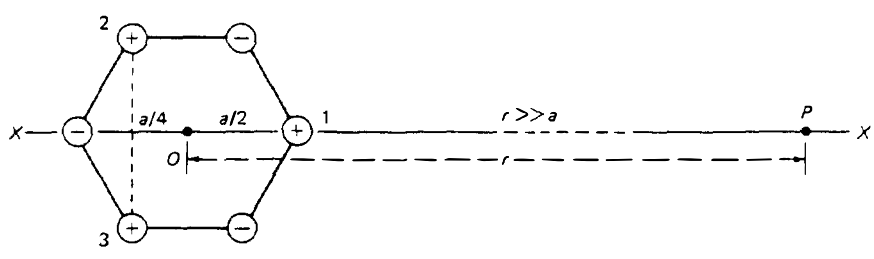

Fig. 4.2. Two-dimensional configuration of electric charges.

This is exactly the potential at P due to a charge of $+3q$ located at point O. Thus we have the important result that the potential, and the field intensity, at a distant point is the same for the three charges as for three coincident charges at the "center of gravity." Naturally the same result holds for the three negative charges, so that the potential and field at P are zero because the two contributions cancel.

Now suppose, however, that forces are applied along the Y axis causing the system of charges to be distorted, as shown in Fig. 4.3*a*. The center of gravity of the three positive charges moves to the left and that of the three negative charges moves to the right. If we assume that the strain causes the line from O to charge q_2 to be rotated counterclockwise by a small angle $d\theta$, it is easy to show that the X component of the displacement of q_2 is given by $(a/2)\cos 30^\circ\, d\theta$. The same is true of charge q_3. It is then easy to see that the center of gravity of the three positive charges has been displaced to the left by an amount $(\sqrt{3}\, a\, d\theta)/2$ and that of the three negative charges to the right by the same amount. Thus a dipole has been created having a dipole moment of

$$p = 3\sqrt{3}\, qa\, d\theta \qquad \text{coulomb meters in mks units}$$

If we imagine a crystal made up of molecules consisting of ions arranged like the charges of Fig. 4.3*a*; that the crystal contains N

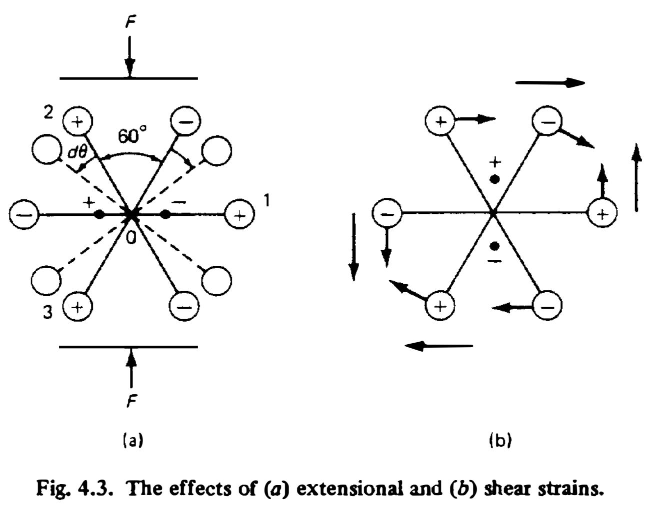

Fig. 4.3. The effects of (*a*) extensional and (*b*) shear strains.

such molecules per unit volume; and that each molecule is subjected to the same strain; then the dipole moment per unit volume is

$$P = Np = 3\sqrt{3}\ N\,qa\ d\theta$$

Although the model which we have been considering is hypothetical and certainly cannot agree in detail with a real crystal, it is of some interest to compute the piezoelectric coefficient e which it would have. The coefficient e is defined by the equation $P = e\,x$ [see Eq. (16)], where P is the polarization and x is the strain, which in this case is $d\theta$. Therefore, in our simple model,

$$e = 3\sqrt{3}\,N\,q\,a$$

If we take a to be 2.5 Å = 2.5×10^{-10} m, $N = 6 \times 10^{27}\ \mathrm{m}^{-3}$, both of which are typical values, and $q = 1.6 \times 10^{-19}$ C we obtain

$$e = 1.2\ \mathrm{C/m^2}$$

For purposes of comparison the value of e for various crystals are: quartz, $e_{11} = 0.173$, $e_{14} = 0.040$; Rochelle salt, $e_{25} = 0.15$, $e_{36} = 0.10$; tourmaline, $e_{15} = 0.25$, $e_{22} = 0.018$, $e_{31} = 0.103$, $e_{33} = 0.32$. Thus the value of e computed from even such a simple model differs by a factor of the order of 10 from the actual values for typical crystals.

The foregoing discussion is intended merely to give the reader a feel for the origin of the piezoelectric effect. It should not be expected that results derived from such a simple model should agree in detail or magnitude with real crystals.

It is possible to calculate the effect of a shear strain on the arrangement of charges shown in Fig. 4.3*b*. The pure shear, as we have seen in Fig. 3.5, is equivalent to two extensions at right angles. It can be seen from Fig. 4.3*b* that the effect of the shear strain is to cause the center of gravity of the three positive charges to move upward and that of the three negative charges to move downward, again producing a dipole. Calculation of the resulting piezoelectric coefficient is left as an exercise for the reader.

Before leaving the topic, we now show that the polarization (or dipole moment per unit volume) is equal to the piezoelectric displacement (or the surface charge per unit area). This important result can be seen in the following way. Imagine a rectangular parallelepiped of piezoelectric material. Let the surface area be A and the thickness be L. Let the sample contain n dipoles, each having a dipole moment $p = q\,d$ aligned in the direction of L.

The dipole moment per unit volume is obviously given by

$$P = \frac{nqd}{AL}$$

Now the charge per unit area on the surface A is equal to q times the number of charges which are exposed on the surface which is obviously $[n(d/L)]/A$. Therefore the charge per unit area is

$$\sigma = \frac{nqd}{AL}$$

which is the same as P.

We have been discussing the origin of the direct piezoelectric effect, i.e., the polarization resulting from a mechanical strain in a crystal. Within practical limits the polarization can be considered to be proportional to the strain and we may write

$$P = e\,x$$

where P is the polarization and x is the strain. However, as with Hooke's law in elasticity, the linear approximation is valid only for sufficiently small strain. In the design of quartz crystal units the linear approximation is adequate, although such is not necessarily the case with other materials.

THE CONVERSE PIEZOELECTRIC EFFECT

A piezoelectric crystal placed in an electric field may experience one or more kinds of mechanical strain. Again, within limits, the strain can be considered to be proportional to the applied field and we may write

$$x = d\,E$$

where x is the strain and E is the electric field. The constant d is called the *piezoelectric strain coefficient.*

The piezoelectric strains originate in the forces which charged particles experience in an electric field. Positive and negative ions tend to be pushed in opposite directions in an electric field and a dipole tends to rotate to align itself with the direction of the field. The resulting displacements give rise to the mechanical strains known as the converse piezoelectric effect.

Piezoelectric strains are usually quite small. For example, suppose that a potential difference of 100 V is applied to metallic electrodes deposited on the major surfaces of an X-cut plate of quartz having a thickness of 1.00 mm. The field is thus 1.00×10^5 V/m. The resulting strain is therefore $x = 2.27 \times 10^{-12}$ m/V $\times$ 1.00×10^5 V/m = 2.27×10^{-7}. This is the same strain which would be produced in the thickness of the plate by a temperature change of 0.016°C.

THE GENERALIZED PIEZOELECTRIC EQUATIONS

In the example just given, a field in the X direction produces an extensional strain in the X direction. The same electric field might (and often does) produce extensional strains in the Y and Z directions. Moreover, the same electric field may produce shear strains about one or more of the axes. All possible linear relations between the three components of the electric field and the six components of strain are included in the following set of equations.

$$\begin{aligned}
x_x &= d_{11}E_x + d_{21}E_y + d_{31}E_z \\
y_y &= d_{12}E_x + d_{22}E_y + d_{32}E_z \\
z_z &= d_{13}E_x + d_{23}E_y + d_{33}E_z \\
y_z &= d_{14}E_x + d_{24}E_y + d_{34}E_z \\
z_x &= d_{15}E_x + d_{25}E_y + d_{35}E_z \\
x_y &= d_{16}E_x + d_{26}E_y + d_{36}E_z
\end{aligned} \tag{15a}$$

where $x_x, \ldots, x_y$ are the extensional and shear strains and E_x, E_y, and E_z are the components of the electric field. The d_{ij} are the piezoelectric strain coefficients. Equation (15) may be written in matrix form

$$x = d\,E \tag{15b}$$

The three components of polarization may be written in terms of the six components of strain in the following way.

$$\begin{aligned} P_x &= e_{11} x_x + e_{12} y_y + e_{13} z_z + e_{14} y_z + e_{15} z_x + e_{16} x_y \\ P_y &= e_{21} x_x + e_{22} y_y + e_{23} z_z + e_{24} y_z + e_{25} z_x + e_{26} x_y \\ P_z &= e_{31} x_x + e_{32} y_y + e_{33} z_z + e_{34} y_z + e_{35} z_x + e_{36} x_y \end{aligned} \tag{16a}$$

In matrix notation,

$$P = e\,x \tag{16b}$$

Equations (15) and (16) relate the polarization and the field to the strain. It is sometimes necessary to have the equations relating the polarization and the field to the stress. We already have

$$\begin{aligned} x &= d\,E && \text{from Eq. (15}b\text{)} \\ P &= e\,x && \text{from Eq. (16}a\text{)} \\ -x &= s\,X && \text{from Eq. (12}a\text{)} \\ -X &= c\,x && \text{from Eq. (13}a\text{)} \end{aligned}$$

Eliminating x between the second and third equation gives

$$-P = es\,X \tag{17}$$

And eliminating x between the first and fourth equation gives

$$-X = cd\,E \tag{18}$$

Equations (17) and (18) are the required equations, but we can show that $es = d$ and $cd = e$, so that we can write

$$-P = d\,X \quad \text{and} \quad -X = eE$$

The proof is a little complex depending on arguments from thermodynamics. We imagine a piezoelectric crystal to be placed in an electric field and at the same time subjected to a mechanical stress. The temperature is held constant. The electric field E produces polarization P and the stress X produces a strain x. Both represent energy stored in the crystal called the internal energy U. We now imagine the field to be changed by an infinitesimal amount dE and the stress by an infinitesimal amount dX. The change in the internal energy is[1]

$$dU = P\,dE - x\,dX \tag{19}$$

$$\left(\frac{\partial U}{\partial E}\right)_X = P \qquad \text{and} \qquad \left(\frac{\partial U}{\partial X}\right)_E = -x$$

$$\frac{\partial^2 U}{\partial E \partial X} = \frac{\partial p}{\partial X} \qquad \text{and} \qquad \frac{\partial^2 U}{\partial X \partial E} = -\frac{\partial x}{\partial E}$$

If the process is reversible, i.e., if energy is conserved, then Eq. (19) is an exact differential and the order of differentiation is immaterial; therefore,

$$\frac{\partial P}{\partial X} = -\frac{\partial x}{\partial E}$$

But from Eq. (17),

$$\frac{\partial P}{\partial X} = -es$$

and from Eq. (15*b*),

$$\frac{\partial x}{\partial E} = d$$

so that we have

$$d = es$$

By writing $dU = P\,dE - X\,dx$ and using the same procedure, one can show that $e = cd$. We may now write the piezoelectric stress equations as follows.

[1] The reader who is familiar with the subject of thermodynamics will recognize the analogy between Eq. (19) and the enthalpy equation for a reversible system.

$$
\begin{aligned}
-X_x &= e_{11}E_x + e_{21}E_y + e_{31}E_z \\
-Y_y &= e_{12}E_x + e_{22}E_y + e_{32}E_z \\
-Z_z &= e_{13}E_x + e_{23}E_y + e_{33}E_z \\
-Y_z &= e_{14}E_x + e_{24}E_y + e_{34}E_z \\
-Z_x &= e_{15}E_x + e_{25}E_y + e_{35}E_z \\
-X_y &= e_{16}E_x + e_{26}E_y + e_{36}E_z
\end{aligned}
\tag{20}
$$

and

$$
\begin{aligned}
-P_x &= d_{11}X_x + d_{12}Y_y + d_{13}Z_z + d_{14}Y_z + d_{15}Z_x + d_{16}X_y \\
-P_y &= d_{21}X_x + d_{22}Y_y + d_{23}Z_z + d_{24}Y_z + d_{25}Z_x + d_{26}X_y \\
-P_z &= d_{31}X_x + d_{32}Y_y + d_{33}Z_z + d_{34}Y_z + d_{35}Z_x + d_{36}X_y
\end{aligned}
\tag{21}
$$

To summarize, we have (written in matrix notation)

$$x = dE \tag{22}$$

$$-P = dX \tag{23}$$

$$-X = eE \tag{24}$$

$$P = ex \tag{25}$$

where Eq. (22) is shorthand for

$$
\begin{pmatrix} x_x \\ y_y \\ z_z \\ y_z \\ z_x \\ x_y \end{pmatrix}
=
\begin{pmatrix}
d_{11} & d_{21} & d_{31} \\
d_{12} & d_{22} & d_{32} \\
d_{13} & d_{23} & d_{33} \\
d_{14} & d_{24} & d_{34} \\
d_{15} & d_{25} & d_{35} \\
d_{16} & d_{26} & d_{36}
\end{pmatrix}
\begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}
\tag{22a}
$$

and Eq. (23) means

$$
-\begin{pmatrix} P_x \\ P_y \\ P_z \end{pmatrix}
=
\begin{pmatrix}
d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\
d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\
d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36}
\end{pmatrix}
\begin{pmatrix} X_x \\ Y_y \\ Z_z \\ Y_z \\ Z_x \\ X_y \end{pmatrix}
\tag{23a}
$$

Note that the rows and columns are interchanged in the d matrices of Eqs. (22*a*) and (23*a*). This is necessary in order to be able to perform the required multiplications. Not being square matrices, neither the d nor e matrix has a reciprocal matrix, so it is not possible to "solve" for the variables as in the case of the square matrix.

THE PIEZOELECTRIC MATRIX FOR QUARTZ

Although the piezoelectric matrix contains 18 terms in the general case, symmetry conditions usually require many of the terms to be zero and establish relations between others. To determine the relationships between the terms in the piezoelectric strain matrix for quartz it is sufficient to perform a rotation of 120° about the Z axis followed by a rotation of 180° about the X axis.

The strain matrix is rotated by use of the appropriate matrix[2] to obtain

$$x' = \alpha_3 x$$

where α_3 is the 6×6 matrix for rotation about the Z axis.

The electric field, being a vector, is rotated by the 3×3 matrix of Eq. (10c). We then have

$$E' = c E \qquad \text{or} \qquad E = c^{-1} E'$$

Substituting in the piezoelectric strain matrix from Eq. (22) we have

$$x' = \alpha_3 x = \alpha_3 d E = \alpha_3 d c^{-1} E' = d'E' \qquad \text{where } d' = \alpha_3 d c^{-1}$$

Repeating the same process for a rotation of 180° about the X axis we have

$$\begin{aligned} x'' &= \alpha_1 x' \\ E'' &= a E' \qquad \text{and} \qquad E' = a^{-1} E'' \\ x' &= d' E' \end{aligned}$$

from which

$$x'' = \alpha_1 x' = \alpha_1 d'E' = \alpha_1 d'a^{-1} E'' = \alpha_1 \alpha_3 d c^{-1} a^{-1} E''$$

$$\text{or} \qquad x'' = d''E'' \qquad \text{where} \qquad d'' = \alpha_1 \alpha_3 d c^{-1} a^{-1}$$

[2] See Walter L. Bond, "The Mathematics of the Physical Properties of Crystals," *B.S.T.J.*, 22: 1-72 (January 1943). This article includes tables of the matrices required to perform the rotations required in work in piezoelectricity.

Now the double rotation which is compatible with the symmetry of quartz must leave the piezoelectric matrix unchanged. Therefore, each term of d'' must be equal to the corresponding term of the matrix d. This leads to 18 simultaneous equations, the solution of which requires that 13 of the d_{ij} be zero and that only 2 of the remaining coefficients be independent.

In this way the d matrix for quartz is found to be

$$d = \begin{pmatrix} d_{11} & 0 & 0 \\ -d_{11} & 0 & 0 \\ 0 & 0 & 0 \\ d_{14} & 0 & 0 \\ 0 & -d_{14} & 0 \\ 0 & -2d_{11} & 0 \end{pmatrix} \qquad (26)$$

The d matrix for quartz thus contains five nonzero terms but only two of them are independent. The five nonzero terms tell us the nature of the strains which can be produced by the three components of the electric field. The X-component of the electric field produces three types of strain; an extensional strain in the X-direction, a (negative) extensional strain in the Y-direction, and a shear strain about the X-axis, i.e., in the YZ-plane. The Y-component of the field produces a shear strain about the Y- axis and a shear strain about the Z-axis. The latter is used in the Y-cut family of piezoids which includes the AT- and BT-cuts. The former is the basis of the strain utilized in the CT- and DT-cuts. The Z-component of the field produces no piezoelectric strain.

The e matrix can be calculated from the d matrix by using the equation $e = cd$ (see page 58). Using Eqs. (13b) and (26) we have

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & 0 & c_{14} & \dfrac{c_{11}-c_{12}}{2} \end{pmatrix} \begin{pmatrix} d_{11} & 0 & 0 \\ -d_{11} & 0 & 0 \\ 0 & 0 & 0 \\ d_{14} & 0 & 0 \\ 0 & -d_{11} & 0 \\ 0 & -2d_{11} & 0 \end{pmatrix} = \begin{pmatrix} e_{11} & 0 & 0 \\ -e_{11} & 0 & 0 \\ 0 & 0 & 0 \\ e_{14} & 0 & 0 \\ 0 & -e_{14} & 0 \\ 0 & -e_{11} & 0 \end{pmatrix}$$

By carrying out the indicated operations it is seen that

$$e_{11} = (c_{11} - c_{12})d_{11} + c_{14}\, d_{14} \quad \text{and} \quad e_{14} = 2c_{14}\, d_{11} + c_{44}\, d_{14}$$

Hence, if we measure d_{11} and d_{14} and know the elastic constants c_{11}, c_{12}, c_{14}, and c_{44}, we can calculate all the terms of the e matrix.

We show in Chap. 6 that the characteristics of AT- and BT-cut resonators depend upon the value of e'_{26} which is obtained by rotating the e matrix about the X axis by the angle θ. The value is found to be

$$e'_{26} = (e_{14}\, sc - e_{11}\, c)c$$

where c = cos θ and s = sin θ.

Note: In Chaps. 6 and 7 the symbol e for the piezoelectric strain coefficient is replaced with ϵ to avoid confusion with the symbol e, which designates thickness.

Table 4.1. The Piezoelectric Coefficients of Alpha Quartz.

$d_{11} = +2.27 \times 10^{-12}$ m/V	$e_{11} = +0.173$ C/m^2
$d_{14} = -0.67$	$e_{14} = +0.040$