8
THE FREQUENCY CONSTANTS AND TEMPERATURE COEFFICIENTS OF FREQUENCY

INTRODUCTION

In this chapter we show how the frequency constant of a given piezoid is determined by the density, the dimensions and the elastic constants. Then we show how the temperature coefficient of the resonant frequency is determined by the temperature dependence of the same factors.

THE FREQUENCY CONSTANTS

We have seen [Eqs. (39), (40), and (43)] that the fundamental and the harmonic resonant frequencies of an infinite plate, i.e., one in which the length and width, or diameter, are very large compared with the thickness, is given approximately by

$$f_n = \frac{nv}{2e} \quad n = 1, 3, 5, \ldots$$

where v is the velocity with which the longitudinal or shear wave is propagated in the plate and e is the thickness. These are the "harmonic" frequencies utilized in high-frequency quartz crystal units.

The velocity of propagation of a wave in the thickness direction of a thin plate is given by

$$v = \sqrt{\frac{c_{ij}}{\rho}}$$

where c_{ij} is the ratio of the stress to the strain associated with the elastic wave which is being propagated in the quartz and ρ is the density of quartz.

In the case of an X-cut piezoid in which the wave is a longitudinal wave in the thickness direction, the appropriate elastic modulus is c_{11}. For a Y-cut plate, in which the wave is transverse, the stress and strain are related by the modulus c_{66}. If the plate is cut in such a way that the thickness is not parallel to either the X- or Y-axis, as in the AT- and BT-cut plates, the applicable modulus becomes a function of two or more of the elastic moduli and of the angles between the crystallographic axes and the direction of propagation of the wave. The value of the applicable elastic modulus is then determined by the use of matrix algebra, as outlined in Chap. 2.

The resonant frequency of an infinite plate vibrating in a thickness mode is therefore

$$f_n = \frac{n}{2e}\sqrt{\frac{c_{ij}}{\rho}} \qquad n = 1, 3, 5, \ldots \tag{85a}$$

Since all the quantities on the right-hand side of Eq. (85) are constant except e, we may write

$$f_n = n\left(\frac{K}{e}\right) \tag{85b}$$

where $K = \frac{1}{2}\sqrt{c_{ij}/\rho} = \frac{1}{2}\,v$ is called the *frequency constant*. K has the dimensions of velocity but is usually expressed in kilohertz-inches or kilohertz-millimeters.

The values of K are the same if expressed in megahertz-mils (a mil is 0.001 in) or in megahertz-microns (a micron is 0.001 mm). Thus the frequency of a given plate is found by dividing the thickness into the frequency constant. For example, an AT-cut plate having a thickness of 10.0 mils has a frequency of 65.5/10.0 = 6.55 MHz.

Table 8.1 Frequency Constants of a Few Quartz Piezoids.

	K, kHz·in	K, kHz·mm
X-cut	112.1	2849
Y-cut	76.9	1954
AT-cut	65.5	1664
BT-cut	100.3	2549
SC-cut	70.9	1800

The frequencies of the harmonic modes ($n = 1, 3, 5, \ldots$) are not precisely integral multiples of each other in actual resonators. This is due to the differences between the vibrating areas and the plated areas in the different modes. The harmonic frequency f_n may be either slightly larger or smaller than nf_1.

LINEAR COEFFICIENTS

Many physical quantities are approximately linear functions of other physical quantities. Ohm's law, Hooke's law, and the gas law are examples in which a linear approximation is sufficiently accurate for many purposes. When greater accuracy is required the relationship may be expressed as a power series with sufficient terms to provide the required accuracy.

The temperature dependence of the thermal expansion of a solid can be expressed by the equation

$$L = L_0 \left[1 + \alpha (T - T_0) + \beta (T - T_0)^2 + \cdots \right]$$

where L_0 is the length at temperature T_0 and L is the length at temperature T. For many purposes we may keep only the first term and write

$$L = L_0 \left[1 + \alpha (T - T_0)\right]$$

or

$$L - L_0 = L_0 \alpha (T - T_0)$$

from which

$$\alpha = \frac{1}{L_0} \frac{L - L_0}{T - T_0} = \frac{1}{L_0} \frac{\Delta L}{\Delta T}$$

The constant α is called the *temperature coefficient of linear expansion.*

THE TEMPERATURE COEFFICIENT OF FREQUENCY

Since the frequency of a resonator depends on its thickness, density, and the elastic constant and each of these changes with the temperature, it follows that the frequency is also temperature-dependent. To a first approximation we may treat each of the temperature dependences as linear and then compute the linear temperature coefficient of the frequency. To do so we write Eq. (85a) in logarithmic form in the following way.

$$\log f_n = \log\left(\frac{n}{2}\right) - \log e + \tfrac{1}{2}\log c_{ij} - \tfrac{1}{2}\log \rho$$

We then differentiate the resulting equation with respect to the temperature to obtain

$$T_f = \frac{1}{f}\frac{df}{dT} = -\frac{1}{e}\frac{de}{dT} + \frac{1}{2}\;\frac{1}{c_{ij}}\frac{c_{ij}}{dT} - \frac{1}{2}\;\frac{1}{\rho}\frac{d\rho}{dT} \qquad (86)$$

The quantity on the left is called the *temperature coefficient* (actually it is the linear temperature coefficient of the frequency) and it is usually expressed in parts per million (ppm) per degree Celsius, or in percent change in frequency per degree Celsius.

Equation (86) indicates that T_f is independent of the harmonic order n, which is true to a first approximation. However, since actual plates are far from infinite, the value of T_f is slightly dependent on n, so plates of a given size are cut at slightly different angles for operation on different harmonic modes.

Since quartz expands when heated, it is easily seen that $d\rho/dT$, the change of density with temperature, is a negative quantity, while the change in thickness with temperature de/dT is a positive quantity and thus from Eq. (86) their effects on T_f are opposite in effect. While the effects do not cancel, it does suggest that the value of T_f might be made zero by balancing out the effects of temperature on these and the elastic modulus. It is fortunate that this is possible in quartz. The usefulness of several otherwise useful crystals is limited by the impossibility of finding any orientation at which the temperature coefficient is zero.

The temperature coefficients of linear expansion in the directions perpendicular and parallel to the Z-axis are called α_1 and α_3, respectively. We have already shown in Chap. 2 that the coefficient of linear expansion is a direction making an angle θ with the Y-axis is given by

$$\alpha' = T_e = \alpha_1 \cos^2\theta + \alpha_3 \sin^2\theta \tag{87}$$

where $\alpha_1 = 14.3 \times 10^{-6}$ and $\alpha_3 = 7.8 \times 10^{-6}/°C$.

With these two values and Eq. (87) the value of the T_e can be calculated for any direction in quartz.

The value of T_ρ can also be calculated. Consider a small cube of quartz having dimensions x, y, and z in the X-, Y-, and Z-directions, respectively. Let m be the mass of the cube. The density is thus

$$\rho = \frac{m}{xyz}$$

The temperature coefficient of the density T_ρ is found as before by taking the logarithmic derivative to obtain

$$\frac{1}{\rho}\frac{d\rho}{dT} = T_\rho = \frac{1}{m}\frac{dm}{dT} - \frac{1}{x}\frac{dx}{dT} - \frac{1}{y}\frac{dy}{dT} - \frac{1}{z}\frac{dz}{dz}$$

But

$$\frac{dm}{dT} = 0 \qquad \frac{1}{x}\frac{dx}{dT} = \frac{1}{y}\frac{dy}{dT} = \alpha_1 \quad \text{and} \quad \frac{1}{z}\frac{dz}{dT} = \alpha_3$$

Therefore the temperature coefficient of the density is

$$T_\rho = -(2\alpha_1 + \alpha_3) = -36.4 \times 10^{-6}/°C \tag{88}$$

The values of the temperature coefficients of the elastic moduli have been determined by Mason.[1] His values are given in Table 8.2. It should be noted that all the values are negative except Tc_{66}. It

[1] W. P. Mason, *Piezoelectric Crystals and Ultrasonics.* New York: Van Nostrand, 1950, p. 103.

Table 8.2. Values of the Temperature Coefficients of the Elastic Constants of Quartz.

$Tc_{11} = -46.5 \times 10^{-6}\ °C^{-1}$	$Tc_{33} = -205$
$Tc_{12} = -3300$	$Tc_{44} = -166$
$Tc_{13} = -700$	$Tc_{66} = +164$
$Tc_{14} = -90$	

is due to the fact that this temperature coefficient is positive that a zero temperature coefficient of frequency is possible in quartz.

We now have all the information necessary to compute the value of T_f for the X- and Y-cut plates. The thickness of the X-cut plate is in the X-direction and therefore $T_e = \alpha_1 = 14.3 \times 10^{-6}$. The elastic modulus is c_{11} and $Tc_{11} = -46.5 \times 10^{-6}$. Therefore, for the X-cut plate,

$$T_f = \left[\tfrac{1}{2}(-46.5) - 14.3 - \tfrac{1}{2}(-36.4)\right] \times 10^{-6} = -19.4 \times 10^{-6}\ °C^{-1}$$

which is in agreement with the measured value.

For the Y-cut plate we have that the thickness is in the Y-direction and therefore $T_e = \alpha_1 = 14.3 \times 10^{-6}$. The elastic modulus is c_{66} and Tc_{66} is $+\ 164 \times 10^{-6}$. Therefore, for the Y-cut plate, vibrating in thickness shear,

$$T_f = \left[\tfrac{1}{2}(164) - (14.3) - \tfrac{1}{2}(-36.4)\right] \times 10^{-6} = 86 \times 10^{-6}\ °C^{-1}$$

To determine T_f for a plate in which the direction of wave propagation is not parallel to one of the crystallographic axes, it is necessary to determine the temperature coefficient of expansion in the thickness direction of the plate and the temperature coefficient of the applicable elastic modulus. The temperature coefficient of the density is, of course, independent of direction.

We illustrate the process by computing the T_f for a rotated Y-cut plate, i.e., an orientation reached by considering a Y-cut plate to be rotated about the X-axis which lies in the plane of the plate.

The angle of rotation θ is measured as shown in Fig. 8.1a. This angle convention conforms to the convention used by Bond[2] and to the usual method of specifying the orientation of AT, BT, and other

[2] *B. S. T. J.*, 22. (1):12 (January 1943).

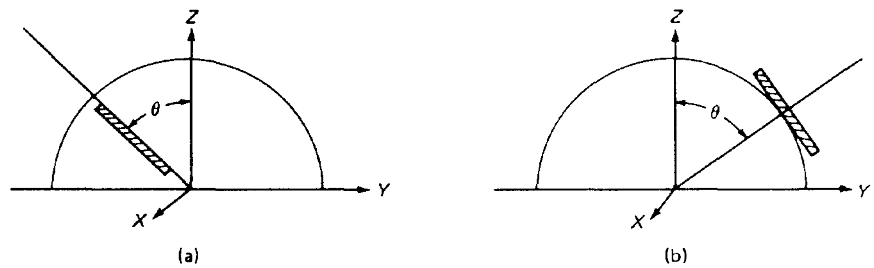

Fig. 8.1. Methods of specifying the angular rotation of piezoids of the *Y*-cut family. (*a*) System used by Bond. (*b*) IRE (IEEE) system.

piezoids. It differs from the convention adopted by the Technical Committee on Piezoelectric Crystals in the 1945 report of the Institute of Radio Engineers (now IEEE). The latter convention is illustrated in Fig. 8.1*b*. Although the IEEE convention is preferable in some respects, the older system is used to avoid the necessity of converting all the rotation matrices which have been given by Bond[3]. Calculations are most easily made in the older system and the results may be expressed according to the IEEE convention where desirable.

The calculation of the values of the elastic moduli for rotated plates is somewhat more complicated than that for the dielectric constants because the elastic moduli are described by 6 X 6 matrices while the dielectric constants are described by 3 X 3 matrices. However the procedure is the same in principle.

The stress matrix transforms according to the relation

$$X' = \alpha X$$

where α is the matrix which performs a rotation about the X axis.

The strain matrix transforms as

$$x' = \alpha_c^{-1}\, x \qquad \text{or} \qquad x = \alpha_c\, x'$$

[3] (*Loc. cit.*)

where α_c^{-1} is the reciprocal matrix of the congugate matrix of α. All the required matrices have been tabulated by Bond.[4] Using the methods of matrix algebra developed in Chap. 2 we have

$$X = c\,x$$
$$X' = \alpha c\,x$$
$$X' = \alpha\, c\, \alpha_c\, x'$$

or

$$X' = c'\, x'$$

where c' is written for $\alpha\, c\, \alpha_c$.

The matrix c' corresponding to a rotation by an angle θ about the X axis is found by performing the following matrix multiplications.

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & c^2 & s^2 & 2sc & 0 & 0 \\ 0 & s^2 & c^2 & -2sc & 0 & 0 \\ 0 & -sc & sc & c^2-s^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & c & -s \\ 0 & 0 & 0 & 0 & s & c \end{pmatrix} \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & 0 & c_{14} & c_{66} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & c^2 & s^2 & -sc & 0 & 0 \\ 0 & s^2 & c^2 & sc & 0 & 0 \\ 0 & 2sc & -2sc & c^2-s^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & c & s \\ 0 & 0 & 0 & 0 & -s & c \end{pmatrix}$$

where, as usual, c stands for $\cos\theta$ and s for $\sin\theta$.

Fortunately, to determine a single element of a matrix, it is not necessary to compute the entire matrix. In this case we are interested only in c'_{66}, which is the coefficient required to determine the frequency constant and the temperature coefficients of all members of the rotated Y-cut family of piezoids.

To obtain the value of c'_{66} we need compute only the last row of the matrix obtained by multiplying α by c. This row is found to be

$$0 \quad 0 \quad 0 \quad 0 \quad (c_{44}s + c_{14}c) \quad (c_{14}s + c_{66}c)$$

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[4] (*Loc. cit.*)

We then multiply the row just obtained by the last column in α_c. This gives

$$c'_{66} = c_{44}s^2 + 2\,c_{14}sc + c_{66}c^2 \tag{89}$$

For $\theta = 0$ corresponding to a Y-cut, $c'_{66} = c_{66}$; and if $\theta = 90°$ corresponding to a Z-cut, $c'_{66} = c_{44}$. Both are correct.

The value of c'_{66} for any angle of rotation about the X-axis can be calculated by using Eq. (89) and the values of the elastic moduli from Table 3.1. In this way the value of c'_{66} for the AT-cut ($\theta = 35\frac{1}{4}°$) is found to be

$$c'_{66} = 29.3 \times 10^9 \text{ N/m}^2$$

and for the BT-cut ($\theta = -49°$)

$$c'_{66} = 68.9 \times 10^9 \text{ N/m}^2$$

We are now able to compute the frequency constants using Eq. (85b) and the density of quartz, which is 2650 kg/m^3.

It must be remembered, however, that the elastic constants are themselves temperature-dependent and therefore c'_{66} is also temperature-dependent. The temperature coefficient of c'_{66} is calculated in the following way. We differentiate Eq. (89) with respect to T and divide both sides by c'_{66}. This gives

$$Tc'_{66} = \frac{1}{c'_{66}}\,\frac{dc'_{66}}{dT} = \frac{s^2\,c_{44}\,Tc_{44} + c^2\,c_{66}\,Tc_{66} + 2sc\,c_{14}\,Tc_{14}}{c'_{66}} \tag{90}$$

The values of the temperature coefficients of the elastic constants c_{66}, c_{44}, and c_{14} have been determined experimentally and are given in Table 8.2. From Eq. (86) we have for the rotated Y-cut family of quartz plates:

$$T_f = -T_e + \tfrac{1}{2}\,Tc'_{66} - \tfrac{1}{2}\,T_\rho \tag{91}$$

Substituting from Eqs. (87), (88), and (90) into Eq. (91) gives the temperature-frequency coefficient for the entire Y-cut family.

$$T_f = -(\alpha_1 c^2 + \alpha_3 s^2) + \frac{1}{2}\,\frac{s^2 c_{44} Tc_{44} + c^2 c_{66} Tc_{66} + 2sc\, c_{14} Tc_{14}}{c_{44} s^2 + c_{66} c^2 + 2sc\, c_{14}} + \frac{1}{2}(36.4 \times 10^{-6}) \qquad (92)$$

The values of the angle θ for which the temperature-frequency coefficient is zero is found, in principle, by setting the equation above equal to zero and solving for θ. It would be a very laborious task to solve this equation in closed form. With the aid of a computer the values can be obtained readily or solutions can be obtained by successive approximation methods.

If $\theta = 0$ is substituted into Eq. (92), we find $T_f = 86 \times 10^{-6}\ °C^{-1}$. This is, of course, the temperature coefficient of the Y-cut piezoid.

If $\theta = 90°$, corresponding to the Z-cut, is substituted, the value of $T_f = -73 \times 10^{-6}$. It is not possible to excite the Z-cut plate into oscillation through the piezoelectric effect because no piezoelectric strains are produced in quartz by electric fields in the Z-direction. However, if the thickness shear mode were excited by driving the plate in some way, it would have a negative temperature coefficient of about −73 ppm/°C. Since the temperature coefficient changes from positive to negative as θ is changed from 0° to 90°, it follows that it must be zero at some point between.

The value of T_f actually becomes zero at two values of θ. These are at approximately $\theta = -35\frac{1}{4}°$ and at $\theta = +49°$ corresponding to the AT- and BT-cuts, respectively.

The position of the two cuts relative to the major and minor rhomb faces, R and r, are shown in Fig. 8.2.

We have derived the expression for T_f using the room-temperature values of the elastic moduli and their temperature coefficients, and the linear coefficient of expansion. We therefore obtain the value of T_f for room temperature. If all the coefficients were constants and independent of temperature, then T_f would be independent of temperature.

However, none of the quantities is truly independent of temperature and therefore T_f must also be temperature-dependent. Bechman[5] has determined the second- and third-order terms in the power-series

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[5] *Proc. I. R. E.*, 50:1812 (August, 1962).

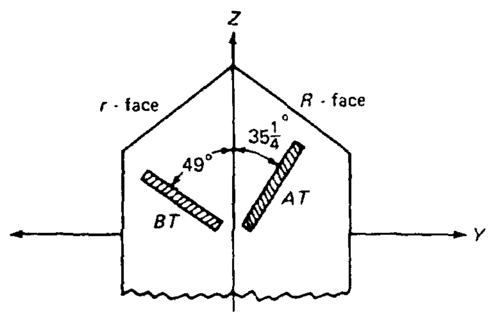

Fig. 8.2. The AT- and BT-cuts in quartz relative to the major and minor rhomb faces. The X-axis is normal to the plane of the diagram. The r- and R-faces make an angle of 38° 13′ with the Z-axis.

expression for the elastic moduli of quartz. Using these values it is possible, in principle, to calculate the value of T_f for any member of the rotated Y-cut family of piezoids at any temperature between -196 and +170°C.

Excellent experimental data exist showing the temperature-frequency curves for the AT- and BT-cut plates for the range of angles over which these cuts are used. Figure 8.3, which is adapted from the Final Report of the Union Thermoelectric Company on Contract No. DA49-025-sc-118, shows the temperature-frequency curves for AT-cut piezoids operating at 100 MHz on the fifth-harmonic mode. The blanks were 0.375 in in diameter and 0.0033 in thick, giving them a diameter/thickness ratio of more than 100. Their behavior, therefore, closely approximates that of an infinite plate.

Figure 8.4 shows the frequency-temperature curves of AT-cut plates operating at a frequency of 4.0 MHz. The blanks had diameters of 0.550 in and thicknesses of 0.0166 in, making the diameter/thickness ratio approximately 33. The blanks were designed for optimum performance by making the major surfaces conform to a spherical surface having a radius of curvature of 0.5 m.

From the curves of Figs. 8.3 and 8.4 it is apparent that no single angle can be prescribed for the AT-cut piezoid. The optimum value of the angle θ depends on (1) the nominal frequency, (2) the harmonic order, (3) the diameter/thickness ratio, (4) the temperature range, and to a lesser degree on (5) the size of the electrodes, (6) the drive level, (7) the countour, and (8) the material and thickness of the plated elec-

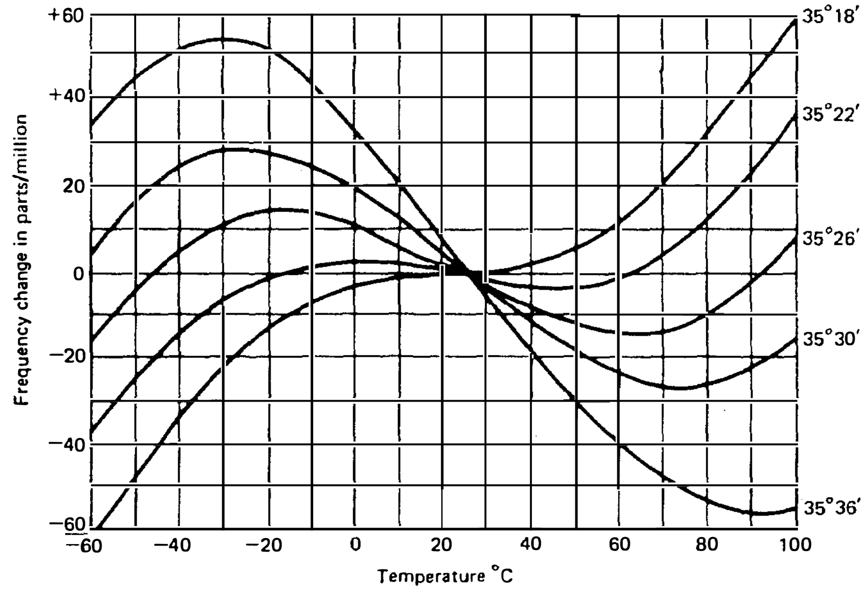

Fig. 8.3. Frequency-temperature curves for the AT-cut operating on the fifth harmonic mode at 100 MHz vs. the orientation angle.

trodes. Consequently, some experimentation is usually necessary to determine the correct value of θ and the allowable tolerances.

The temperature-frequency curves for the BT- cut are shown in Fig. 8.5. The frequency of a BT-cut plate cut at an angle of 49° has a maximum value near room temperature and the frequency decreases both at higher and lower temperatures. Consequently, the frequency is set above the nominal frequency at room temperature. Whereas an AT-cut plate can be made with a frequency tolerance of ±15 ppm over the temperature range −60 to +100°C, the BT-cut plate deviates by ±100 ppm over the same temperature range. For this reason the BT-cut has fallen into disfavor although it was formerly used very extensively.

However, the BT-cut does have certain advantages over the AT-cut. The frequency constant is 50 percent greater and therefore the blanks are 50 percent thicker for a given frequency. This is a distinct advantage at the highest frequencies. The turning point of the BT- but is easily adjusted to any desired temperature and the angular tolerances are less severe, so that the BT-cut has some advantages in applications in which the temperature of the crystal unit is controlled. Activity dips

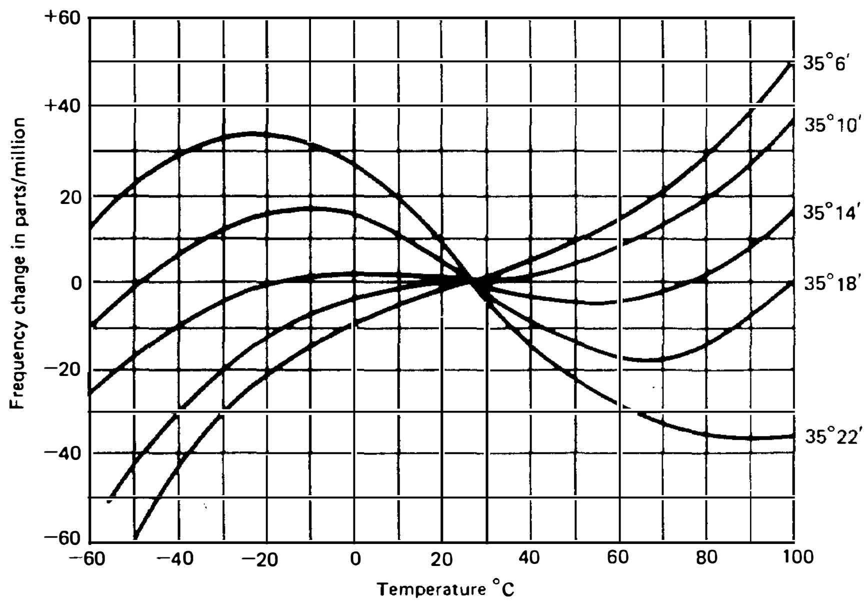

Fig. 8.4. Frequency-temperature curves for the AT-cut operating at 4 MHz vs. the angle of orientation.

are a bit less severe in BT- than in AT-cuts because the piezoelectric constant is smaller. The higher capacitance ratio, larger motional inductance, and smaller piezoelectric coupling sometimes offer advantages in filter applications.

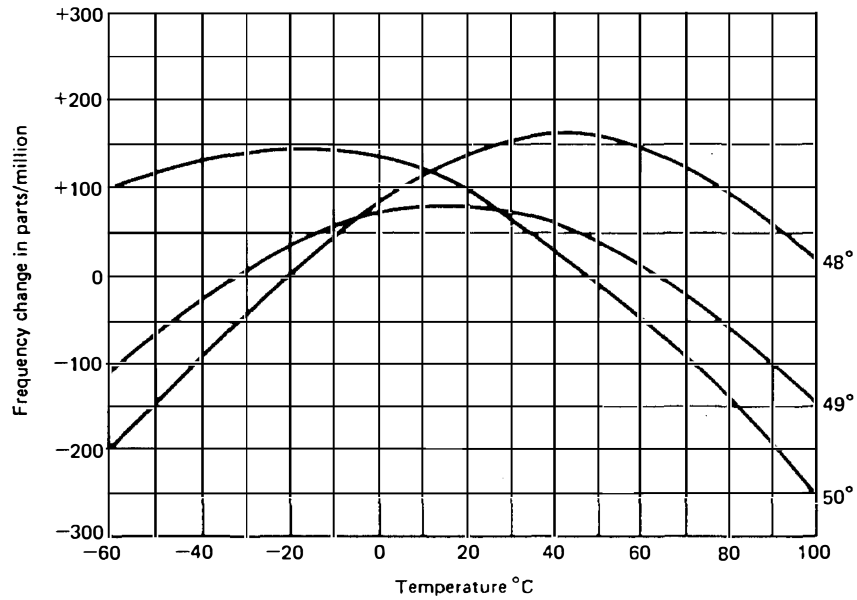

Fig. 8.5. Frequency-temperature curves for the BT-cut at different values of the angle θ.