

Part 1

## **The crystal as a physical device**

# 1 Quartz resonators

## 1.1 NATURAL AND CULTURED QUARTZ

Quartz is a crystalline form of silicon dioxide,  $\text{SiO}_2$ . It is a hard, brittle, transparent material with a density of  $2649 \text{ kg m}^{-3}$  and a melting point of  $1750^\circ\text{C}$ . When quartz is heated to  $573^\circ\text{C}$  its crystalline form changes. The stable form above this transition or inversion temperature is known as ‘high-quartz’ or ‘beta-quartz’, the stable form below  $573^\circ$  is known as ‘low-quartz’ or ‘alpha-quartz’. For resonator applications, only alpha-quartz is of interest and unless stated otherwise the term ‘quartz’ in the sequel always refers to alpha-quartz. Quartz is insoluble in ordinary acids, but soluble in hydrofluoric acid and in hot alkalis.

Quartz is one of the commonest naturally occurring crystalline minerals, sand for example being largely made up of grains of quartz produced by the weathering of larger crystals. Despite this natural abundance, crystals of sufficient size and purity for processing into quartz resonators are very rare. The occurrence and characteristics of natural quartz are fully described by Willard in Chapter IV of Heising (1946). For all but very exceptional requirements, natural quartz has now been superseded by cultured quartz in resonator manufacture. Cultured quartz has a long history (Cady, 1964), but no significant progress was made until the shortage of raw material for the war effort in 1939–45 spurred an intensive post-war program of research on both sides of the Atlantic. Cultured quartz is now routinely grown from aqueous alkaline solutions under conditions of high pressure and temperature in massive underground steel autoclaves. The lower part of the autoclave is maintained at a temperature of about  $400^\circ\text{C}$  and contains nutrient in the form of pure silica ( $\text{SiO}_2$ ). At this temperature and at pressures of the order of a thousand atmospheres, the solubility of silica is relatively high and a saturated solution is formed. Convection currents transport the saturated solution up to the upper part of the autoclave which is maintained at a slightly lower temperature of about  $350^\circ\text{C}$ . At this lower temperature the solution is supersaturated and quartz is deposited on seed crystals suspended in the cooler region of the autoclave. Over periods of many days or weeks crystals of substantial size can be grown. Brice (1985) gives more details of the process.

## 1.2 CRYSTALLOGRAPHY AND SYMMETRY

Alpha-quartz belongs to the crystallographic class 32. It has a single axis of threefold symmetry (trigonal axis) and perpendicular to this three axes of twofold symmetry (digonal axes). The digonal axes are spaced  $120^\circ$  apart and are polar axes, that is a definite sense can be assigned to them. The presence of polar axes implies the lack of a centre of symmetry and is a necessary condition for the existence of the piezoelectric effect. The digonal axes are known as the electric axes of quartz, since in the original experiments of the Curies the electrical polarization produced by pressure was developed along a polar axis. In crystals with fully developed natural faces the two ends of each polar axis can be differentiated by the presence or absence of the *s* and *x* faces (Fig. 1.1). When pressure is applied in the direction of the electric axis a negative charge is developed at that end of the axis modified by these faces. The trigonal axis, also known as the optic axis or *c*-axis, is not polar, since the presence of digonal axes normal to it implies that the two ends of the trigonal axis are equivalent. Thus no piezoelectric polarization can be produced along the optic axis.

Alpha-quartz is an optically active material. When a beam of plane-polarized light is transmitted along the optic axis a rotation of the plane of polarization occurs, the amount of the rotation depending on the distance traversed in the material. The sense of the rotation can be used to differentiate between the two naturally occurring forms of alpha-quartz known as left quartz and right quartz. In right quartz the plane of polarization rotates clockwise when seen by an observer looking towards the source of light, and in left quartz it rotates anti-clockwise. In crystals with fully developed *s* and *x* faces their orientation with respect to the major prism faces also provides a means of differentiation between right and left quartz (Fig. 1.1).

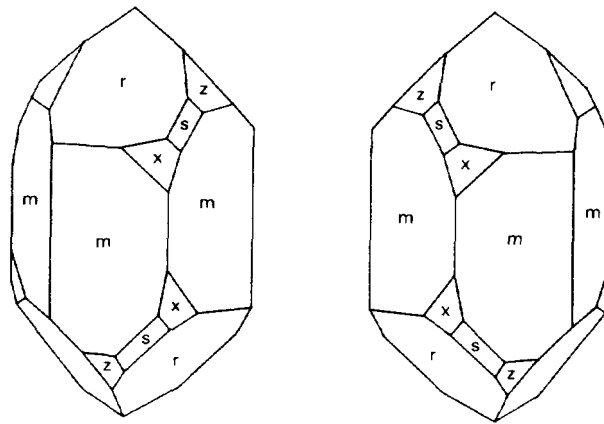


Fig. 1.1 Right and left hand quartz crystals.

The handedness of cultured quartz depends on the handedness of the seed crystals used. Most cultured quartz produced is right quartz, whereas in natural quartz left and right forms are about equally distributed. Either form can equally well be used in the manufacture of resonators, but material in which left and right forms are mixed, that is *optically twinned* material, cannot be used. *Electrically twinned* material is all of the same hand, but contains regions where the sense of the electric axis is reversed, thus reducing the overall piezoelectric effect. Such material is also not suitable for resonator application. The presence of twinning and other defects in natural quartz crystals is the major reason for the shortage of suitable natural material, and the absence of significant twinning in cultured quartz constitutes one of its main advantages.

When alpha-quartz is heated to above 573°C, the crystalline form changes to that of beta-quartz, which has hexagonal rather than trigonal symmetry. On cooling down through 573° the material reverts to alpha-quartz, but in general will be found to be electrically twinned. Similarly the application of large thermal or mechanical stresses can induce twinning, so it is necessary in resonator processing to avoid any such thermal or mechanical shocks.

The precise description of the physical properties of anisotropic materials requires the definition of a coordinate system. In the past several different conventions and standards have been used; the coordinate system used here follows the 1978 *IEEE Standard on Piezoelectricity* (IEEE, 1978). The reference system is a rectangular system of coordinates *OXYZ* in which the + *Z* direction is chosen parallel to the optic axis. The *X* direction is chosen to be parallel to an electric axis with the positive sense in right quartz being towards the end of the axis modified by the *s* and *x* faces. The *Y* direction is then chosen so as to form a right-handed coordinate system. In left quartz the sense of the *X* direction is reversed, so that the positive sense is away from the modified end of the electric axis, but still the *Y* direction is selected to keep a right-handed system. Adoption of this standard results in all the piezoelectric constants of left quartz having the opposite sign to those of right quartz.

### 1.3 MATERIAL CONSTANTS

The behaviour of quartz resonators, at least in the linear theory, is described by the field equations and boundary conditions discussed in Appendix 4. In order to be able to apply these equations a knowledge of the material constants appearing in them is required. The relevant parameters are the elastic constants  $c_{ikmp}$ , the piezoelectric constants  $e_{ikm}$ , the dielectric constants  $\epsilon_{ik}$  and the density  $\rho$ . In addition, in order to be able to understand the variation of resonator characteristics with temperature, knowledge is

required both of the thermal expansion coefficients and also of the temperature coefficients of the constants already listed.

In a completely anisotropic material, there are 21 independent elastic constants, 18 piezoelectric constants and 6 dielectric constants. Along with the density, there are therefore a total of 46 independent quantities needed to describe the relevant properties of the material at a given temperature. In the context of resonator theory, it is usual to describe the temperature dependence of a quantity  $f(T)$  by giving the temperature coefficients  $T_f^{(r)}$  of order  $r$  for  $r=1, 2$  and  $3$ . The  $T_f^{(r)}$  are defined for a given reference temperature  $T_0$  by expanding  $f(T)$  in a Taylor series about  $T_0$  and setting

$$T_f^{(r)} = f^{(r)}(T_0)/(r! f(T_0))$$

where  $f^{(r)}(T_0)$  denotes the  $r$ th derivative of  $f$  with respect to its argument  $T$ , evaluated at  $T_0$ .

Then neglecting terms higher than third order in  $(T - T_0)$ ,  $f(T)$  can be written

$$f(T) = f(T_0)\{1 + T_f^{(1)}(T - T_0) + T_f^{(2)}(T - T_0)^2 + T_f^{(3)}(T - T_0)^3\}$$

In a completely anisotropic material, the number of temperature coefficients required is therefore  $3 \times 46 = 138$ .

The thermal expansion coefficients of order  $r$  are defined in a similar way by expanding the thermally induced strain in a Taylor series and retaining up to third order terms. If  $S_{ik}$  is the strain at temperature  $T$  referred to the configuration of the material at temperature  $T_0$  then the expansion coefficients of order  $r$  are the coefficients of  $(T - T_0)^r$  in the expansion

$$S_{ik}(T) = \alpha_{ik}^{(1)}(T - T_0) + \alpha_{ik}^{(2)}(T - T_0)^2 + \alpha_{ik}^{(3)}(T - T_0)^3$$

The expansion coefficients are all symmetric second order tensors and so in the general case have six independent components. Therefore up to third order an additional 18 quantities are required, making a grand total of  $46 + 138 + 18 = 202$ . Since in fact the temperature coefficients of the density are determined by the thermal expansion coefficients, the final count of the number of independent parameters required to specify the characteristics of a completely anisotropic material in the linear approximation reduces to 199.

Fortunately the completely anisotropic material is of little practical importance, and in commonly used materials the number of independent parameters is much reduced by the presence of crystal symmetries. In the particular case of quartz, with one trigonal and three digonal axes, it can be shown by the methods illustrated in Appendix 5 that the numbers of independent parameters for second, third and fourth rank tensor properties are 2, 2 and 6, respectively. Using the matrix notation also explained in Appendix 5, the dielectric, piezoelectric and elastic constants have the following forms.

## Dielectric constants

$$\begin{pmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{11} & 0 \\ 0 & 0 & \epsilon_{33} \end{pmatrix}$$

## Piezoelectric constants

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

## Elastic constants

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & 0 & c_{14} & c_{66} \end{pmatrix}$$

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

Table 1.1 gives values for these independent parameters at a reference

**Table 1.1** Material constants of right quartz

Property	Value at 25°C	Temperature coefficients		
		First order, 10 <sup>-6</sup> /°C	Second order, 10 <sup>-9</sup> /°C <sup>2</sup>	Third order, 10 <sup>-12</sup> /°C <sup>3</sup>
Thermal expansion				
$\alpha_{11}$	—	+ 13.71	+ 6.5	- 1.9
$\alpha_{33}$	—	+ 7.48	+ 2.9	- 1.5
Density (kg/m <sup>3</sup> )				
$\rho$	2648.6	- 34.9	- 15.9	+ 5.3
Elastic constants (10 <sup>9</sup> N/m <sup>2</sup> )				
$c_{11}$	86.74	- 48.5	- 107	- 70
$c_{33}$	107.20	- 160	- 275	- 250
$c_{12}$	6.97	- 3000	- 3050	- 1260
$c_{13}$	11.90	- 550	- 1150	- 750
$c_{44}$	57.93	- 177	- 216	- 216
$c_{66}$	39.89	+ 178	+ 118	+ 21
$c_{14}$	17.91	+ 101	- 48	- 590
Piezoelectric constants (C/m <sup>2</sup> )				
$e_{11}$	0.171	- 160	—	—
$e_{14}$	0.0406	- 1440	—	—
Dielectric constants (10 <sup>-12</sup> F/m)				
$\epsilon_{11}$	39.97	—	—	—
$\epsilon_{33}$	41.03	—	—	—

temperature of 25°C along with their temperature coefficients. There is reasonable agreement in the literature on the room temperature values but considerably less in respect of the temperature coefficients, with the uncertainty increasing as the order increases. In the case of the piezoelectric constants  $e_{11}$  and  $e_{14}$  even the first order coefficients are uncertain, and no information is available on the higher order coefficients of the dielectric constants  $\epsilon_{11}$  and  $\epsilon_{33}$ . The values presented in Table 1.1 are not intended to be definitive; for more detailed information on the material constants of quartz and references to the original papers recent review articles, such as that of Brice (1985), should be consulted.

#### 1.4 MODES OF VIBRATION

Of the many different modes of vibration that may exist in a piezoelectric body, it is only those that are capable of being driven by an applied electric field that are of direct relevance in resonator applications. When the constitutive relations for a linear piezoelectric material are written in the form

$$S = sT + dE$$

$$D = dT + \epsilon E$$

where all quantities are understood to be expressed in the matrix form of Appendix 5, the first of these can be used to gain an understanding of the types of deformation that result from an applied field.

In the absence of mechanical stresses, the strain  $S$  is just  $dE$  or in terms of the matrix components,

$$S_k = d_{jk} E_j$$

where  $k = 1$  to 6 and  $j$  runs from 1 to 3, with the summation over  $j$  understood. The  $d$  matrix is subject to the same symmetry conditions and the matrix  $e$ , and so for the particular case of quartz has the form

$$\begin{pmatrix} d_{11} & -d_{11} & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14} & -2d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

where the factor 2 in the component  $d_{26}$  arises from the corresponding factor of 2 in the definitions of the matrix components of strain  $S_4$ ,  $S_5$  and  $S_6$  in Appendix 5. From the vanishing of the third row and third column of the  $d$  matrix it follows that an electric field component  $E_3$  cannot produce any mechanical strain, and also that a longitudinal strain component  $S_3$  cannot be produced by a field in any direction. (Note however that in the dynamic case where the stresses  $T$  are not zero,  $S_3$  strains will be produced by elastic coupling due to the non-zero off-diagonal elastic constants.)

For field components  $E_1$  and  $E_2$ , the possible non-zero strains are

$$\begin{aligned} S_1 &= d_{11}E_1 \\ S_2 &= -d_{11}E_1 \\ S_4 &= d_{14}E_1 \\ S_5 &= -d_{14}E_2 \\ S_6 &= -2d_{11}E_2 \end{aligned}$$

Taking these in turn illustrates the basic modes of vibration commonly used in quartz resonators. In practical cases, these simple modes generally suffer from the disadvantages of high temperature coefficients of frequency, excessive unwanted coupling to other modes, or inconvenient dimensions in particular frequency ranges, and are consequently little used. However, they form the basis for the understanding of the more sophisticated resonators that have been developed for specific purposes and which are also briefly described in the following sections. Thickness mode resonators, which are currently the most important type in frequency control applications, are discussed in more detail in the following chapter. For further details of the other resonator types, reference should be made to the standard works by Heising (1946), Mason (1950) and Vigoreux and Booth (1950). A comprehensive review, especially with regard to low frequency units, is to be found in the US Government Report, *Handbook of Piezoelectric Crystals for Radio Equipment Designers* (Buchanan, 1956).

#### 1.4.1 Thickness extensional modes in X-cut plates

The relation  $S_1 = d_{11}E_1$  shows that an electric field along the  $X$  or electric axis produces a longitudinal strain along the same axis. Therefore if a plate is cut normal to the electric axis and provided with electrodes on its major faces, as in Fig. 1.2, a voltage applied to the electrodes will produce a strain along the thickness of the plate. An alternating voltage will therefore generate longitudinal waves in the plate with both the particle displacement and the direction of propagation along  $X$ . In a first approximation, mechanical resonance will occur when the frequency is such that the thickness of the plate contains an integral number  $n$  of half wavelengths of the longitudinal or extensional wave. Under such conditions, standing waves will be set up in the plate, with the plate surfaces being antinodes of vibration. With  $n$  odd the displacements of the two major surfaces are in anti-phase, whereas with  $n$  even the displacements are in phase. Consequently, as explained in more detail in the following chapter, the even order modes cannot be excited electrically because the applied potentials on the resonator electrodes are always in anti-phase. The integer  $n$  is the *overtone order*, and so in this case, and for thickness modes in general, only the odd overtones can be excited.



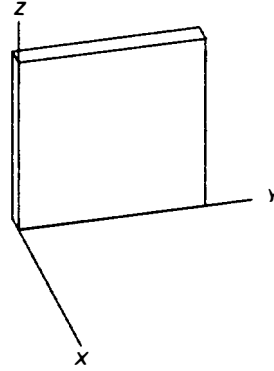


Fig. 1.2 X-cut plate.

The  $n = 1$  mode is commonly termed the *fundamental* mode. Again to a first approximation, the velocity  $V$  of the extensional waves depends only on the material constants and is independent of the frequency  $f$ . The wavelength is  $(V/f)$ , so the condition for resonance may be written

$$t = n(V/f)/2$$

or

$$f = nV/(2t)$$

where  $t$  is the thickness of the plate and  $n$  is an odd integer. Thus the resonance frequencies are inversely proportional to the thickness  $t$ . The product  $k = ft$ , known as the *frequency-thickness constant*, is  $nV/2$  and so depends only on the material constants and the overtone order. In the present case of thickness extensional modes in  $X$ -cut plates,  $k$  has a value of approximately 2870 kHz mm and the temperature coefficient of frequency is about  $-20$  ppm/ $^{\circ}\text{C}$ . A plate of thickness 1 mm therefore has a frequency of approximately 2.87 MHz.

Besides the longitudinal strain  $S_1$ , an electric field along the electric axis also produces strains  $S_2$  and  $S_4$ .  $S_2$  is a longitudinal strain along the  $Y$  axis, which lies in the plane of an  $X$ -cut plate, and  $S_4$  is a shear strain, again in the plane of the plate. Additionally, a strain  $S_3$  is produced by elastic cross-coupling. All three strain types give rise to other families of resonances in  $X$ -cut plates, but with resonance frequencies essentially determined by the lateral dimensions and not the thickness. So long as the length and width of rectangular plates, and the diameter of circular plates, are kept much larger than the thickness, the fundamental thickness mode frequency will be much higher than the fundamental frequencies of these lateral modes, and will be essentially determined by the simple formula above. However, coupling between the thickness mode and higher order overtones of the lateral modes

cannot be avoided, and this together with the large temperature coefficient effectively rules out the  $X$ -cut resonator from frequency-control applications. The  $X$ -cut nevertheless remains useful as an ultrasonic transducer.

#### 1.4.2 Length extensional modes in $X$ -cut bars

Even in the absence of the factors mentioned in the previous section which limit the use of  $X$ -cut thickness mode resonators, at frequencies below the megahertz region the plate dimensions would become too unwieldy for practical use. For such frequencies it becomes necessary to make use of those modes where the frequency is determined by dimensions other than the thickness. If instead of the plate in Fig. 1.2, the crystal blank is cut in the form of a bar with the length along the  $Y$  axis, as in Fig. 1.3, and width along  $Z$ , thickness along  $X$  as before, then a field  $E_1$  applied via electrodes on the  $YZ$  faces can excite the bar into longitudinal vibration along  $Y$  via the relation  $S_2 = -d_{11}E_1$ . In an analogous way to the thickness mode case, an alternating field can be thought of as generating longitudinal waves propagating along  $Y$  with a velocity  $V$  essentially determined by the material constants and independent of the dimensions. Resonance occurs when an integral number of half wavelengths is included in the length  $l$  of the rod, so that if  $f$  is the frequency

$$f = nV/2l$$

For the  $X$ -cut bar, the frequency constant  $k = fl$  is approximately 2730 kHz mm, so that for a length of 25 mm, the fundamental frequency is roughly 109 kHz. The frequency-temperature characteristic is parabolic in nature with a zero coefficient around room temperature but a total shift of around 100 ppm in a temperature range  $-20$  to  $+70^\circ\text{C}$ .

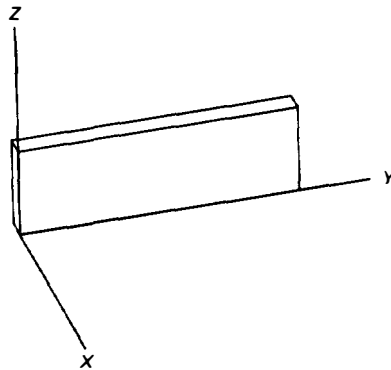


Fig. 1.3  $X$ -cut bar.

Just as in the case of the  $X$ -cut plate, the additional strains  $S_1$  and  $S_4$  will also be excited. The  $S_1$  strain, corresponding to the thickness mode, will have a fundamental mode frequency much higher than the length mode provided the thickness of the bar is sufficiently small, and outside the frequency range of interest. The  $S_4$  strain, which is not only piezoelectrically driven but also coupled to the  $S_2$  strain via the elastic compliance  $s_{24}$ , can, however, generate interfering modes of both face shear and flexural type. Interfering modes can also be generated in the width or  $Z$  direction through elastic cross coupling to the strain  $S_3$ , even though this strain is not piezoelectrically excited. Hence the width-to-length ratio for  $X$ -cut bars needs to be carefully chosen to avoid unwanted couplings in the desired frequency range.

### 1.4.3 Face shear modes in $X$ -cut and $Y$ -cut plates

The strain-field relations  $S_4 = d_{14}E_1$  and  $S_5 = -d_{14}E_2$  indicate that a shear in the plane of the plate is produced by a field along the thickness in both  $X$ -cut and  $Y$ -cut crystals. These shears are called *face shears* to distinguish them from *thickness shears* in which the deformation occurs in a plane containing the thickness of the crystal, as illustrated in Fig. 1.4. A static face shear would deform an initially square plate into a rhombus; however, the Figure shows in schematic form the deformation expected in the dynamic case when the driving field is an alternating one. In contrast to the previously considered cases of extensional modes along either the length or thickness of a plate, and to the case of thickness shear modes to be considered next, there is no comparable simple explanation of face shear modes in terms of one-dimensional standing wave systems. This is due to their essentially two-dimensional nature. For rectangular plates of length  $l$  and width  $w$ , the face shear resonance frequencies depend upon both  $l$  and  $w$ , and the overtone frequencies are not harmonically related. Because of the strong coupling that exists to other modes and their unfavourable temperature coefficients, face

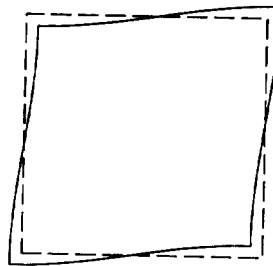


Fig. 1.4 Face shear deformation of a square plate.

shear modes in  $X$ - and  $Y$ -cut plates are not used in practice; however, in oblique cuts, ie, plates cut at an angle to the crystallographic axes, the face shear mode is very important.

#### 1.4.4 Thickness shear modes in $Y$ -cut plates

The strain-field relation  $S_6 = -2d_{11}E_2$  shows that a shear strain in the  $XY$  plane is developed by a field along  $Y$ . Since the strain involves the thickness direction, it is termed a *thickness shear* as opposed to the face shears considered in the previous section. As shown in the following chapter, the principal displacement in the thickness shear deformation of a  $Y$ -cut plate is in the  $X$  direction and therefore perpendicular to the thickness (Fig. 1.5). An alternating field can thus be thought of as generating transverse waves propagating along the thickness with a velocity  $V$  dependent in a first approximation only on the material constants, and just as in the case of thickness extensional modes in  $X$ -cut plates, resonance will occur when the thickness contains an integral number of half wavelengths. The resonance frequencies will again be given by the expression

$$f = nV/2t$$

and a frequency-thickness constant  $k = ft = nV/2$  can be defined. Once again, only odd order overtones can be electrically excited.

For the  $Y$ -cut resonator,  $k$  is approximately 1950 kHz mm and the temperature coefficient of frequency is about +75 ppm/°C. Not only is the temperature coefficient rather large, but the actual frequency-temperature

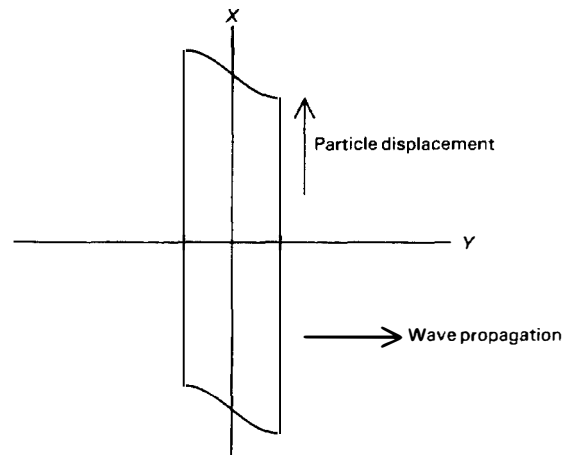


Fig. 1.5 Thickness shear deformation in  $Y$ -cut plate.

characteristic is subject to large discontinuities as a result of the very strong coupling to overtones of the face shear and other interfering modes. Consequently the *Y*-cut is no longer used in frequency control applications, although it still finds application as an ultrasonic transducer for the generation of shear waves.

#### 1.4.5 Flexural modes

The modes of vibration discussed so far all have direct links with the matrix strain-field relationship  $S = dE$  insofar as the principal strain involved is one of those excited by a field component along a crystallographic axis. Flexural modes need a rather more complex electrode arrangement for their piezoelectric excitation, but in themselves represent probably the most obvious and widespread vibration type. Everyday examples are provided by tuning forks, xylophones, and all types of wind instruments dependent on vibrating reeds. The major advantage of flexural modes in the context of frequency control is that in the low frequency range, say below about 50 kHz, other types of resonator become unmanageably large, whereas the flexural type can be kept compact. This is illustrated admirably by the modern application in electronic watches of miniature crystals at 32.768 kHz utilizing flexural modes in a tuning fork structure (cf. the paper by Walls in Gerber and Ballato, 1985, 2, p. 276, for a brief review and references).

Length extensional vibrations in an *X*-cut bar with its length along the *Y* axis have already been considered in Section 1.4.2. Such a bar can be excited in a flexural mode by reversing the field direction over half the width of the bar, so that the upper half contracts while the lower half expands and vice versa (Fig. 1.6). The fundamental mode of such a resonator has two nodal points, as shown in Fig. 1.7, with the middle and both ends of the bar being anti-nodes. This is termed a *free-free* mode in contrast to a *clamped-free* mode where one end of the bar is clamped and thus constrained to be a node, as in a tuning fork. A further type of flexural resonator, of importance in the lowest frequency ranges, is the *bimorph* or *duplex* resonator. This consists of

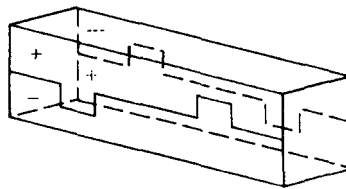
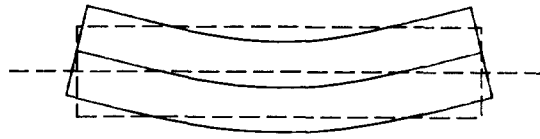


Fig. 1.6 Excitation of flexural modes in a bar.



**Fig. 1.7** Flexural deformation of a bar.

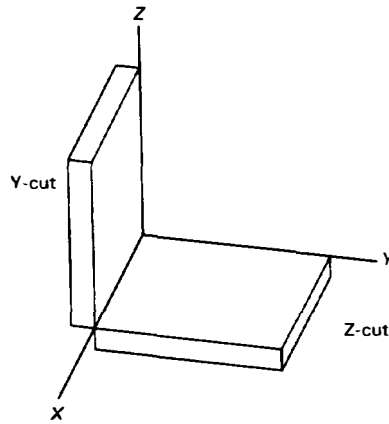
two length extensional bars of opposite hand cemented together such that one bar expands while the other contracts. The frequency range covered is from a few hundred Hz up to about 10 kHz.

For all types of flexural mode resonator, the resonance frequencies are in general complicated functions of the dimensions. In particular, it is not possible except in special limiting cases to define a useful frequency constant, and the overtone mode frequencies are not harmonically related to the fundamental.

#### **1.4.6 Coupled mode resonators: the GT-cut**

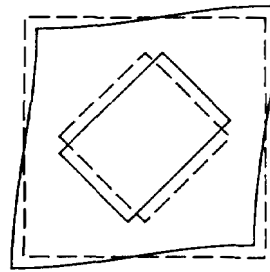
The crystal resonators so far described have all been in the form of bars or plates cut along or normal to the crystallographic axes. They suffer either from large temperature coefficients of frequency, or severe unwanted coupling to other modes of vibration, or both. As such, although offering significant advances in frequency stability as compared to previous techniques, the performance of early crystal units utilizing these cuts still fell short of the requirements of radio communications systems. Noting that the temperature coefficients of the simple cuts had both positive and negative values, early workers in the field were led to investigate two avenues of approach. In the first, the objective was to produce a resonator that by virtue of coupling between two modes of motion with different temperature coefficients, would have a zero resultant temperature coefficient. In the second, the objective was to find orientations such that plates cut accordingly would have a zero temperature coefficient for a simple uncoupled mode of vibration.

The culmination of the work in the first direction was the invention by Mason (1940) of the GT-cut resonator. This rests on the facts that (a) plate orientations can be found such that the face shear mode of vibration has a positive temperature coefficient; that (b) a face shear motion can be resolved into two extensional motions at right angles; and that (c) it can be shown that all pure extensional modes have negative or zero temperature coefficients. It follows that the positive temperature coefficient of the face shear mode must be due to the coupling between the two component extensional modes, and Mason recognized that by reducing this coupling the coefficient of the original mode must eventually pass through zero.

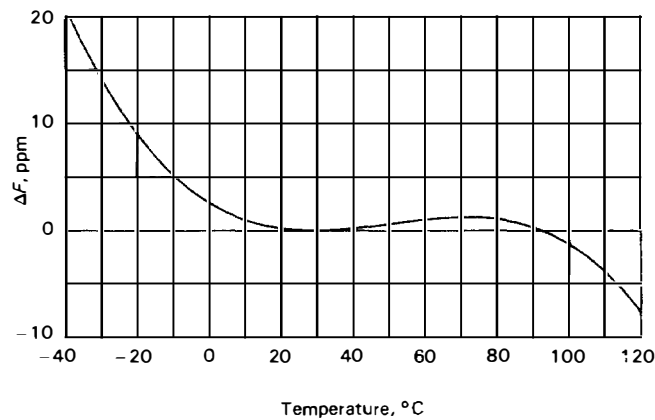


**Fig. 1.8** Y-cut and Z-cut plates.

The procedure by which the coupling is controlled can be explained as follows. Consider first a square Y-cut plate, that is a plate cut normal to the  $Y$  axis with its length and width along the  $X$  and  $Z$  axes. As described in Section 1.4.3, such a plate may be driven in a face shear mode by a field along  $Y$  through the  $d_{14}$  piezoelectric constant. The temperature coefficient of the face shear mode is negative, but it turns out that as the plate is rotated about the  $X$  axis towards the limiting case of a Z-cut plate (Fig. 1.8), the temperature coefficient increases through zero to a positive value. (At the same time the degree of piezoelectric excitation decreases to zero, as the component of the applied field along the crystallographic  $Y$  axis decreases and that along the non-piezoelectric  $Z$  axis increases.) Suppose that an orientation is selected such that the face shear mode has a positive temperature coefficient, but that the plate is cut with its length at  $45^\circ$  to the  $X$  axis. Then the face shear character of the piezoelectrically driven motion will disappear and be replaced by a pair of coupled extensional vibrations along the length and width of the rotated plate (Fig. 1.9). These vibrations will be close in



**Fig. 1.9** Face shear and coupled extensional modes.



**Fig. 1.10** GT-cut frequency-temperature characteristic.

frequency to that of the face shear mode and at least one will have a positive temperature coefficient. If now either the length or the width of the plate is altered, the coupling between the extensional modes will be reduced as the separation between the uncoupled mode frequencies is increased. As the coupling is further and further reduced by altering the width-to-length ratio of the plate, then the temperature coefficients of the two modes must both approach those of the pure extensional modes, which are negative. Hence at one particular value of the width-to-length ratio, the temperature coefficient of one of the coupled modes must vanish. As it turns out, by judicious choice of the angle of rotation about the  $X$  axis and also of the dimensional ratio, both first and second order temperature coefficients of frequency can be made to vanish at room temperature, resulting in a frequency-temperature characteristic extremely flat over a range of 100 $^{\circ}\text{C}$  or more (Fig. 1.10).

The GT-cut resonator was originally conceived by Mason as one of a family of similar cuts varying in rotation angle about  $X$  and width-to-length ratio. The optimum values given by Mason for the temperature range  $-25^{\circ}\text{C}$  to  $+75^{\circ}\text{C}$  are a rotation angle of  $-51^{\circ} 7.5'$  and a width-to-length ratio of 0.859. In this case the zero temperature coefficient mode is the width extensional one, with a frequency constant of 3370 kHz mm, so that the frequency can be adjusted by modifying the width while small corrections to the temperature coefficient can be independently made by adjusting the length. The subsidiary length extensional mode has a frequency some 15% lower than the main width mode.

Despite its excellent frequency stability, early application of the GT-cut was mainly limited to frequency standards in the frequency range 100 to 500 kHz, primarily because of manufacturing difficulty. To achieve maximum performance requires extreme care and precision in the orientation and dimensioning of the crystal blank, accompanied by equal care in



mounting. Compared to the relative ease of manufacture of AT-cut plates, the high manufacturing costs of the GT could only be justified in rare cases. In the last few years, however, this situation has been changed by the application of photolithographic manufacturing techniques and computer-aided design to the production of miniature GT resonators in the frequency range 1 to 3 MHz. An interesting feature of these units is the fabrication of both resonator and support structure out of a single quartz blank (Kawashima *et al.*, 1980).

#### 1.4.7 Rotated crystal cuts

The second avenue of approach to the objective of improved frequency stability was, as mentioned in the previous section, to search for orientations such that crystals cut accordingly had favourable characteristics in respect of either freedom from unwanted coupled modes, or frequency-temperature coefficient or both. The pioneering research in this area was mainly done by a team of workers at the Bell Telephone Laboratories, and is fully described in the books by Heising (1946) and Mason (1950).

The basic theory and results for thickness mode resonators in arbitrarily oriented plates are considered in Chapter 2, and it is shown there that the first-order temperature coefficient of frequency of such resonators is given by

$$T_f = \frac{1}{2}T_c - \frac{1}{2}T_\rho - T_t$$

where  $T_c$ ,  $T_\rho$  and  $T_t$  are, respectively, the temperature coefficients of the effective elastic constant, the density and the thickness. Both  $T_\rho$  and  $T_t$  are determined by the thermal expansion coefficients, and it can easily be shown (Chapter 2) that their combined contribution to  $T_f$  is always small and positive, ranging from a minimum of about 4 ppm/°C to a maximum of 10 ppm/°C. As the first-order coefficients of the elastic constants listed in Table 1.1 are typically an order of magnitude greater than this, it is clear that  $T_f$  is primarily determined by  $T_c$ .

The *rotated Y-cut* family of plates can be thought of as obtained from a Y-cut plate by rotation about the crystallographic  $X$  axis, which lies in the plane of the plate. For all plates in this family, it can be shown (Chapter 2) that the only one of the three possible thickness modes that can be piezoelectrically excited is a thickness shear mode with the particle displacement along the  $X$  axis, with the effective elastic constant  $c_{66}'$ . The prime indicates that the indices refer to a plate coordinate system with  $X$  axis coincident with the crystal  $X$  axis,  $Y$  axis along the thickness of the plate and the  $Z$  axis chosen to form a right-handed system. As shown in Appendix 5,  $c_{66}'$  is then given in terms of the rotation angle  $\theta$  by

$$c_{66}' = s^2 c_{44} + 2sc_{14} + c^2 c_{66}$$

where  $s = \sin(\theta)$  and  $c = \cos(\theta)$ . Hence as  $\theta$  varies between 0 and  $90^\circ$   $c_{66}'$  varies from  $c_{44}$  to  $c_{66}$ . But Table 1.1 shows that the temperature coefficients of  $c_{44}$  and  $c_{66}$  are roughly equal in magnitude but opposite in sign, so that the temperature coefficient of  $c_{66}'$  must vary continuously from large negative values to large positive values. Therefore there must be at least one angle  $\theta$  for which  $T_c$  just compensates for the contributions of  $T_p$  and  $T_t$  to give a zero  $T_f$ .

In fact there are two such angles when positive and negative rotations are considered, corresponding to the AT- and BT-cuts first reported by Lack, Willard and Fair (Lack *et al.*, 1934). The corresponding angles are approximately  $-35.25^\circ$  and  $+49.20^\circ$  for AT and BT, respectively, the precise angles being varied in manufacture to suit the requirements of particular specifications. The actual frequency-temperature characteristics of the AT and BT are, respectively, found to be cubic and parabolic in nature, with the AT-cut having the distinct advantage that both first *and* second order temperature coefficients can be made to vanish around room temperature, thus giving a flatter frequency-temperature curve over a wider range of temperature than the BT.

As remarked in Section 1.4.4, one of the problems with the simple Y-cut thickness shear resonator is the strong coupling with overtones of the face shear mode involving an  $S_y$  strain. Not only is the face shear mode directly driven through the  $d_{14}$  piezoelectric constant, it is also coupled to the thickness shear motion through the  $c_{56}$  elastic constant. This coupling is also present in the rotated Y-cuts. Again referring to Appendix 5, in the plate coordinate system the constant  $c_{56}'$  is determined in terms of the rotation angle by

$$c_{56}' = c_{14}(c^2 - s^2) - (c_{66} - c_{44})sc$$

This is easily shown to vanish when

$$\tan(2\theta) = 2c_{14}/(c_{66} - c_{44})$$

that is, for rotation angles of  $-31.6^\circ$  and  $+58.4^\circ$ . Hence at these angles, known respectively as the AC- and BC-cuts and also introduced by Lack, Willard and Fair, the mechanical coupling to the face-shear mode vanishes. As the AC and BC angles are quite close to the AT and BT, it also turns out that the latter cuts are also relatively free from this coupling. However they do remain prone to coupling to flexural modes.

The AC, BC, AT and BT are the most important thickness mode resonators in the rotated Y-cut family, but are not suitable for low frequency applications, say below 1 MHz. In the frequency region down to about 200 kHz, the face shear resonators designated the CT- and DT-cuts and introduced by Hight and Willard (1937) are commonly used. These are closely related to the AT- and BT-cuts as shown in Fig. 1.11 for the AT and DT case. It is clear from the figure that the face shear motion in the DT plate involves the same strain component  $S_6'$  as does the thickness shear motion in

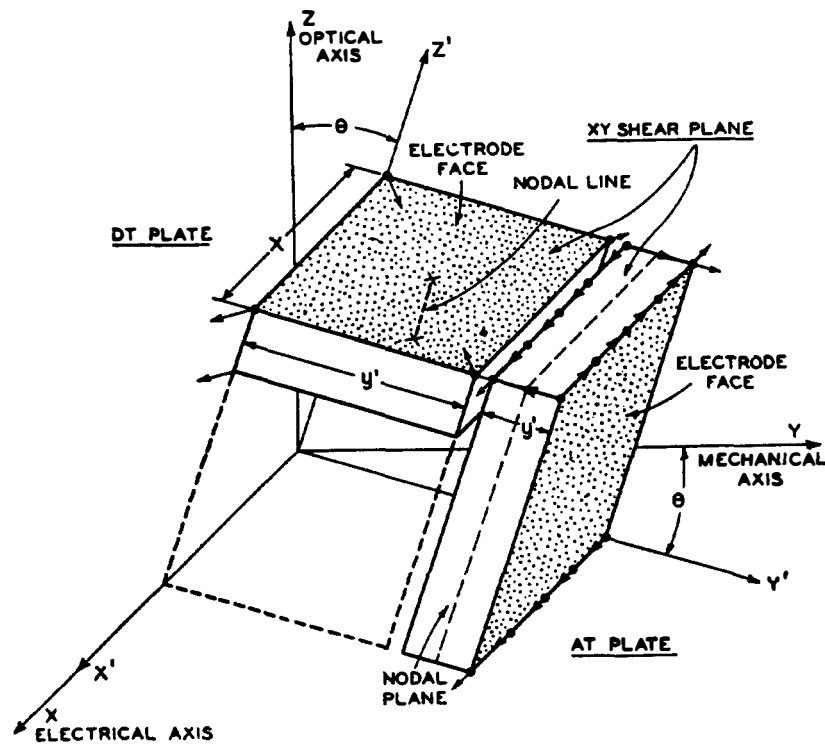


Fig. 1.11 Relation of AT and DT crystal cuts. (Reproduced, with permission, from R.A. Heising, *Quartz Crystals for Electronic Circuits*, Electronic Industries Association, 1978.)

the AT plate, and should therefore be governed by the same elastic constant,  $c_{66}'$ . Since this has a near zero temperature coefficient, it is also to be expected that the face shear mode will have a near zero frequency-temperature coefficient. Willard and Hight found in practice that this was achieved with a difference in angle of  $87^\circ$  rather than the  $90^\circ$  of the figure, corresponding to a rotation angle for the DT-cut of  $+52^\circ$ . The CT is similarly related to the BT, and has a rotation angle of  $-38^\circ$ .

The manufacture of crystal blanks in the rotated Y-cut family is relatively straightforward. In the initial cutting or sawing operations and in the subsequent lapping and polishing processes, precise control is necessary of the angle by which the plate is rotated about the X axis. Tolerances on this angle of the order of a minute of arc are common, but on the other hand the tolerances on the incidental rotations that may also occur about the Y and Z axes are much wider, with errors of the order of a degree being quite tolerable.

Such a situation no longer exists when the performance requirements imposed on the crystal are such as to demand more complicated cuts. The

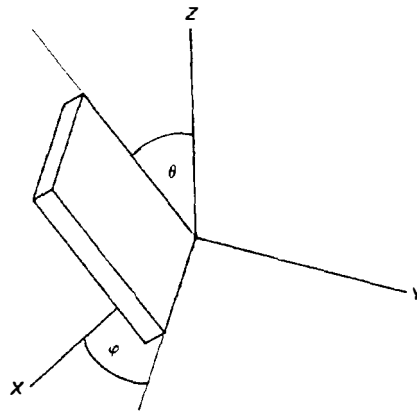


Fig. 1.12 Doubly rotated crystal plate.

AT-cut, for example, although the most widely used thickness mode resonator, has certain disadvantages in relation to its performance when mechanically and thermally stressed. These can be overcome by introducing the extra degree of freedom allowed by the use of *doubly rotated* cuts. As illustrated in Fig. 1.12, a doubly rotated cut can be thought of as being obtained from a Y-cut plate by an initial rotation about the Z axis through an angle  $\phi$ , followed by a second rotation about the  $X'$  axis through an angle  $\theta$ , so that the angles  $\phi, \theta$  specify the orientation of the blank. In the special case of the rotated Y-cuts, the first rotation  $\phi$  is zero.

The benefit of allowing  $\phi$  to vary over its permissible range is that a whole family of crystal cuts having a zero frequency-temperature coefficient at or around room temperature is obtained. In fact two distinct families of zero coefficient crystals are generated, one containing the AT as a special case, the other containing the BT. Particularly extensive investigations of the properties of the family containing the AT-cut have been carried out, culminating in the introduction of the *stress-compensated*, or SC-cut, with  $\phi \sim 22^\circ$  and  $\theta \sim -34.3^\circ$  (EerNisse, 1975).

The specific advantages of the SC are that for a plate so oriented, the resonance frequencies of the plate are largely independent of mechanical stresses in the plane of the plate. Such stresses can arise from external forces, from the mounting of the crystal, from stresses in the electrode films, and also from thermal gradients set up in the crystal when subject to varying ambient temperatures. Frequency shifts due to these causes are relatively large in AT-cut resonators and limit the frequency stability available. Consequently, the SC-cut is currently preferred for those applications where the highest stability is required.

As already intimated, the advantages of the doubly rotated cuts are accompanied by significant disadvantages. Firstly, the manufacturing difficulties

**Table 1.2** Rotated X-cuts

Cut	Mode of vibration	Frequency range, kHz
X	Thickness extensional	350 to 20 000
X	Length extensional	40 to 350
+5°X	Length extensional	50 to 500
+5°X	Length-width flexure	10 to 100
+5°X	Duplex	0.4 to 10
MT	Length extensional	50 to 500
NT	Length-width flexure	4 to 100
-18°X	Length extensional	60 to 300

are considerably complicated by the need to maintain close tolerances on both rotation angles. Secondly, whereas in the rotated *Y*-cut case only a single thickness mode is excited, in the general doubly rotated cases all three modes can be excited. For the SC, the second thickness-shear mode is nearly equal in strength to the desired mode, and only some 10% above it in frequency. This makes it necessary to either use additional circuitry to suppress the unwanted mode, or else to use special manufacturing techniques to reduce its relative strength. The advantages and disadvantages of doubly rotated cuts are considered in detail by Ballato (1977).

To complete the discussion on rotated crystal cuts, brief mention must be made of the crystals in the *rotated X-cut* family that are used for low frequency applications. Table 1.2 lists the commonly used cuts, giving their usual designations, the mode of vibration and the frequency range in which they operate. As for the thickness mode resonators already discussed, the motivation for introducing these rotated cuts is to improve the frequency-temperature characteristics or to reduce interference from unwanted coupled modes, or both. For a full discussion, reference should be made to Heising (1946) or Buchanan (1956).