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SECTION 1
INTRODUCTION

1. PROGRAM OBJECTIVE

The objective of this program is the exploratory development of doubly rotated cuts of quartz possessing superior Surface Acoustic Wave (SAW) properties for applications involving environmentally hardened devices. The key properties examined and optimized both theoretically and experimentally are: first, second and third order Temperature Coefficients of Delay (TCD), piezoelectric coupling factor, power flow angle, Bulk Acoustic Wave (BAW) inverse velocity surfaces, leaky waves, and sensitivities of the above quantities to misorientations and manufacturing tolerances.

2. PROGRAM SCOPE

The program consists of two major task areas comprising an interactive numerical/experimental approach. Task I involves the numerical computation of the key SAW properties for doubly rotated quartz substrates for the purpose of locating promising angular ranges with properties superior to the singly rotated cuts now in existence. More detailed calculations follow to refine the angular coordinates in order to specify cuts for experimental verification in Task II. In Task II, sets of substrates with promising orientations identified in Task I are prepared and SAW device patterns fabricated for evaluation of the key SAW properties. The experimental results of this task are correlated with the theoretical predictions and an iterative process develops for refinement of both theoretical and experimental parameters. As the program proceeds, working SAW device models will be delivered as a demonstration of progress and an indication of the future potential of the doubly rotated cuts. Depending upon the progress made and time and budget limitations, additional properties in the area of nonlinear elasticity will be investigated.

3. TECHNICAL APPROACH SUMMARY

To accurately characterize the properties of doubly rotated quartz, three basic capabilities are essential:

a. Theoretical approach and associated computer software which will accurately and quickly locate promising zero TCD cut angles and characterize the other key SAW parameters

b. Source of rotated quartz substrates of superior quality which can be quickly fabricated and the angular orientation which can be determined with a high degree of precision

c. Required fabrication facilities and measurement tools to accurately determine the key SAW device parameters.
In the theoretical area, this program has characterized two basic theoretical approaches for the identification of zero TCDs on rotated cuts of quartz. For this study, two computer programs available at Motorola are used. The first program calculates the first, second and third order TCDs of rotated cuts using a finite difference method. This technique is simple, well established, and has been used for analytically determining the temperature coefficient curves for singly and doubly rotated cuts of quartz. To more accurately refine the temperature coefficient properties, a second program which encompasses lattice skewing effects is used. This more complete theoretical approach is based on the work of Sinha and Tiersten; its utility has been verified.

The final theoretical work is the characterization of the other key parameters with standard SAW programs used routinely for material characterization and device development.

Accurately oriented quartz bars, supplied by Motorola, Carlisle, are cut, lapped and finely polished at Motorola. A mechanical polishing procedure is used. During this program, several substrates from a single bar with incremental angular deviations about a promising angular position are fabricated. By careful organization of the angle selection and cut procedures, a substantial savings in time and money is achieved.

The angular orientation of the doubly rotated substrates are defined to an accuracy of within ±5 minutes using X-ray diffractometry. Equipment used includes Laue pattern X-ray equipment, X-ray diffractometers, and precision wafer cut and polishing equipment.

A complete SAW test area and optical laboratory form the basis for evaluating the key SAW parameters of the doubly rotated quartz delay lines, oscillators and resonators. The equipment will be set up for rapid display and recording of the SAW parameters.

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SECTION II
TECHNICAL DISCUSSION

The following section discusses the technical approaches used in this program. A comparison of numerical approaches is made and the numerical approach used is described in paragraph 1 (Task I). Experimental techniques (Task II) will be outlined in paragraph 2.

1. INTRODUCTION

Quartz is the most commonly used substrate for fabricating Surface Acoustic Wave (SAW) devices. In SAW narrowband filter, oscillator, and resonator applications, the temperature stability of the device is an important design parameter. Currently, almost all SAW devices fabricated on quartz use the ST-Cut, which exhibits a parabolic frequency dependence in temperature. For many applications, the temperature dependence of devices fabricated on ST quartz is too large. Thus it is desirable to find crystal cuts with superior temperature performance. Of course, many other design parameters must be considered when choosing a crystal cut. Some of the more important ones are the piezoelectric coupling coefficient, acoustic losses, dependence of device performance on cut misorientation, excitation of bulk modes, and beam steering angle. These parameters are all easily determined for a given cut.

The objectives of this program are to find crystal cuts which exhibit zero temperature coefficients of delay so that there will be no frequency-temperature dependence observed in temperature stable oscillators, resonators and filters. We have used computer models to investigate the temperature dependence of different cuts of crystal for SAW devices.

Defining \( r \) as the delay time for an acoustic wave to propagate between two points on the surface of the crystal, we wish to find orientations for which \( r \) is constant in temperature, or more formally \( (1/r) (d(r/dT)) \mid \gamma = 25 \) degrees \( \epsilon = 0 \).

If \( F \) is the frequency of a SAW resonator, we have \( (1/F) (d(F/dT)) = -(1/r) (d(r/dT)) \). Of course, we would also like the higher order derivatives to be as close to zero as possible, or \( (1/2r) (d^2(r/dT^2)) \mid \gamma = 25 \) degrees \( \epsilon = 0 \), etc.

Letting \( \rho \) be the length between two points, \( (r) \) is simply given by \( r = (\rho/V,). \)\((1/r)(d(r/dT)) = (1/\rho)(d(\rho/dT)) - (1/V,)(dV,/dT) \).

We have computer programs for calculating \( r \) as a function of the stress, the dielectric and piezoelectric constants of a substrate material. Furthermore, we have at our disposal the temperature variation of those constants for quartz allowing one to calculate \( (1/V,)(dV,/dT) \) by a finite difference method (note that higher order terms can be calculated the same way). If the crystal expansion coefficients are known, it is then a simple matter to calculate \( (1/r)(d(r/dT)) \) for any particular orientation. Perturbation
programs developed by Sinha and Tiersten to calculate \((1/\tau)(d\tau/dT)\) are also available. Combined with a search method, we are able to find cuts for which first order temperature coefficient of frequency vanishes.

a. Calculation of Temperature Coefficients

It has been shown that determining the temperature dependence of \(\tau\) (time delay) is equivalent to determining the temperature dependence of \(F\) (frequency) via the relation \(F \propto 1/\tau\).

Since our experimental data is derived from frequency measurements, we determine the frequency characteristics of the devices. The relation between the temperature coefficient of frequency (TCF) and temperature coefficient of delay (TCD) are related as follows (See Appendix E):

\[
\begin{align*}
\alpha_F^{(i)} &= -\alpha_{\tau}^{(i)} \\
\alpha_{\tau}^{(i)} &= -\alpha_F^{(i)} + (\alpha_{\tau}^{(i)})^2 \\
\alpha_{\tau}^{(i)} &= -\alpha_F^{(i)} + 2\alpha_F^{(i)} \alpha_{\tau}^{(i)} - (\alpha_{\tau}^{(i)})^3
\end{align*}
\]

where \(\alpha_F^{(i)}\) is the ith order TCF, \(\alpha_{\tau}^{(i)}\) is the ith order TCD.

Using the relations above, one can always relate one set of the temperature coefficients to the other.

The various procedures outlined in the following sections will yield the quantities \(\alpha_{\tau}^{(i)}\), \(i = 1, 2, 3\), with \(V_{\tau}(T) = V_{\tau}(T_o)(1 + \alpha_{\tau}^{(1)} dT + \alpha_{\tau}^{(2)} dT^2 + \alpha_{\tau}^{(3)} dT^3)\) and \(dT = T - T_o\).

The problem of interest is not only, however, in finding the \(\alpha_{\tau}^{(i)}\)'s but in finding the delay time \(\tau\) and the frequency dependence \(F\) of a device. The frequency dependence \(F(T) = F(T_o)(1 + \alpha_F^{(1)} dT + \alpha_F^{(2)} dT^2 + \alpha_F^{(3)} dT^3)\) is a function of not only \(V\), but of \(z(T_o) = z(T_o)(1 + \alpha_z^{(1)} dT + \alpha_z^{(2)} dT^2 + \alpha_z^{(3)} dT^3)\), the spacing between reflectors in a resonator (or the length of the delay line in an oscillator).

From the above relations and \((1 + X)^{-1} = 1 - X + X^2 - X^3\) if \(X << 1\), we see that:

\[
\begin{align*}
F &= V_{\tau}(T) \\
&= F(T_o)(1 + \alpha_F^{(1)} dT + \alpha_F^{(2)} dT^2 + \alpha_F^{(3)} dT^3) \\
&- \alpha_F^{(1)} dT - \alpha_F^{(1)} \alpha_F^{(1)} dT^2 - \alpha_F^{(1)} \alpha_F^{(1)} dT^3 \\
&- \alpha_F^{(2)} dT^2 - \alpha_F^{(2)} \alpha_F^{(1)} dT^3 - \alpha_F^{(2)} dT^3 \\
&+ (\alpha_F^{(1)})^2 dT^2 + (\alpha_F^{(1)})^2 \alpha_F^{(1)} dT^3 \\
&+ 2\alpha_F^{(1)} \alpha_F^{(1)} dT^3 - (\alpha_F^{(1)} \alpha_F^{(1)})^3
\end{align*}
\]

or
\begin{align*}
\alpha_i^{(1)} &= \alpha_i^{(11)} - \alpha_i^{(11)} \\
\alpha_i^{(2)} &= \alpha_i^{(11)} - \alpha_i^{(11)} + (\alpha_i^{(11)})^2 - \alpha_i^{(12)} \\
\alpha_i^{(3)} &= \alpha_i^{(11)} - \alpha_i^{(11)} + \alpha_i^{(11)} (\alpha_i^{(11)})^2 - (\alpha_i^{(11)})^3 + 2 \alpha_i^{(11)} - \alpha_i^{(11)} - \alpha_i^{(11)}
\end{align*}

\text{giving the frequency dependence directly. The calculation of the temperature coefficients of velocity, } \alpha_i^{(1)}, \text{ is achieved by calculating the phase velocity with the Finite Difference Technique or other techniques discussed below for a variety of temperatures. As the velocity is a function of temperature, a linear regression program is used in the finite difference technique to curve fit the data to a third order polynomial. The constants } \alpha_i^{(1)}, \alpha_i^{(2)} \text{ and } \alpha_i^{(3)} \text{ are thus obtained by optimum curve fitting of the data points to the polynomial. The temperature coefficients of length, } \alpha_i^{(4)}, \text{ are found in standard references. It should be noted that the } \alpha_i^{(s)} \text{ also depend on the direction of propagation, and must be calculated for each direction of propagation considered by a simple geometrical transformation analogous to that used to rotate all of the other physical constants.}

\text{b. Rayleigh Wave}

\text{We will briefly discuss the Rayleigh wave solutions in their general form in this section. The coordinate system is defined with the Z or 1 axis being the direction of propagation and the } -Y \text{ or 3 axis normal to the crystal surface. } V, \text{ will denote the Rayleigh wave velocity, } \beta_n = \omega/V, \text{ the wave number, } u_i (i = 1, 2, 3), \text{ the particle displacements along the 1, 2, or 3 axis, } u_4 = \phi, \text{ the electric potential. Also, } T, \text{ denotes the stress tensor.}

\text{S}, \text{ is } (1/2)(du_i/dx_j + du_j/dx_i), \text{ the strain tensor, } c_{ijkl}, \text{ the elastic tensor, } \rho \text{ the density of the substrate, } D, \text{ the electric displacement, } E, \text{ the electric field, } e_i \text{ the dielectric constant, and } e_{ik} \text{ the piezoelectric constant. We also use } \Delta \text{ for the difference, where, for example,}

\Delta \rho = \rho(T_i) - \rho(T_0) = \rho(T_0)[(\alpha_1^{(11)}d\rho + \alpha_2^{(2)}d\rho^2 + \alpha_3^{(3)}d\rho^3)], \text{ and let } P = \text{power/unit width in the } x \text{ direction.}

\text{We assume relations such as}

\begin{align*}
T &= -e \cdot E + e^6: S \text{ or } S = e \cdot E + S^6 \cdot T \\
D &= e^5 E + e \cdot S \quad D = e^5 E + d \cdot T \\
\rho \partial^2 u_i / \partial t^2 - c_{ijkl} \partial u_k / \partial x_j \partial x_k - e_{ik} \partial^2 \phi / \partial x_i \partial x_k = 0 \\
e_{ikl} \partial^2 u_k / \partial x_i \partial x_l - e_{ik} \partial^2 \phi / \partial x_i \partial x_k = 0
\end{align*}
The general solution for a wave traveling on the surface can be written

\[ u_j = \left[ \sum_{m=1}^n c_m \alpha_j^{(m)} \exp\left(-i\omega/V_j\right) \sum_{i=1}^4 b_i^{(m)} x_i \right] \exp(\omega t) \text{ for } j = 1 \text{ to } 4 \] 

(12)

For the Rayleigh wave, this reduces to

\[ u_j = \sum_{m=1}^n c_m \alpha_j^{(m)} \exp\left(-i\beta_n b^{(m)} y\right) \exp(i\omega z - i\omega t) \] 

(13)

where the coefficient \( c_m \), \( \alpha_j^{(m)} \) (weighting factors), \( \beta_n \) (wave number), and \( b^{(m)} \) (complex decay constants) are to be calculated by the standard iterative procedure on a computer.

The fields are calculated as \( E = \nabla u \), with \( E_x = 0 \), \( E_y = (-i\beta_n b^{(m)} y)u_x \), and \( E_z = (i\beta_n)u_x \).

c. Methods for Calculating the Temperature Dependence of the Rayleigh Velocity

In the following sections, four methods for calculating the temperature characteristics of the Rayleigh wave are discussed.

(1) Finite Difference Technique of Calculating Temperature Dependence of the Rayleigh Velocity

Before \( \text{TCD} = (1/n)(\partial V/\partial T) \) can be calculated, one must first calculate the dependence of the Rayleigh wave velocity on temperature. The most straightforward method for doing this is the finite difference method. The Rayleigh wave velocities are calculated for different temperatures, yielding the values \( V_i(T_i), i = 1, 2, \ldots, n \). This is done by first calculating the fundamental constants at the temperature of interest. The fundamental constants are then rotated into the coordinate system of interest. An iterative procedure is used to calculate a velocity \( V_i \) for which Christoffel's equation and the boundary conditions are satisfied simultaneously (see Appendix D). Simple finite difference techniques can be used to calculate \( (1/V_i)(\partial V_i/\partial T) \), \( (1/2V_i)(\partial^2 V_i/\partial T^2) \), etc. For example, after calculating \( V_i(T_i) \) for \( T_1 = T_0, T_2 = T_0 + \Delta T, T_3 = T_0 - \Delta T \), we can use \( (1/V_i)(\partial V_i/\partial T) \) at \( T_0 \equiv (1/V_0(T_0))(V_0(T_0 + \Delta T) - V_0(T_0 - \Delta T))/2\Delta \). Alternately, standard linear regression of polynomials may be employed to yield those coefficients. Another approach consists of calculating directly the frequency-temperature characteristics of the orientation for several widely differing temperatures. A measure of the temperature stability is then used. Letting \( F(T) \) be the frequency of the device, the measure of deviation is calculated as

\[ \text{RMS frequency deviation} = \left[ \frac{1}{n} \sum_{i=1}^n (F(T_i) - F(T_0))^2 \right]^{1/2} \text{ with} \]

(14)

\[ F(T) = V_i(T)/2(1 + \alpha_i^{(1)}(\Delta T) + \alpha_i^{(2)}(\Delta T)^2 + \alpha_i^{(3)}(\Delta T)^3). \]

although \( \alpha_i^{(1)}, \alpha_i^{(2)}, \text{ and } \alpha_i^{(3)} \) are calculated for purposes of comparison.
In much of the earlier work, the SAW velocities were calculated at three temperature points, $T_1 = -50^\circ C$, $T_2 = 25^\circ C$, and $T_3 = 100^\circ C$, to save on computer time. The following formulas were used for the calculations of first and second order temperature coefficients of velocity.

$$\alpha_{1V}^{(1)} = \frac{[V(T_1) - V(T_3)]}{[V(T_2) - V(T_3)]}$$  \hspace{1cm} (15)

$$\alpha_{1V}^{(2)} = \frac{[V(T_1) + V(T_3) - 2 \cdot V(T_2)]}{[V(T_2) - 2 \cdot (T_1 - T_3)]}$$  \hspace{1cm} (16)

In the more recent works, six temperature points were calculated for each orientation to provide data for the linear regression analysis. The six temperature points were $100^\circ C$, $85^\circ C$, $75^\circ C$, $-25^\circ C$, $-10^\circ C$, and $-50^\circ C$. The results were used to calculate $TCF^{(1)}$, $TCF^{(2)}$, and $TCF^{(3)}$.

(2) Perturbation Technique of Calculating Temperature Dependence of the Rayleigh Velocity

Perturbation theory may be applied to the problem of calculating the first, second and third order dependence of the Rayleigh velocity $V$, of a piezoelectric substrate, once the solution to the Rayleigh wave propagation at a temperature reference $T_0$ is known.

Perturbation techniques allow calculations of small changes in the solutions to a problem caused by small changes in the physical parameters of the problem, once the solution to the unperturbed problem is known. One can apply perturbation techniques either to boundary perturbation such as mass loading on the surface or to volume perturbations such as adding a thin conducting layer to the interior of piezoelectric substrates. As the boundary conditions are unaffected by changes in temperature while material constants such as $c$, are temperature dependent, one can apply the volume perturbation theory to the problem.

The general approach to the problem of determining the temperature dependence of $V$, will be as follows. First, the Rayleigh wave propagation problem will be solved in the standard way in its entirety at room temperature, $T_0$. Given the solution of the problem at $T_0$ and the dependence of the physical constants (such as $c$) on temperature at $T_0$, one will apply the volume perturbation formula, calculating the temperature dependence of $V$. The dependence of $V$, on $T$ is then used to calculate the frequency characteristics of the actual device given the thermal expansion coefficients as a function of temperature. At this point, the frequency temperature dependence of the substrate as a function of the crystal cut and direction can be thoroughly explored. See Appendix A for a complete discussion of this method.
(3) Approach of Sinha and Tiersten

The primary difficulty with the perturbation technique is that it does not take into account the change of coordinate systems induced by the thermal expansion in the material. This comes about because the material distorts as temperature changes. Thus, the set of axis is to which the fundamental elastic constants refer, which is fixed to the crystal, is no longer equivalent to the axis used to calculate $V$. This problem is elegantly solved by Sinha and Tiersten. The first simplification which occurs is that the density of the material remains constant with temperature. Furthermore, the $\alpha_i^{(0)}$ simply become $\alpha_i^{(0)} = \alpha_i^{(0)}$, as the length in this coordinate system does not change. The only difficulty is that the elastic constants previously used no longer refer to the proper coordinate system and must be rederived from the original experimental data. This procedure has already been carried out for the first order temperature derivation of quartz but has not been done for the second and third order coefficients. Nonetheless, the procedure yields more accurate results for the first order dependence. See Appendix B for a mathematical description of the salient features of this technique.

(4) Differentiation Method

A method for determining the theoretical temperature dependence of Rayleigh Surface Waves consists of formally differentiating the wave equation and boundary conditions. The boundary conditions and wave equation must be true at all temperatures, placing constraints on how the parameters of the wave equation may vary. In this technique, the derivatives of these equations with respect to temperature are set to zero and solved for the velocity-temperature dependence. This method follows the methods used by Bechmann, Ballato, and Lukaszek to compute the temperature dependence of the fundamental elastic constants from frequency data, except that the simplifying assumptions of assuming bulk wave solutions cannot be made. This method was later used by Hauden to search for temperature stable cuts of quartz. See Appendix C for a discussion of this method.

(5) Summary of Approaches

Of all the techniques presented, the finite difference technique satisfies all of the basic requirements for calculating temperature coefficients of delay. Arbitrary crystal structures may be

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investigated once the density, piezoelectric, elastic, and dielectric constants and their temperature variation are known. When double precision on the computer is used and when the velocity over a large temperature range is calculated, it becomes a very accurate numerical approach. The computational efficiency of the finite difference method is not as high as some of the other techniques, owing to the need for repeated calculation of the surface wave velocity.

A comparison between the experimental results of Schulz and Motorola's finite difference program adapted from Jones et al. as shown in Figure 1. The results for this cut and many other orientations studied have been found to be very good. The slight shift of the analytical curve versus experimental curve can be explained by a crystal misorientation.

![Finite Difference Method Versus Experiment ST-Cut (Quartz)](image)

Figure 1. Finite Difference Method Versus Experiment ST-Cut (Quartz)


Figure 2 displays a phase delay versus temperature plot for the orientation (YXwlt) 56/40/27 in quartz obtained from Hauden's graphs. Using the differentiation approach, he calculated \( \alpha_1^{(1)} = 0, \alpha_2^{(1)} = -0.04 \times 10^{-1} \text{ ppm/}^\circ\text{C}, \varphi_3^{(1)} = -22.7 \times 10^{-6} \text{ ppm/}^\circ\text{C} \) for a cut close to (YXwlt) 56/40/27. The Finite Difference approach was used to verify his first order calculation but is in disagreement on the second and third order calculations. This can be resolved by experiment.

![Finite Difference Method Calculation for Hauden's Cut](image)

Figure 2. Finite Difference Method Calculation for Hauden’s Cut (YXwlt) 56°/40°/27°

Tiersten’s Perturbation program, while very difficult to extend to higher orders, is available for calculating the first order TCD.

Figure 3 shows the results of Tiersten’s calculation and compares those results with the Finite Difference method as well as experiment. The cut used for comparison is the AT-Cut. The improvement in accuracy is substantial. It offers the significant advantages of being quite cost efficient, as well as being more accurate in the first order on off-axis cuts, our primary area of interest. In the task of making quartz cuts along the surface of zero TCD, accurate values for the first order TCD prove more useful than the less exact values for the first, second, and third order TCD's provided by other methods, because it is a necessary (but not sufficient) condition for zero TCD cut to get a zero first order. Since it is the dominating term, it is important to first get an accurate first order zero TCD locus. Then one may search for the intersection of this locus with the zero second and third order terms with the finite difference technique.


Figure 3. Tiersten's Method Versus Finite Difference and Experiment

6. Investigative Approach

A necessary but not sufficient condition to find a temperature stable cut of quartz is that \( \alpha_{T}^{(1)} = 0 \). In practice, a sufficient condition for finding a zero temperature cut is that \( \alpha_{T}^{(1)} = \alpha_{T}^{(2)} = \alpha_{T}^{(3)} = 0 \). Thus every zero temperature cut must be on the locus of angles which satisfy the condition \( \alpha_{T}^{(1)} = 0 \). Thus the first problem is to locate accurately such cuts. Both the finite difference approach and Tiersten's method are being used now to calculate the TCF.

The approach used in this program is to identify the areas (angles) where TCF\(^{(1)}\), TCF\(^{(2)}\) and TCF\(^{(3)}\) are relatively low by using the Finite Difference Approach and then define the exact orientation that has zero TCF\(^{(1)}\) in those areas by the Sinha and Tiersten approach.

In case the condition TCF\(^{(1)}\) = TCF\(^{(2)}\) = TCF\(^{(3)}\) = 0 cannot be met, a compromise approach would be to find an orientation where the first and third order effects tend to cancel out in the temperature range of interest and to find the minimum second order effect orientation amount for those cuts. This approach would provide an effective low TCF cut of quartz for SAW application.
Analytical Results on Zero TCF on Quartz

IRE standard angle definitions (YX wink) PHI/THETA/PSI for quartz were used throughout the investigation. Consider the TCFs to be functions of these angles, which define an angular volume $0 < \text{PHI} \leq 30^\circ$, $-90^\circ < \text{THETA} < 90^\circ$, $0 < \text{PSI} < 180^\circ$, which spans the space of possible cuts and propagation directions. The set of points at which $\text{TCF}^{(1)}(\text{PHI}, \text{THETA}, \text{PSI}) = 0$ forms a surface in this angular volume. Likewise, the set of points at which $\text{TCF}^{(2)}(\text{PHI}, \text{THETA}, \text{PSI}) = 0$ also form surfaces in this angular volume.

Our object is to find a point where $\text{TCF}^{(1)} = \text{TCF}^{(2)} = \text{TCF}^{(3)} = 0$. If the surface of zero $\text{TCF}^{(1)}$ intersected with the surface of zero $\text{TCF}^{(2)}$, the result would be a line (or a point if the two surfaces are tangent to each other) of angular points on which $\text{TCF}^{(1)} = \text{TCF}^{(2)} = 0$. The intersection of this line with the surface on which $\text{TCF}^{(3)} = 0$ would yield a single point at which $\text{TCF}^{(1)} = \text{TCF}^{(2)} = \text{TCF}^{(3)} = 0$. Neglecting higher order terms, we would have found a temperature stable cut.

The calculated values of $\text{TCF}^{(1)}$ versus propagation angles are shown in Figure 4. The zero $\text{TCF}^{(1)}$ is identified by the areas where $\text{TCF}^{(1)}$ changes sign.

Using the Finite Difference approach with the available crystal constants, the calculated results show that the zero $\text{TCF}^{(1)}$ surfaces do not intersect with the zero $\text{TCF}^{(2)}$ surfaces, based on the interpolated results of the $10^\circ \times 10^\circ \times 10^\circ$ resolution. It is not likely that a finer resolution will provide contrary information because $\text{TCF}^{(1)}$ and $\text{TCF}^{(2)}$ are relatively slow varying functions as shown in Figure 4.

Figure 4A. Calculated values of TCF versus propagation angles.
Figure 4B. Calculated Values of TCF$^{11}$ Versus Propagation Angles
Figure 4C. Calculated Values of TCF\(^{(1)}\) Versus Propagation Angles
Figure 4E. Calculated Values of TCF$^{III}$ Versus Propagation Angles
Figure 4I. Calculated Values of TCF* Versus Propagation Angles
Figure 4J. Calculated Values of TCF\(^{11}\) Versus Propagation Angles
Figure 4N. Calculated Values of TCF$^{iii}$ Versus Propagation Angles
Figure 40. Calculated Values of TCF\textsuperscript{11} Versus Propagation Angles
Figure 4P. Calculated Values of TCF$^{11}$ Versus Propagation Angles
Figure 4R. Calculated Values of TCF\textsuperscript{111} Versus Propagation Angles
Figure 4T. Calculated Values of TCF\textsuperscript{m} Versus Propagation Angles
Figure 4U. Calculated Values of TCF$^{(1)}$ Versus Propagation Angles
Figure 4V. Calculated Values of TCF versus Propagation Angles
Figure 42. Calculated Values of TCF\(^{(1)}\) Versus Propagation Angles
Figure 4DD. Calculated Values of $TCF^{(1)}$ Versus Propagation Angles
Figure 4H. Calculated Values of TCF vs. Propagation Angles
Figure 4II. Calculated Values of TCF\textsuperscript{111} Versus Propagation Angles
Figure 4JJ. Calculated Values of TCF\textsuperscript{III} Versus Propagation Angles
Figure 4KK. Calculated Values of TCF Versus Propagation Angles
Figure 4LL. Calculated Values of TCF\textsuperscript{th} Versus Propagation Angles
Calculations were performed on a $10^\circ \times 10^\circ \times 10^\circ$ grid over the angular ranges $0 \leq \text{PHI} \leq 30^\circ$, $0 \leq \text{PSI} \leq 180^\circ$, and $-90^\circ \leq \text{THETA} \leq 90^\circ$. These angular ranges, due to the symmetry of quartz, include all possible angular orientations. These initial calculations defined the "angular volumes" of low TCF orientations. Calculations were then performed on a $2.5^\circ \times 2.5^\circ \times 2.5^\circ$ grid near promising orientations. In this way, the entire angular range was explored and a large computer-based data file built. Maps of first and second order TCF's are shown in Figure 5. Zero first order TCF contours are drawn. In addition, contours of the second order TCF are drawn. In addition, contours of the second order TCF are drawn and shaded in areas where the second order TCF is less than 0.01 PPM/°C. This represents a substantial improvement over ST quartz, for which the second order for TCF is approximately 0.03 PPM/°C. Where data points were missing, lines were connected by interpolation.

Figure 5. TCF Map of SAW Device on Quartz

Despite the number and density of points at which the first and second order TCFs were calculated, wherever TCF was found to be less than or equal to zero, we found TCF to be less than 0. The reason for this probably lies in the lack of independence of the crystal constants themselves. Using the volume perturbation approach of Auld\textsuperscript{1}, one obtains equation A-8 of Appendix A.

For small changes in \(\rho\) and \(c^{(0)}\), one might expect that the TCFs are well correlated with the temperature derivatives of the fundamental constants for Rayleigh waves in quartz. A list of some of the crystal elastic constants' temperature derivatives is in Table 1.

**TABLE 1. CRYSTAL ELASTIC CONSTANTS' TEMPERATURE DERIVATIVES**

<table>
<thead>
<tr>
<th>(C_{ij})</th>
<th>(TC^{(1)})</th>
<th>(TC^{(2)})</th>
<th>(TC^{(3)})</th>
</tr>
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<tr>
<td>(C_{11})</td>
<td>(-48.5 \times 10^{-9})</td>
<td>(-107 \times 10^{-9})</td>
<td>(-70 \times 10^{-12})</td>
</tr>
<tr>
<td>(C_{12})</td>
<td>(-3000)</td>
<td>(-3050)</td>
<td>(-1260)</td>
</tr>
<tr>
<td>(C_{44})</td>
<td>(-550)</td>
<td>(-1150)</td>
<td>(-750)</td>
</tr>
<tr>
<td>(C_{14})</td>
<td>(-160)</td>
<td>(-275)</td>
<td>(-250)</td>
</tr>
<tr>
<td>(C_{44})</td>
<td>(-177)</td>
<td>(-216)</td>
<td>(-216)</td>
</tr>
<tr>
<td>(C_{an})</td>
<td>(178)</td>
<td>(118)</td>
<td>(21)</td>
</tr>
<tr>
<td>(\rho)</td>
<td>(-34.92)</td>
<td>(-15.9)</td>
<td>(5.3)</td>
</tr>
<tr>
<td>(\alpha_{11})</td>
<td>(13.7)</td>
<td>(6.5)</td>
<td>(-1.9)</td>
</tr>
<tr>
<td>(\alpha_{44})</td>
<td>(7.5)</td>
<td>(2.9)</td>
<td>(-1.5)</td>
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</table>

Figure 6 shows a plot of these values. The correlation is quite high, except for the case of \(C_{14}\) and suggests that the TCFs should be correlated also. Plots of \(TC^{(1)}\) and \(TC^{(2)}\) versus angles shown in Figure 4A through 4NN reflect this correlation.

Of course, if the two TCF surfaces do not intersect to form a line of zero \(TC^{(1)}\) and \(TC^{(2)}\), we must use a slightly different approach to finding temperature stable cuts. The largest variation in constants occurs for \(C_{11}\). As we are interested in the temperature range from \(-50^\circ C\) to \(100^\circ C\), the maximum deviation of \(T\) from \(T_n = 25^\circ C\) is \(|T - T_n| = 75^\circ C\). Calculating the changes in the constant \(C_{12}\) for this maximum temperature change gives:

\[
\left| \frac{1}{C_{12}} \right| \Delta C_{12} = 2.25 \times 10^{-1}
\]

\[
\left| \frac{1}{C_{12}} \right| \Delta C_{12} = 1.72 \times 10^{-1}
\]

\[
\left| \frac{1}{C_{12}} \right| \Delta C_{12} = 5.32 \times 10^{-4}
\]

---

Figure 6. Temperature Coefficients of the Fundamental Constants of Quartz
Thus the most significant term is the first order term. The second order term is still quite significant but one order of magnitude below the first, while the third order term is almost three orders of magnitude below the first. Since the delay time $\tau$ is dependent on the crystal constants, the most significant term should be $\text{TCF}^{11}$. The least significant term should be $\text{TCF}^{13}$. After numerous calculations of the TCFs for many orientations, this appears to be the case.

The investigative approach used has been to first locate the surfaces of zero $\text{TCF}^{11}$ (the most significant term) with the finite difference program. Near these surfaces of zero $\text{TCF}^{11}$, low values of $\text{TCF}^{13}$ are sought, using already calculated results of the finite difference programs. Where low values of $\text{TCF}^{13}$ have been found, the perturbation approach was used to more accurately locate the zero $\text{TCF}^{11}$ surface, this being the most significant term in the total temperature dependence. $\text{TCF}^{13}$'s are then calculated to assure that their effect on the total temperature dependence is small. To date, this has always been found to be the case.

(8) Results of the Investigative Approach

Table 2 consists of a summary of the results of using the investigative approach described in paragraph (7) above. There are three areas where low TCF cuts have been located. These areas are centered near (YX wlt) 0/27/138, (YX wlt) 7/27/135.5, and (YX wlt) 15/40/40. These orientations have zero $\text{TCF}^{11}$, calculated by the Sinha and Tiersten approach, with $\text{TCF}^{13}$ and $\text{TCF}^{13}$ calculated with Finite Difference approach. These areas were chosen because of zero $\text{TCF}^{11}$, low $\text{TCF}^{12}$, and a low $\text{TCF}^{13}$ which can be mostly cancelled out by the first order TCF if the propagation direction is slightly rotated away from the zero $\text{TCF}^{11}$ direction. Then the $\text{TCF}^{12}$ term will dominate the performance characteristics. The angular resolution in these areas is $1^\circ \times 1^\circ \times 1^\circ$. The cuts potentially have one half to one third the temperature coefficients of ST-Cut quartz.
## Table 2. Propagation Characteristics of Selected Orientations

<table>
<thead>
<tr>
<th>Phi</th>
<th>Theta</th>
<th>Psi</th>
<th>( \text{TCF}^{(1)}/\text{C}^2 \times 10^{-4} ) Program</th>
<th>( \text{TCF}^{(2)}/\text{C}^2 \times 10^{-4} ) Program</th>
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</thead>
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57
Piezoelectric Coupling Factor

The piezoelectric coupling factor, denoted by $k^2$, is a measure of the coupling efficiency for an interdigitated electrode.

We can express $k^2$ in terms of the interdigital transducer's input conductance as

$$G_n(\omega_n) = -\pi^2 \omega_n M^2 \varepsilon_{\infty} \varepsilon_0 G, P_{n-1}^{-2} (\cos \eta \pi) / K^2 (\cos \eta \pi/2)$$

where $\omega_n = 2\pi (2n - 1) / \lambda S_n$, $M$ is the number of electrode pairs, $w$ is the length of the electrodes, $\lambda$ is the spatial periodicity of the array, the width of each electrode is $\eta^2 / 2$, $\varepsilon_{\infty}$ is the value of the effective permittivity at zero velocity, $K$ is the complete elliptic integral of the first kind, and $P_n$ are the Legendre polynomials. $G_\eta$ is the residue of $1/(s \eta)$.

$k^2$ is defined by

$$k^2 = -2\varepsilon_{\infty} G_\eta$$

Thus (18) becomes

$$G_n(\omega_n) = (1/2) \pi^2 \omega_n M^2 \varepsilon_{\infty} \varepsilon_0 G, P_n^{-1} (\cos \eta \pi) / K^2 (\cos \eta \pi/2)$$

and we see that $k^2$ is related to the input conductance and hence to the coupling efficiency. A good approximation to $k^2$ is given by

$$k^2 \approx 2(V_n - V_\omega) / V_\omega = 2\Delta V / V$$

where $V_n$ is the shorted Rayleigh wave velocity and $V_\omega$ is the free Rayleigh wave velocity.

It is seen that the quantity $\Delta V / V$ is an important parameter as it is a direct measure of the coupling efficiency and conductance of an interdigitated electrode pair on a piezoelectric substrate. Furthermore, $\Delta V / V$ is easily determined once the shorted and free surface problems have been solved. Programs are available for calculating the Rayleigh wave velocity with either shorted or free boundary conditions.

The shorted velocity calculations assumes a massless, perfectly conducting layer on the surface of the crystal. The boundary condition which must be satisfied is that $\phi = 0$ at $x_3 = 0$. The free surface boundary conditions are such that the potential $\phi$ and the normal component of the displacement, $D$, are continuous at the surface. Furthermore, $\phi$ must satisfy Laplace's equation above the surface, resulting in

$$\phi = \phi_0 \exp(-kx_3) \exp(-ik(x_3 - Vt)), \quad (x_3 \geq 0)$$

---

In both calculations the mechanical boundary conditions are the same, that there be no force component in the \( x \), direction, or
\[
T_{11} = T_{12} = T_{13} = 0 \text{ at } x = 0
\]  
(23)

\( \Delta V/V \) for different crystal types with various orientations were calculated. Results have been found to be in good agreement with experiments.

For example, on ST-quartz,
\[
V_0 = 3.1586 \times 10^7 \text{ m/s} \\
V_0 = 3.1569 \times 10^7 \text{ m/s}
\]
(24)
\[
\Delta V/V = 5.4 \times 10^{-4}
\]
To insure the suitability of the cuts described in paragraph (8) above for SAW applications, the coupling coefficients have been calculated for these cuts and are summarized in Table 3.

### TABLE 3. PROPAGATION CHARACTERISTICS OF SELECTED ORIENTATIONS

<table>
<thead>
<tr>
<th>Angles of ZTCF(^{(1)} ), degrees (S &amp; T's program)</th>
<th>Velocity (msec)</th>
<th>( K^2 ) (x10(^{-3} ))</th>
<th>Power Flow Angle (Degrees)</th>
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TABLE 3. PROPAGATION CHARACTERISTICS OF SELECTED ORIENTATIONS (CONT)

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<th>Angles of ZTCF°, degrees</th>
<th>Velocity (msec)</th>
<th>K² (x10⁻¹)</th>
<th>Power Flow Angle (Degrees)</th>
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</tr>
<tr>
<td>16 40 39.605 3314.03 0.98 -8.4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16 41 39.825 3323.15 0.92 -9.0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

e. Power Flow Angle

The power flow angle for a particular direction of propagation is an important design parameter. While the phase fronts always remain parallel to the source transducer, the wave, as a whole, does not propagate perpendicular to the wave fronts (see Figure 7). This is a characteristic of anisotropic substrates where the phase velocity is asymmetric about the propagation direction; i.e., \( V(\psi + \Delta \psi) \neq V(\psi - \Delta \psi) \). The major problem which arises is that the acoustic beam may steer off of the desired propagation track, missing the output transducer unless it is properly designed.

The power per unit width carried in a surface wave is found by integrating the mechanical and electrical Poynting vectors to obtain

\[
P_i = -\frac{1}{2} \text{Re} \left\{ \int_\infty^0 T_i \mu_i^* dx_3 - i \omega \int_\infty^\infty \phi D_i dx_3 \right\}, \quad i = 1, 2
\]

(25)

\( P_1 \) gives the power flow perpendicular to the wave front and \( P_2 \) gives the power flow parallel to the wave front. \( P_1 = 0 \) for the Rayleigh wave which is confined to the surface. The power flow angle may be defined as

\[
\theta = \arctan(P_2/P_1) = P_2/P_1 \text{ for } P_2 \ll P_1
\]

(26)

The power flow angles are calculated using either the perturbation programs or the finite difference routine. Table 4 gives results of calculations for the ST-Cut quartz. Note that for \( \psi = 0 \), the power
flow angle is zero, within the single precision accuracy used, as a result of the crystal symmetry. Power flow angles as high as 20 degrees are not uncommon on quartz.

TABLE 4. POWER FLOW ANGLES ST-CUT

<table>
<thead>
<tr>
<th>( \psi )</th>
<th>Transverse/Incident Power</th>
<th>Power Flow Angle ( \theta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°</td>
<td>( 6.159 \times 10^6 )</td>
<td>0</td>
</tr>
<tr>
<td>10°</td>
<td>( 6.145 \times 10^6 )</td>
<td>3.5 degrees</td>
</tr>
<tr>
<td>20°</td>
<td>( 9.502 \times 10^5 )</td>
<td>5.4 degrees</td>
</tr>
</tbody>
</table>

The beam steering angle will be calculated for the selected cut of quartz with TCF = 0. The analytical results will be compared with experimental measurements. Table 3 contains the results of calculations for the selected orientations described in paragraph (8) above.

Figure 7. Nonzero Power Flow Angle

f. Proximity and Excitation Strength of Bulk Acoustic Waves (BAW) Spectrum

The purpose of this task is to analytically determine the strength of spurious signals caused by BAW. With this knowledge, one can predict the quality of the SAW device which has been selected for its zero TCD cut.

Interdigital transducers do not couple all of their field energy into surface waves. Bulk waves are also generated at various frequencies in the piezoelectric medium. These bulk waves can bounce off of the bottom surface, undergoing mode conversions in the process, and be received by the output transducer, resulting in unacceptable spurious signals. In most cases, this problem can be virtually eliminated by proper preparation of the bottom surface.

A transducer with periodicity \( \lambda \) excites surface waves at center frequencies

\[
f_{\text{SAW}} = (2n + 1)V_{\text{SAW}}/\lambda \tag{27}
\]
where \( V_{\text{sw}} \) is the surface wave velocity and \( n \) is an integer, \( n = 0, 1, 2 \ldots \). The coupling to higher harmonics depends on transducer design. Bulk waves are radiated into the medium at an angle \( \theta \) at a center fundamental frequency

\[
f_\gamma = V_b(\theta)/[\lambda \cos(\theta)]
\]

where \( V_b(\theta) \) is the velocity of the bulk wave in that particular direction. Equation 28 is a statement of the Bragg condition (see Figure 8). If the medium is isotropic for each mode, \( V_b \) is a constant. In the general case, \( V_b \) depends on the direction of propagation and hence on \( \theta \). To calculate \( V_b(\theta) \), the matrix of elastic constants are rotated through the angle \( \theta \) in the standard way. The quasi-longitudinal velocity and quasi-shear velocities are calculated as:

\[
\begin{align*}
V_{ll} &= |[C_{ll}(\theta) + e_{ii}^2(\theta)/\epsilon_{ii}(\theta)]/\rho|^{1/2} \\
V_{nl} &= |[C_{nn}(\theta) + e_{ii}^2(\theta)/\epsilon_{ii}(\theta)]/\rho|^{1/2} \\
V_{ns} &= |[C_{ns}(\theta) + e_{ii}^2(\theta)/\epsilon_{ii}(\theta)]/\rho|^{1/2}
\end{align*}
\]

Figure 8. Bragg Condition for Excitation of BAW

The inverse values of these velocities, plotted as a function of \( \theta \), form the inverse velocity curves. Inverse velocity plots as a function of propagation are particularly useful, for as long as \( V_b/\cos \theta \), the effective velocity of the bulk wave on the surface, is greater than \( V_{\text{SAW}} \), the effects of bulk mode generation may be suppressed by appropriate design and by proper conditioning of the bottom surface. Should \( V_b/\cos \theta \) be less than \( V_{\text{SAW}} \) for any bulk mode, the SAW may couple to the BAW, resulting in a

leaky surface wave. Inverse velocity plots have been made for orientations with promising SAW temperature characteristics to check for the possibility of leaky surface waves and minimum values of \( f_s \) calculated and compared with \( f_{\text{SAW}} \).

The polar plots of the inverse velocities for a (YXwlt) 0/27/137.8 and 7/27/135.59 are shown in Figure 9 and Figure 10, respectively. The values of \( 1/v_{\text{bulk}} \) for the two shear modes and one longitudinal mode for different propagation directions (\( \theta \)) into the crystal are also shown in Figures 9 and 10. The inverse surface wave velocity for 0/27/137.8 is \( 3.06 \times 10^{-3} \), that for 7/27/137.8 is \( 3.03 \times 10^{-3} \). These values are larger than the maximum \( (1/v_{\text{bulk}}) \cos \theta (\leq 2.9 \times 10^{-4}) \), therefore, the analysis indicates that a leaky mode does not exist (see Table 3 for the SAW velocities).

Figure 9. Polar Plots of Inverse Velocities for a (YXwlt) 0/27/137.8
Degeneracies

Degenerate waves occur when the physical constants are such that equations (30) and (32) decouple.

\[
\begin{bmatrix}
\Gamma_{11} - \rho V_i^2 & \Gamma_{12} & \Gamma_{13} & \Gamma_{14} \\
\Gamma_{12} & \Gamma_{22} - \rho V_i^2 & \Gamma_{23} & \Gamma_{24} \\
\Gamma_{13} & \Gamma_{23} & \Gamma_{33} - \rho V_i^2 & \Gamma_{34} \\
\Gamma_{14} & \Gamma_{24} & \Gamma_{34} & \Gamma_{44}
\end{bmatrix}
\begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3 \\
\alpha_4
\end{bmatrix}
= 0
\]  

(30)
where

\[
\begin{align*}
\Gamma_{11} &= c_{55} b^2 + 2c_{45} b + c_{11} \\
\Gamma_{22} &= c_{66} b^2 + 2c_{46} b + c_{66} \\
\Gamma_{13} &= c_{15} b^2 + 2c_{55} b + c_{15} \\
\Gamma_{12} &= c_{45} b^2 + (c_{14} + c_{16}) b + c_{16} \\
\Gamma_{13} &= c_{15} b^2 + (c_{11} + c_{15}) b + c_{15} \\
\Gamma_{23} &= c_{45} b^2 + (c_{16} + c_{45}) b + c_{46} \\
\Gamma_{44} &= -(\epsilon_{33} b^2 + 2\epsilon_{13} b + \epsilon_{11}) \\
\Gamma_{14} &= e_{35} b^2 + (e_{15} + e_{32}) b + e_{11} \\
\Gamma_{24} &= e_{36} b^2 + (e_{14} + e_{36}) b + e_{16} \\
\Gamma_{34} &= e_{33} b^2 + (e_{13} + e_{33}) b + e_{15}
\end{align*}
\]  

(31)

The boundary conditions become, in matrix form,

\[
\begin{bmatrix}
\cdots (c_{133} + c_{333} b^{(m)}) \alpha_1^{(m)} + (\theta_{133} + c_{333} b^{(m)}) \alpha_4^{(m)} \\
\cdots (c_{133} + c_{333} b^{(m)}) \alpha_1^{(m)} + (\theta_{133} + c_{333} b^{(m)}) \alpha_4^{(m)} \\
\cdots (c_{323} + c_{133} b^{(m)}) \alpha_1^{(m)} + (c_{323} + c_{333} b^{(m)}) \alpha_4^{(m)} \\
\cdots (e_{333} b^{(m)}) \alpha_1^{(m)} - (c_{133} + c_{333} b^{(m)} - i\epsilon_4) \alpha_4^{(m)}
\end{bmatrix}
\begin{bmatrix}
C_1 \\
C_2 \\
C_3 \\
C_4
\end{bmatrix} = 0
\]

(32)

The definition of the constants and derivation of the equations are given in Appendix C. The condition for decoupling requires that the matrix in equation 30 has zero elements such that independent, non-Raleigh wave solutions may exist. Equation 30 may decouple in many ways. If, for example, \(\Gamma_{12} = \Gamma_{14} = \Gamma_{34} = 0\), \(u_1\) and \(u_3\) are found to be coupled and \(u_2\) and \(\phi\) are found to be coupled, however \(u_1\) and \(u_3\) are decoupled from \(u_2\) and \(\phi\). If the physical constants are such that these two solutions are not coupled through the boundary conditions (equation 32) then we find the Rayleigh like wave \((u_1\) and \(u_3\)) is not coupled to \(\phi\), the potential term, and cannot be excited by electrodes in this cut.

The displacement \(u_2\) which is coupled to \(\phi\) is called the Bleustein—Gulyaev wave and is excited by interdigital transducers. These two waves \((u_1, u_3, u_2, \phi)\) are degenerate as they propagate with the same velocity. The simplest method to determine whether equation 30 has decoupled for a particular orientation is to calculate the matrix of equation 30. This is presently accomplished using the Rayleigh wave velocity calculation program, which calculates and prints the matrix in equation 30. Because of the variety of special cases which may arise, some of which may ultimately prove useful, each case in which we find the wave equation decouples will be considered on an individual basis.


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The analytical results of this section allow us to determine which modes can be generated on the selected zero TCD cut of quartz. At the three areas tabulated in Table 2, only Rayleigh wave modes were found.

h. Sensitivities Due to Crystal Misorientation

In cutting quartz and aligning masks on it, there is always some maximum achievable accuracy. Thus it is useful to know how all of the acoustic quantities considered vary with angle. Quantities such as TCD, phase velocity, power flow angle, $\Delta V/V$, bulk wave spectrums, and bulk wave velocity surfaces, are of interest to this program. These quantities can be accurately determined by directly calculating the quantities at $\phi = (\phi_0 + \Delta \phi)$, $\theta = (\theta_0 + \Delta \theta)$, and $\psi = (\psi_0 + \Delta \psi)$ with the same computer program discussed in paragraph 1, where $\phi_0$, $\theta_0$, and $\psi_0$ are the desired angles, $\Delta \phi$, $\Delta \theta$ and $\Delta \psi$ are the actual directional deviation from the desired direction due to the fabrication tolerance. It is important to calculate the sensitivity of the parameters to the crystal misorientation; i.e., amount of change of a function as a result of small angular misorientation.

For case of the power flow angle (PFA)

$$\frac{d[PFA (\phi = 0, \theta = 42.75, \psi = 10^\circ)]}{d\psi} = (PFA (\psi = 20^\circ) - PFA (\psi = 0^\circ))/20^\circ = 0.27^\circ/\text{degree}.$$  

The quantities $d[PFA (\phi = 0^\circ, \theta = 42.75^\circ, \psi = 10^\circ)]/d\phi$ and $d[PFA (\phi = 0^\circ, \theta = 42.75^\circ, \psi = 10^\circ)]/d\theta$ are computed in an equivalent manner.

In the case of TCD:

$$d(TCD) = \frac{\partial(TCD)}{\partial \theta} d\theta + \frac{\partial(TCD)}{\partial \phi} d\phi + \frac{\partial(TCD)}{\partial \psi} d\psi$$

$$\frac{\partial(TCD)}{\partial \theta} = \frac{[TCD(\phi_0, \theta_0, \psi_0) - TCD(\phi_0, \theta_0 + \Delta \theta, \psi_0)]}{\Delta \theta}$$

$$\frac{\partial(TCD)}{\partial \phi} = \frac{[TCD(\phi_0, \theta_0, \psi_0) - TCD(\phi_0 + \Delta \phi, \theta_0, \psi_0)]}{\Delta \phi}$$

$$\frac{\partial(TCD)}{\partial \psi} = \frac{[TCD(\phi_0, \theta_0, \psi_0) - TCD(\phi_0, \theta_0, \psi_0 + \Delta \psi)]}{\Delta \psi}$$

All the TCD $(\phi, \theta, \psi)$ and TCD $(\phi, \theta, \psi + \Delta \psi)$ etc., are calculated with the computer programs discussed in paragraph 1. Therefore, all the $\partial(TCD)/\partial \theta, \partial(TCD)/\partial \psi, \partial(TCD)/\partial \phi$ can be accurately calculated. Hence the sensitivities due to crystal misorientation are determined.

Calculation of the angular dependence on the first, second, and third order TCDs is, of course, our primary task. Of these three quantities, the first order TCF is most sensitive to angular variation. The
angular dependence on these parameters will be calculated in the same way as all of the other quantities but on a much smaller angular grid $(\Delta \theta, \Delta \phi$ and $\Delta \psi$) about the zero TCD locus. The size of this grid will vary, depending on the magnitude and smoothness of the variation about each point on the locus of zero first order TCD orientations as verified by experiment and calculation. In case the function is smooth or linearly varying with angles, large $\Delta$ angles may be used.

By performing the above mentioned calculations, we have precise information on the sensitivities due to crystal misorientation. This information will allow us to impose a practical tolerance limit on fabrication and still be able to achieve the required superior performance specification.

Quantities such as velocity (Table 3), power flow angles (Table 3), BAW spectrum (Figures 50 and 51), coupling coefficients (Table 3), and second and third order TCFs (Table 2) do not vary quickly with angle. This is not the case for $\text{TCF}^{iii}$. Table 5 contains a summary of $\text{aTCF}^{iii}/\partial \psi$. The large values of $\text{aTCF}^{iii}/\partial \psi$ impose strict fabrication tolerances on the SAW cuts and mask alignment. Fabrication accuracy to within 6 minutes is required to keep the total temperature variation due to $\text{TCF}^{iii}$ within 45 ppm for $\text{aTCF}^{iii}/\partial \psi = 3(\text{PPM/}^\circ\text{C})/\text{degree}$ over the temperature range $-50^\circ\text{C}$ to $100^\circ\text{C}$. Table 6 contains summaries of $\text{aTCF}^{iv}/\partial \phi$ and $\text{aTCF}^{iv}/\partial \theta$. These values impose fabrication tolerances on the rotated quartz plate angles $\phi$ and $\theta$ of 12 minutes to keep the total temperature variation due to $\text{aTCF}^{iv}(15/40/40)/\partial \phi$ within 45 ppm over the temperature range $-50^\circ\text{C}$ to $100^\circ\text{C}$. This linear temperature variation may be compensated for by varying $\psi$ on any particular cut if all other cut parameters vary slowly with angle.

**TABLE 5. $\text{aTCF}^{iii}/\partial \psi$ FOR SELECTED CUTS**

<table>
<thead>
<tr>
<th>Phi</th>
<th>Theta</th>
<th>Psi</th>
<th>$\text{aTCF}^{iii}/\partial \psi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>26</td>
<td>136.31</td>
<td>+2.7 (ppm/°C)/degree</td>
</tr>
<tr>
<td>6</td>
<td>27</td>
<td>135.93</td>
<td>+2.7</td>
</tr>
<tr>
<td>6</td>
<td>28</td>
<td>135.59</td>
<td>+2.7</td>
</tr>
<tr>
<td>7</td>
<td>26</td>
<td>135.99</td>
<td>+2.7</td>
</tr>
<tr>
<td>7</td>
<td>27</td>
<td>135.64</td>
<td>+2.7</td>
</tr>
<tr>
<td>7</td>
<td>28</td>
<td>135.27</td>
<td>+2.7</td>
</tr>
<tr>
<td>8</td>
<td>26</td>
<td>135.74</td>
<td>+2.7</td>
</tr>
<tr>
<td>8</td>
<td>27</td>
<td>135.36</td>
<td>+2.7</td>
</tr>
<tr>
<td>8</td>
<td>28</td>
<td>134.97</td>
<td>+2.7</td>
</tr>
<tr>
<td>1</td>
<td>26</td>
<td>137.78</td>
<td>+2.8</td>
</tr>
</tbody>
</table>
TABLE 5. $\alpha_{\text{TCF}^{(1)}}/\alpha_1$ FOR SELECTED CUTS (CONT)

<table>
<thead>
<tr>
<th>Angles of ZTCF$^{(1)}$, degrees</th>
<th>$\alpha_{\text{TCF}^{(1)}}/\alpha_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(S &amp; T's program)</td>
<td></td>
</tr>
<tr>
<td>Phi</td>
<td>Theta</td>
</tr>
<tr>
<td>-----</td>
<td>--------</td>
</tr>
<tr>
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<td>28</td>
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<td>27</td>
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<td>28</td>
</tr>
<tr>
<td>-1</td>
<td>26</td>
</tr>
<tr>
<td>-1</td>
<td>27</td>
</tr>
<tr>
<td>-1</td>
<td>28</td>
</tr>
<tr>
<td>14</td>
<td>39</td>
</tr>
<tr>
<td>14</td>
<td>40</td>
</tr>
<tr>
<td>14</td>
<td>41</td>
</tr>
<tr>
<td>15</td>
<td>39</td>
</tr>
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<td>15</td>
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<tr>
<td>16</td>
<td>40</td>
</tr>
<tr>
<td>16</td>
<td>41</td>
</tr>
</tbody>
</table>

TABLE 6. $\alpha_{\text{TCF}^{(1)}}/\alpha_1$ AND $\alpha_{\text{TCF}^{(1)}}/\alpha_2$ FOR SELECTED CUTS

<table>
<thead>
<tr>
<th>Angles of ZTCF$^{(1)}$ (S&amp;T's Program), Degrees</th>
<th>$\alpha_{\text{TCF}^{(1)}}/\alpha_1$</th>
<th>$\alpha_{\text{TCF}^{(1)}}/\alpha_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phi</td>
<td>Theta</td>
<td>Psi</td>
</tr>
<tr>
<td>-----</td>
<td>--------</td>
<td>------</td>
</tr>
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<td>27</td>
<td>135.64</td>
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<td>137.78</td>
</tr>
<tr>
<td>15</td>
<td>40</td>
<td>40.00</td>
</tr>
</tbody>
</table>

2. WAFER FABRICATION

During the developmental phase of the doubly rotated cut SAW Devices program, a large number of wafers with 30 different crystal orientations will be fabricated and evaluated. To perform this task with good quality control, minimum cost and in a short time, Motorola has developed the techniques and processes to fabricate the doubly rotated cut of quartz wafers internally. The crystal boules are supplied by Motorola.
Carlisle, Pennsylvania; the X-ray wafer cutting is performed at Motorola's Semiconductor Group; polishing, fabrication and testing are performed at the Motorola Government Electronics Division. The methods used to fabricate the quartz wafers are described in the following sections.

A computer program was developed to calculate the incident angles and reflected angles for any given cut of crystal. The basic mathematical relations were derived in R.A. Heising's "Quartz Crystals for Electrical Circuits." The relations were formulated to computer programs. The flow diagram is shown in Figure 11. The results are shown in the printout (see Appendix F). The incident angle $G$, exit angle $(G + G')$, are defined for each plate position. The plate positions are determined by the direction of the rotated axis. $(\pm 1, \pm 2, \pm 3)$, relative to the measuring stage. Once the angles of $(YX$ wlt) $\phi/\theta/\psi$ are defined, all of the reflection angles will be calculated for the different reflection planes, defined by Miller indicies. The useful reflection planes that provide intense reflection with low skewed angles ($<5$ degrees) are selected for printout. These results, after modification due to change in standards, are used to check the accuracy of the cuts.

a. Face Definitions

The following is an outline of the procedure to be used in this program to make a doubly rotated cut $(YX$ wlt) $\phi/\theta/0$. The quartz bars have four lumbered faces with the minus X axis marked. The opposite face is marked by coloring it with a magic marker (blue). One other face not opposite the -X face is colored also with a magic marker (red). The red face is now defined to be the +Z axis as in Figure 12. The direction of the +Y axis may be found by using the right-hand rule (+X crossed into +Y gives +Z). The +Y axis will lie along the length of the crystal. Note that there are two ways to set up the axes on the crystal corresponding to choice of the red face (see Figure 12).

b. Running the X-Ray Program

The X-ray orientation program XRAY is run with the angles $\phi/\theta/0$. The sequence of instructions on the Honeywell 560 under the CP-V operating system is as follows:

\[\text{SET F:103 DC/MILDAT .538; IN}\]

(This instruction assigns to unit 103 the file containing all of the Miller indicies to be searched.)

\[\text{SET F:104 DC/ERRDAT .538;IN}\]

(This instruction assigns to unit 104 the file containing all of the angle perturbations defined in Heising for use with the Laue photographs.)

\[\text{XRAYL M.538}\]

(This instruction loads and begins execution of the program.)

The program will ask for the angles $\phi/\theta/0$. These angles are entered in 3G format [i.e., 10.0, 3.0, 0.0 (carriage return)] and the results of the X-ray analysis printed.

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Figure 11. Flow Diagram of Calculation for Reflected Angles in Doubly Rotated Cut of Quartz
c. Analysis of X-Ray Program

The X-ray program used follows the development of Heising's which uses a book written before the 1949 IRE Standard we use now. His X, Y, and Z axes will be denoted as $\bar{X}$, $\bar{Y}$, and $\bar{Z}$. The relation to our standard is as follows:

<table>
<thead>
<tr>
<th>Heising</th>
<th>1949 IRE Standard</th>
</tr>
</thead>
<tbody>
<tr>
<td>$+\bar{X}$</td>
<td>$-X$</td>
</tr>
<tr>
<td>$+\bar{Y}$</td>
<td>$-Y$</td>
</tr>
<tr>
<td>$+\bar{Z}$</td>
<td>$+Z$</td>
</tr>
</tbody>
</table>

Furthermore, Heising's incident beam comes from the left, while our incident beam comes from the right. When these differences are accounted for, the "position chart" shown in Figure 13 must be used instead of the charts Heising uses in order that our X-ray machine and the 1949 standard may be used. $P_1$, $P_2$, and $P_3$ in the "position chart" are the $+X$, $+Y$, and $+Z$ axes of the rotated plate. An important note of caution: the $\phi$ crystal face off of which we reflect the X-ray beam has $\bar{Y}$ or $-Y$ as its normal. Since we may not assume that the crystal faces are parallel, we must propagate the surface wave on this face. This is important, because to achieve the same crystal properties, we must rotate by $\phi$ about the $+Y$ axis, resulting in a change of the sign of the third rotation (see Figure 14).
$P_1$, $P_2$, and $P_3$ are the rotated plate axes $X$, $Y$, and $Z$.

Figure 13. X-ray Position Chart
d. Determination of the Actual $\psi$ Angle

The third angle of rotation must be measured from a reference. The reference used is the face opposite the red face of the crystal (−Z face). To determine the actual orientation of the finished crystal edge, we must know the orientation of this plane exactly (see Figure 15).

---

**Figure 14.** Direction of Mask Alignment Angle Rotation $\psi$

**Figure 15.** Crystal Rotation (YX wlt) $\phi/\theta/0$
If the angles $\alpha$ and $\beta$ in Figure 16 are measured using the (003) plane, which is parallel to the X and Y axes, $\Delta \psi$ is given by:

$$\Delta \psi = -\tan^{-1}\left(\frac{\cos \phi \sin \alpha - \sin \phi \sin \beta}{\sin \phi \sin \alpha - \sin \phi \cos \phi \cos \beta + \cos \phi \sqrt{1 - \sin^2 \alpha - \sin^2 \beta}}\right)$$

(36)

Thus, given a $\psi$ desired which we wish to obtain, we must actually rotate the mask by $\psi_{\text{actual}} = \psi_{\text{des}} - \Delta \psi$ as shown in Figure 17.

**e. Determination of $\alpha$ and $\beta$**

The most appropriate crystal plane to use for determining $\alpha$ and $\beta$ is the 003 plane. This plane has all of its atoms lying in planes perpendicular to the Z axis, and for a perfect Z face the X-ray deflection angles will be:

- $G = \text{Angle of incidence} = 25 \text{ degrees } 19 \text{ minutes}$
- $G + G' = \text{Exit angle} = 50 \text{ degrees } 38 \text{ minutes}$

For all positions on the X-ray machine with the +Z or −Z face being X-rayed. To determine $\alpha$ and $\beta$ for the −Z face, we use the following relationships.

$$\alpha = \frac{1}{2} (G_{X \text{ toward incident}} - G_{X \text{ toward incident}})$$

(37)

$$\beta = \frac{1}{2} (G_{Y \text{ toward incident}} - G_{Y \text{ toward incident}})$$

(38)
To determine $\alpha$ and $\beta$ for the $+Z$ face we use:

$$\alpha' = \frac{1}{2} (G_{\text{X to Incident}} - G_{\text{X to Incident}})$$  \hspace{1cm} (39)\]

$$\beta' = \frac{1}{2} (G_{\text{Y to Incident}} - G_{\text{Y to Incident}})$$  \hspace{1cm} (40)\]

$\alpha'$ and $\beta'$ are the $\alpha$ and $\beta$ we would have measured for a $-Z$ face that is parallel to the $+Z$ face measured. This means that equation (36) is still valid for $\alpha'$ and $\beta'$.

The quartz crystal will now have the orientation (YX wrt) $\phi/\theta_1 - \Delta\phi(\alpha, \beta)$ if we use the $-Z$ edge as a reference and (YX wrt) $\phi/\theta_1 - \Delta\phi(\alpha', \beta')$ if we use the $+Z$ edge as a reference. The computer X-ray program for these angular orientations must be used if we are to get an accurate measurement. The integrity of these measurements of $\alpha$ and $\beta$ is checked by comparing $1/2 (G_{\text{X}} + G_{\text{X}})$ and $1/2 (G_{\text{Y}} + G_{\text{Y}})$ with the theoretical result, $G_{\text{AVG}} = 25$ degrees 19 minutes.

**f. Procedure Used to Zero X-Ray Machine:**

1. Use reference quartz plate marked 10.1
(2) Set X-ray exit angle to 26.5 degrees (marked AT cut on machine).

(3) Set plate in X-ray machine with marking toward you (X-ray bounces off unmarked surface) and blue line up (width direction vertical). (See Figure 18).

(4) Adjust with clutch till X-ray reading occurs at incident angle 13 degrees 18 minutes.

(5) Set plate in X-ray machine with marking toward you (X-ray bounces off unmarked surface) and blue line down (width direction vertical). (See Figure 19).

(6) Angle of incidence should occur at 13 degrees 18 minutes + $\Delta$ angle.

(7) Adjust clutch until angle of incidence is at 13 degrees 18 minutes + $1/2 \Delta$ angle.

(8) Check alignment by measuring in positions of steps 3 and 5. The average of the two readings should be 13 degrees 18 minutes. Any discrepancy represents error in zeroing the machine and may be made less than less than 1 minute.

(9) If the 10.1 cut is not available, the same procedure may be used if, for the cut to be used, the theoretical angles of incidence are equal for the particular crystal plane used in both positions.

---

Figure 18. Position of Step 3, 10.1 Alignment Wafer

Figure 19. Position of Step 5, 10.1 Alignment Wafer Rotated by 180 Degrees About $-Y$ Axis
g. Cutting Techniques for Doubly Rotated Orientations

A slicing machine built by Meyer and Burger Company, model TS3, was used to slice the quartz boule. The 6 inch diamond impregnated blade is supplied by Maurice Dessau, New York. The drift accuracy of the 2 inch cut is approximately 3 mils (~5 minutes).

The stage of the saw has the capability to rotate in two dimensions; it is designed to make the doubly rotated cut. The adjustment accuracies are graded to 0.5 minute. The X-ray beam resolution is about 2 minutes.

The combined accuracy of the wafers obtained experimentally has been better than 15 minutes. Iterative adjustment of the cutting stage can bring the cutting accuracy to within 10 minutes. The cutting procedures are the following:

1. Heat brass plate, glass plate and quartz boule.
2. Melt wax on brass plate and mount glass plate.
3. Melt wax on glass and mount quartz boule on glass.
4. Let cool to room temperature.
5. Screw mount brass plate to slice machine.
6. Initial cut of boule along the XZ plane (or directly to the desired angle if the boule was lumbered).
7. Determine true atomic plane using diffractometer and X-ray computer program.
8. Adjust stage to correct for true atomic planes, and obtain the desired rotation.
10. Measure the reflection angle and check against the calculated result of the X-ray program. Iterative adjustment of stage can be done if cut accuracy is critical.

These procedures are presently used to cut the wafers with low TCF orientation required for this program.

h. Wafer Polishing

The polishing process for the quartz wafers was established during this period. The procedure includes the following:

1. The crystal axis orientation is marked on the back surface of the wafers with marking ink and baked dry. The markings have been demonstrated to stay on the crystal throughout the photolithographic process for easy identification.
(2) The corners of the wafers are ground prior to lapping and polishing to prevent corner breakage.

(3) The polishing is a two step process. The first step is a 15 μm lapping to obtain surface flatness with Microgrit, type WCA, Size 15, on a LAPMASTER, Model 24. The second step is to polish the surface with Cerium oxide on a Logitech, Ltd. Model PM2 polisher. The polish wheel is made of pitch wax supplied by Hacker Instruments, Inc. The polished wafers have a surface finish with no observable grains or pits under a 50X microscope. The wafers are suitable for surface wave application. X-ray orientation was performed before and after the lapping and polishing processes. The change is normally less than 6 minutes.

At the present time, wafers of the following cuts are polished; these are φ/θ/ψ of 6/27/135.9, 6/28/135.6, 7/27/135.6, 7/28/135.3, 8/26/135.7, 8/27/135.4, and 8/28/134.9.

In the coming period, SAW devices will be fabricated on these wafers. Experimental results will be obtained and compared with the theoretical calculations.
The temperature coefficients of frequency (TCF) have been analyzed for doubly rotated cuts of quartz for surface acoustic wave devices. The analysis procedure is shown below:

1. Using Finite Difference program, identify angular areas with zero TCF₁ and low TCF₂ on 10° x 10° x 10° grid.

2. Calculate in these areas with 2.5° x 2.5° x 2.5° grid to locate the rotation with minimum TCF₂ which has TCF₁ = 0.

3. Identify the accurate zero TCF₁ with Sinha and Tiersten's program in areas obtained in (2).

4. Calculate TCF₁, TCF₂ and TCF₃ in selected areas obtained in (3) with 1° x 1° x 1° span.

5. Calculate the coupling coefficients, propagation velocities, power flow angles and inverse bulk wave velocities for these angles.

The conclusions of the initial study are:

(a) The zero TCF₁ surface and zero TCF₂ surface data does not show an intersection in the 10° x 10° x 10° grid. However, orientations with frequency variation ≈ 100 ppm from -50°C to 100°C, better than ST Cut by a factor of two, have been found in several areas where TCF₁ = 0 and TCF₂ is less than 1.5 x 10⁻⁴/°C².

(b) The ∆TCF/∆ angle is normally very large in the areas with zero TCF₁ and low TCF₂, therefore accurate crystal orientation is critical. It is estimated that the orientation accuracy of 6 minutes is required to obtain a TCF₁ of ≈ 50 ppm in the -50°C to 100°C temperature range in the three areas investigated. These are φ/θ/ω of 6/27/135.93 (4.45 x 10⁻² ppm/°C·minute), 14/40/40.415 (5.83 x 10⁻² ppm/°C·minute) and 0/27/137.78 (5.00 x 10⁻² ppm/°C·minute). Orientations with less sensitivity to orientation accuracy have been evaluated. These are the cuts that have ∂[TCF₁]/∂ψ = 0 when TCF₁ = 0. The cuts evaluated were φ/θ/ω = 20/30/155, 20/20/150, 10/40/168. The TCF₂ of these cuts are approximately 4 x 10⁻⁴/°C, comparable or higher than ST cut.

(c) Coupling coefficients, velocities and beam steering angles were defined for the selected areas, no leaky modes were found in these areas.

(d) Methods to X-ray orient the quartz crystals, cut the doubly rotated wafers and polish such crystal wafers were developed. The wafers are ready for SAW device fabrication. The effort in the coming period is to design and fabricate single mode oscillators and to experimentally measure the TCF's of these selected orientations.
APPENDIX A

VOLUME PERTURBATION OF AULD

Perturbation techniques, as used here, allow calculations of small changes in the solutions to a problem caused by small changes in the physical parameters of the problem, once the solution to the unperturbed problem is known.

Our general approach to the problem of determining the temperature dependence of \( V \), will be as follows. First, the Rayleigh wave propagation problem will be solved in the standard way in its entirety at room temperature, \( T_0 \). Given the solution of problem at \( T_0 \) and the dependence of the physical constants (such as \( c_0 \)) on temperature at \( T_0 \), we will apply the volume perturbation formula, calculating the temperature dependence of \( V \). The dependence of \( V \) on \( T \) is then used to calculate the frequency characteristics of the actual device given the thermal expansion coefficients as a function of temperature. At this point, the frequency temperature dependence of the substrate as a function of crystal cut and direction can be thoroughly explored.

The Volume Perturbed Formula.

Denoting \( u_0 (T_0) \) by \( u_0 \), etc., the volume perturbation formula is given by:

\[
\beta_k = \omega \int_0^\infty \frac{[A]}{(1/4) P} \left( \int_0^\infty \left( -u^* \cdot T^* - u^* \cdot T^* \right) \right)
+ \phi^* (i \omega D^*) + \psi (i \omega D^*) \cdot z \, dy
\]

\[
A = [\Delta p u^* \cdot u^* + T^*] \cdot \left( \psi S^* \cdot T^* + \Delta d \cdot E' \right)
+ E^* \cdot (\Delta^e \cdot E + \Delta d \cdot T)]
\]

This equation is exact, but involves knowing the solution \( u' \). However, we can set \( u = u' \) if the temperature dependence of the solution is small and use \( P = (1/2) \) Re \( \int_0^\infty (-u^* \cdot T + E \cdot H^*) \) dy to obtain the approximate solution

\[
\Delta \beta_k = (\omega/4P) \int_0^\infty \left[ \Delta p | u |^2 + S: \Delta c : S \right]
+ E^* \cdot \Delta^e \cdot E + E^* \cdot \Delta e : S + S : \Delta e \cdot E \right) \, dy
\]

The \( u \)'s and \( E \)'s, and \( p \) come directly from the computer solution at \( T_0 \).

\footnote{Auld, B.A., "Acoustic Fields and Waves in Solids," Vol. II.}
The $\Delta$ terms can be written as expansions of the form:

$$\Delta \beta = \beta_T (T) (\alpha_{\beta}^{(1)} dT + \alpha_{\beta}^{(2)} dT^2 + \alpha_{\beta}^{(3)} dT^3)$$  \hspace{0.5cm} (A-3)

$$\Delta \rho = \rho_T (T) (\alpha_{\rho}^{(1)} dT + \alpha_{\rho}^{(2)} dT^2 + \alpha_{\rho}^{(3)} dT^3) = \rho^{(1)} dT + \rho^{(2)} dT^2 + \rho^{(3)} dT^3$$  \hspace{0.5cm} (A-4)

$$\Delta \varepsilon = \varepsilon_T (T) (\alpha_{\varepsilon}^{(1)} dT + \alpha_{\varepsilon}^{(2)} dT^2 + \alpha_{\varepsilon}^{(3)} dT^3, \text{etc.})$$  \hspace{0.5cm} (A-5)

To obtain

$$\Delta \beta = \beta_T (T) \left( \alpha_{\beta}^{(1)} dT + \beta_T (T) \alpha_{\beta}^{(2)} dT^2 + \beta_T (T) \alpha_{\beta}^{(3)} dT^3 \right)$$

$$= (\omega dT/4P) \int_0^\alpha (\rho_T (T) \alpha_{\rho}^{(1)} | u |^2 + S : c^{(1)} : S + E^* \cdot \epsilon^{(1)} \cdot E$$

$$+ E^* \cdot \epsilon^{(1)} \cdot S + S : c^{(1)} : S + E^* \cdot (E - E_0) j dy)$$  \hspace{0.5cm} (A-6)

$$+ (\omega dT^2/4P) \int_0^\alpha (\rho_T (T) \alpha_{\rho}^{(2)} | u |^2 + S : c^{(2)} : S + ...) dy$$

$$+ (\omega dT^3/4P) \int_0^\alpha (\rho_T (T) \alpha_{\rho}^{(3)} | u |^2 + S : c^{(3)} : S + ...) dy$$

Or

$$\alpha_{\beta}^{(3)} = (\omega/4P \beta_T (T)) \int_0^\alpha (\rho_T (T) \alpha_{\rho}^{(3)} | u |^2 + S : c^{(3)} : S + ...) dy$$  \hspace{0.5cm} (A-7)

For the problem of quartz, the electrostatic coupling is small and the electric terms can be ignored. Thus $\Delta d$ and $\Delta \varepsilon$ in (A-8) may be set to zero resulting in the simplified equation.

$$\alpha_{\beta}^{(3)} = (\omega/4P \beta_T (T)) \int_0^\alpha (\rho_T (T) \alpha_{\rho}^{(3)} | u |^2 + S : c^{(3)} : S + ...) dy$$  \hspace{0.5cm} (A-8)

The integrals are calculable, for instance, from (14).

$$\int_0^\alpha \rho_T (T) \alpha_{\rho}^{(3)} | u |^2 dy$$

$$= \rho(T) \alpha_{\rho}^{(3)} \sum_{m,n} \int_0^\alpha \sum_{m,n} C_{mn} \alpha_{\rho}^{(m)} \exp(-i \beta_n b^{(m)} y) \left[ \sum_{n'} \sum_{m'} C_{n'n'} \alpha_{\rho}^{(m')} \exp(i \beta_n b^{(m')} y) \right] dy$$  \hspace{0.5cm} (A-9)
The problem can easily be extended to multi-layered media by simply performing the integral over each layer separately. For the double layer (A-9) becomes:

\[
\int_{a}^{\alpha} \rho_{1} (T_{a}) a_{p_{1}}^{(1)} | u | ^{2} dy + \int_{a}^{\infty} \rho_{2} (T_{a}) a_{p_{2}}^{(2)} | u | ^{2} dy + \ldots
\] (A-11)

Because the dependence of \( u_{i} \) is given explicitly by (13), it is not necessary to use numerical integration procedures, as demonstrated in (A-10).

Once the \( \alpha_{\mu_{i}}^{(i)} \) have been calculated from (A-9) the \( \alpha_{\nu_{i}}^{(i)} \) are simply determined. Using \( \beta = \omega / V_{c} \) and (A-9) we determine \( \alpha_{\nu_{i}}^{(i)} \).
APPENDIX B

VOLUME PERTURBATION FORMULA OF SINHA AND TIERSTEN

The approach used by Sinha and Tiersten includes the effects of distortion caused by heating a substrate of quartz and is based in the coordinate system to which the fundamental elastic constants refer. In this reference system, the density is constant and the $\alpha_{ii}$ are equivalent to the $\alpha_{ii}^\prime$.

In this new reference system, the perturbation formula becomes

$$\frac{\Delta v_i}{v_i} = \left(1/2\beta_k^\prime v_i^3\right) \left(H/N^2\right).$$  \hspace{1cm} (B-1)

$$N^2 = \left(p^\prime \pi/\beta_k^\prime\right) \sum_{m=1}^{n-1} \sum_{n=1}^{m-1} \left(c^{\prime mn} \alpha^{m}\alpha^{n}\right)/\left(\beta_m - \beta_n\right).$$  \hspace{1cm} (B-2)

$$H = -\int_{0}^{\infty} dy \int_{-\pi/\beta_k}^{\pi/\beta_k} \frac{dz}{\beta_k} \left(K_{ie} u_{iie} + K_{ie} u_{iie} + K_{ie} u_{ie} + K_{ie} u_{ie} + K_{ie} u_{ie} + K_{ie} u_{ie}\right).$$  \hspace{1cm} (B-3)

$$K_{L,Y} = \left(c_{L,Y,\alpha} + \Delta c_{L,Y,\alpha}\right) u_{\alpha, \alpha}.$$  \hspace{1cm} (B-4)

For the first order perturbation in $T$ we have:

$$c_{L,Y,\alpha} = \left(c_{L,Y,\alpha} + c_{L,Y,\alpha} + c_{L,Y,\alpha} + c_{L,Y,\alpha} + c_{L,Y,\alpha} + c_{L,Y,\alpha}\right) dT.$$  \hspace{1cm} (B-5)

$$\Delta c_{L,Y,\alpha} = \left(d c_{L,Y,\alpha}/dT\right) dT.$$  \hspace{1cm} (B-6)

Where $c_{L,Y,\alpha}$ are the second order elastic constants previously denoted simply as $c_{L,Y,\alpha}$ and $c_{L,Y,\alpha}$ are the third order elastic constants. The terms $\Delta c_{L,Y,\alpha}$ as calculated by Tiersten is available only to first order in $T$, and the higher order elastic constants $c_{L,Y,\alpha}$ have never been determined.


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APPENDIX C

THE DIFFERENTIATION METHOD

A method for determining the theoretical temperature dependence of Rayleigh Surface Waves consists of formally differentiating the wave equation and boundary conditions. The boundary conditions and wave equation must be true at all temperatures, placing restraints on how the parameters of the wave equation may vary. In this technique, the derivatives of these equations with respect to temperature are set to zero and solved for the velocity temperature dependence. This method follows the methods used by Bechmann, Ballato, and Lukaszek to compute the temperature dependence of the fundamental elastic constants from frequency data, except that the simplifying assumptions of assuming bulk wave solutions cannot be made. This method was later used by Hauden to search for temperature stable cuts of quartz.

Christoffel's wave equation can be written in matrix form as

\[
\begin{bmatrix}
\Gamma_{11} - \rho V_i^2 & \Gamma_{12} & \Gamma_{13} & \Gamma_{14} \\
\Gamma_{12} & \Gamma_{22} - \rho V_i^2 & \Gamma_{23} & \Gamma_{24} \\
\Gamma_{13} & \Gamma_{23} & \Gamma_{33} - \rho V_i^2 & \Gamma_{34} \\
\Gamma_{14} & \Gamma_{24} & \Gamma_{34} & \Gamma_{44}
\end{bmatrix}
\begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3 \\
\alpha_4
\end{bmatrix}
= 0
\]

(C-1)

where

\[
\begin{align*}
\Gamma_{11} &= c_{55} b^2 + 2c_{15} b + c_{11} \\
\Gamma_{12} &= c_{45} b^2 + 2c_{46} b + c_{46} \\
\Gamma_{13} &= c_{35} b^2 + 2c_{33} b + c_{35} \\
\Gamma_{14} &= c_{34} b^2 + (c_{34} + c_{45}) b + c_{34} \\
\Gamma_{22} &= c_{44} b^2 + 2c_{46} b + c_{46} \\
\Gamma_{23} &= c_{33} b^2 + 2c_{35} b + c_{33} \\
\Gamma_{24} &= c_{34} b^2 + (c_{34} + c_{45}) b + c_{34} \\
\Gamma_{33} &= c_{55} b^2 + 2c_{15} b + c_{11} \\
\Gamma_{34} &= c_{34} b^2 + (c_{34} + c_{45}) b + c_{34} \\
\Gamma_{44} &= c_{44} b^2 + 2c_{46} b + c_{46}
\end{align*}
\]

(C-2)


following the notation used in the previous section and in Matthews'\textsuperscript{1}. This equation holds for each of the four modes, hereafter designated by a superscript $m$.

The boundary conditions become, in matrix form,

\[
\begin{bmatrix}
  (c_{11} + c_{333} b'^{m}) \alpha_{1}^{(m)} + (\theta_{11} + \theta_{333} b'^{m}) \alpha_{2}^{(m)} \\
  (c_{11} + c_{333} b'^{m}) \alpha_{1}^{(m)} + (\theta_{11} + \theta_{333} b'^{m}) \alpha_{2}^{(m)} \\
  (c_{11} + c_{333} b'^{m}) \alpha_{1}^{(m)} + (\theta_{11} + \theta_{333} b'^{m}) \alpha_{2}^{(m)} \\
  (e_{33} + e_{333} b'^{m}) \alpha_{3}^{(m)} + (\theta_{33} + \theta_{333} b'^{m}) \alpha_{4}^{(m)}
\end{bmatrix} = 0
\]  

where only the $m$'th column is shown and the $C_i$'s are the amplitudes of each mode. This formulation assumes a normalization of the $a$'s

\[
(a_{1}^{(m)})^2 + (a_{2}^{(m)})^2 + (a_{3}^{(m)})^2 + (a_{4}^{(m)})^2 = 1.
\]  

The first condition we can place on the wave equation is that the determinant of Christoffel's equation vanishes for all temperature, or

\[
\begin{vmatrix}
  \Gamma_{11} - \rho \nu_x^2 & \Gamma_{12} & \Gamma_{13} & \Gamma_{14} \\
  \Gamma_{12} & \Gamma_{22} - \rho \nu_y^2 & \Gamma_{23} & \Gamma_{24} \\
  \Gamma_{13} & \Gamma_{23} & \Gamma_{33} - \rho \nu_z^2 & \Gamma_{34} \\
  \Gamma_{14} & \Gamma_{24} & \Gamma_{34} & \Gamma_{44}
\end{vmatrix} = 0
\]  

For each of the four modes, this equation is valid, resulting in four equations in five unknowns, $dV/dT$, and $db'^{m}/dT$ of the form $F_i^{(m)} (dV_i/dT, db'^{m}/dT) = 0$, $m = 1, 2, 3, 4$.

For each mode, Christoffel's matrix equation (C-1) must vanish, yielding the set of equations

\[
(d/dT) (a_{1}^{(m)} (\Gamma_{11}^{(m)} - \rho \nu_x^2) + \alpha_{2}^{(m)} \Gamma_{12}^{(m)} + \alpha_{3}^{(m)} \Gamma_{13}^{(m)} + \alpha_{4}^{(m)} \Gamma_{14}^{(m)}) = 0
\]

\[
(d/dT) (a_{1}^{(m)} \Gamma_{12}^{(m)} + a_{2}^{(m)} (\Gamma_{22}^{(m)} - \rho \nu_y^2) + a_{3}^{(m)} \Gamma_{23}^{(m)} + a_{4}^{(m)} \Gamma_{24}^{(m)}) = 0
\]

\[
(d/dT) (a_{1}^{(m)} \Gamma_{13}^{(m)} + a_{2}^{(m)} \Gamma_{23}^{(m)} + a_{3}^{(m)} (\Gamma_{33}^{(m)} - \rho \nu_z^2) + a_{4}^{(m)} \Gamma_{34}^{(m)}) = 0
\]

\[
(d/dT) (a_{1}^{(m)} \Gamma_{14}^{(m)} + a_{2}^{(m)} \Gamma_{24}^{(m)} + a_{3}^{(m)} \Gamma_{34}^{(m)} + a_{4}^{(m)} \Gamma_{44}^{(m)}) = 0.
\]  

This results in 16 equations (four per mode) and an additional 16 unknowns (the $a_{i}^{(m)}$s) of the form

\[F_i^{(m)} (dV_i/dT, db'^{m}/dT, d a_{1}^{(m)}/dT, d a_{2}^{(m)}/dT, d a_{3}^{(m)}/dT, d a_{4}^{(m)}/dT) = 0\]

Using (C-3) we obtain the single equation

\[
\left(\frac{d}{dt}\right) \begin{vmatrix}
\cdots \cdots (C_{334} + C_{331}b^{(m)}) \alpha_1^{(m+1)} + (e_{133} + e_{133}b^{(m)}) \alpha_4^{(m)} \\
\cdots \cdots (C_{331} + C_{331}b^{(m)}) \alpha_1^{(m+1)} + (e_{133} + e_{133}b^{(m)}) \alpha_4^{(m)}
\end{vmatrix} = 0
\]

(C-7)

of the form \( F_{1(m)} (\frac{d}{dT}, \frac{d}{dT}, \frac{d}{dT}, \frac{d}{dT}) = 0 \)

and four equations of the form

\[
\left(\frac{d}{dT}\right) \sum_m C_m \left[ (C_{331} + C_{331}b^{(m)}) \alpha_1^{(m)} + (e_{133} + e_{133}b^{(m)}) \alpha_4^{(m)} \right] = 0
\]

(C-8)

\[
\left(\frac{d}{dT}\right) \sum_m C_m \left[ (C_{331} + C_{331}b^{(m)}) \alpha_1^{(m)} + (e_{133} + e_{133}b^{(m)}) \alpha_4^{(m)} \right] = 0
\]

(C-9)

From (5) \( \alpha_1^{(m)} (\frac{d}{d\alpha_1^{(m)}}) + \alpha_2^{(m)} (\frac{d}{d\alpha_2^{(m)}}) + \alpha_3^{(m)} (\frac{d}{d\alpha_3^{(m)}}) + \alpha_4^{(m)} (\frac{d}{d\alpha_4^{(m)}}) = 0 \)

(C-10)

or

\( F_{1(m)} (\frac{d}{dT}) = 0 \)

(C-11)

Combining the above results gives 25 equations in the 25 unknowns.

\( \frac{dV}{dT}, \frac{d}{dV}, \frac{d}{dV}, \frac{d}{dV}, \frac{d}{dV} \)

which are solved simultaneously. Once the temperature dependence of the Rayleigh wave velocity is found, the frequency dependence is found in the usual way.

To obtain the second order dependence of \( V \), the 25 equations are differentiated again. The values of \( \frac{dV}{dT}, \frac{d}{dV}, \frac{d}{dV}, \frac{d}{dV} \) and \( \frac{d}{dV} \) previously obtained are used to obtain \( \frac{d^2V}{dT^2} \), etc.
APPENDIX D

SOLUTION METHOD

Calculating the velocity of a Rayleigh wave requires a complete solution of the problem to be performed. All of the constants in equation (13) must be evaluated. The standard used at Motorola as developed by Campbell and Jones is outlined below.

First the fundamental constants are rotated into the coordinate system of interest.

Next a value of \( V \) is picked. The coefficients \( r_n \) of equation (C-2) are evaluated and the determinant of the matrix in equation (C-1) is set to zero, as it must be if a solution of (C-1) is to be found. This results in an eighth order equation in \( b \). This equation is solved for the eight complex roots. The four roots \( b^{m_1} \) in the lower complex plane are retained, the four discarded roots not satisfying the boundary conditions at infinity. Equation (C-1) is then solved for the four eigenvectors \( \alpha_i^{(m)} \). The \( b_i^{(m)} \) and the corresponding eigenvector \( \alpha_i^{(m)} \) are substituted into equation (C-3) and the determinant of the matrix in equation (C-3) is evaluated. This determinant must be zero for a solution to (C-3) exist. If it is not zero, \( V \) is varied, and the whole procedure repeated, until it is. Once a value of \( V \) is found such that the determinant in equation (C-3) vanishes, the solution to (C-3) is found, giving the values for \( C_m \). These constants completely describe the solution of equation (13), as well as providing the exact velocity.
In the following section, the relations relating the first, second, and third order temperature coefficients of delay and frequency will be derived. These relations show implicitly the equivalence of each representation of the device temperature characteristics, and justify their interchangeable usage.

In the text, we have used the following notation:

\[ \tau = \text{delay time of delay line oscillator} \]  
\[ \alpha_{T} = \text{ith order temperature coefficient of delay} = \frac{T_{N} - T}{\tau_{N}} \]  
\[ F = \text{frequency of delay line oscillator} \]  
\[ \alpha_{F} = \text{ith order temperature coefficient of frequency} \]  
\[ \tau = \tau_{0} \left( 1 + \alpha_{T}^{(1)} (T - T_{0}) + \alpha_{T}^{(2)} (T - T_{0})^{2} + \alpha_{T}^{(3)} (T - T_{0})^{3} + \ldots \right) \]  
\[ F = F_{0} \left( 1 + \alpha_{F}^{(1)} (T - T_{0}) + \alpha_{F}^{(2)} (T - T_{0})^{2} + \alpha_{F}^{(3)} (T - T_{0})^{3} + \ldots \right) \]

where \( T \) is temperature and \( T_{0} \) is a reference temperature, 25°C in our case. For a SAW oscillator, \( F_{0} = \text{constant or} \) 
\[ \frac{\tau}{\tau_{0}} = \frac{F}{F_{0}} \]
\[ = \frac{1}{1 + \alpha_{T}^{(1)} (T - T_{0}) + \alpha_{T}^{(2)} (T - T_{0})^{2} + \alpha_{T}^{(3)} (T - T_{0})^{3} + \ldots} \]  
\[ \frac{1}{1 + X} \approx 1 - X + X^{2} - X^{3} \text{ for } X \ll 1 \]  
\[ 1/(1 + X) \approx 1 - X + X^{2} - X^{3} \text{ for } X \ll 1 \]

Using the relation

\[ 1/(1 + X) \approx 1 - X + X^{2} - X^{3} \text{ for } X \ll 1 \]  
we can write

\[ \frac{\tau}{\tau_{0}} = 1 - \left[ \alpha_{T}^{(1)} (T - T_{0}) + \alpha_{T}^{(2)} (T - T_{0})^{2} + \alpha_{T}^{(3)} (T - T_{0})^{3} \right] \]
\[ + \left[ \left( \alpha_{F}^{(1)} (T - T_{0})^{2} + 2 \alpha_{F}^{(1)} (T - T_{0}) \alpha_{F}^{(2)} (T - T_{0})^{2} \right) \right] \]
\[ - \left[ \alpha_{F}^{(1)} (T - T_{0}) \right]^{3} + \text{higher order terms} \]
\[ = 1 - \alpha_{T}^{(1)} (T - T_{0}) + \left( \alpha_{T}^{(2)} + (\alpha_{T}^{(1)})^{2} \right) (T - T_{0})^{2} + \left( \alpha_{T}^{(3)} + 2 \alpha_{T}^{(1)} \alpha_{T}^{(2)} - (\alpha_{T}^{(1)})^{3} \right) (T - T_{0})^{3} \]  
\[ 1/(1 + X) \approx 1 - X + X^{2} - X^{3} \text{ for } X \ll 1 \]
Equating powers of $T - T_0$ in (E-5) and (E-10), we obtain

$$\alpha_T^{(1)} = \alpha_T^{(1)}$$  \hspace{1cm} (E-11)

$$\alpha_T^{(2)} = \alpha_T^{(2)} + (\alpha_T^{(1)})^2$$  \hspace{1cm} (E-12)

$$\alpha_T^{(3)} = -\alpha_T^{(1)} + 2\alpha_T^{(1)}\alpha_T^{(2)} - (\alpha_T^{(1)})^3$$  \hspace{1cm} (E-13)

As the only assumption on $F$ and $\tau$ used is that of equation (E-7) which is symmetric in $F$ and $\tau$, we immediately obtain

$$\alpha_T^{(1)} = -\alpha_T^{(1)}$$  \hspace{1cm} (E-14)

$$\alpha_T^{(2)} = -\alpha_T^{(2)} + (\alpha_T^{(1)})^2$$  \hspace{1cm} (E-15)

$$\alpha_T^{(3)} = -2\alpha_T^{(2)} - (\alpha_T^{(1)})^3$$  \hspace{1cm} (E-16)

Using (E-11) through (E-16), we can always relate one set of temperature coefficients to the other.
APPENDIX F

X-RAY RUN

The following is an example of the computer results from the FORTRAN X-ray orientation computer program for the doubly rotated cut 7/27/0. File MILDAT contains only the two Miller indices shown on the printout on this run.
16105 APR 10, 80 ID#00847
JOB 536, WILLIAMS (35533.000); FILE=XRAYJOB, ID#63, LINE=22
LIMT (TIME.2), (CD.30), (UD.30)
ASSIGN F109, (FILE, MILDAT).{IN}
ASSIGN F108, (FILE, ERRDAT).{IN}
RUN (LMN, XRAYHL)
INPUT THE THREE ANGLES PHI, THETA, PSI

********* ANGLES ARE (YXMT) 000000 ( 0 MIN), 27,0000 ( 0 MIN), 000000 ( 0 MIN)

************ MILLER INDICES: 0 = 1 1
NORMAL VECTOR = .955336E+01 = .975490 ,197133
THETA = 13.3213

PLATE IN POSITION 1 ( -1 AXIS VERTICAL, 2 AXIS NORMAL)
G = ANGLE OF INCIDENCE 20.0068 ( 80 MIN)
BETA1 = 5,52901 ( 32 MIN)
G PLUS G PRIME=EXIT ANGLE 25,330 ( 32 MIN)
INTENSITY FACTOR1,009521E+01 INTENSITY1,0000000

PLATE IN POSITION 3 ( 1 AXIS VERTICAL, 2 AXIS NORMAL)
G = ANGLE OF INCIDENCE 14,5238 ( 90 MIN)
BETA1 = 2,522001 ( 32 MIN)
G PLUS G PRIME=EXIT ANGLE 25,5310 ( 32 MIN)
INTENSITY FACTOR1,02424% INTENSITY1,000000

************ MILLER INDICES: 0 = 2 1
NORMAL VECTOR = .113399 = .989196 = .029136E+01
THETA = 22.8905

PLATE IN POSITION 2 ( 3 AXIS VERTICAL, 2 AXIS NORMAL)
G = ANGLE OF INCIDENCE 29.9443 ( 33 MIN)
BETA1 = 14,4637 ( 9 MIN)
G PLUS G PRIME=EXIT ANGLE 45.6526 ( 39 MIN)
INTENSITY FACTOR1,362103 INTENSITY1,000000

PLATE IN POSITION 4 ( 3 AXIS VERTICAL, 2 AXIS NORMAL)
G = ANGLE OF INCIDENCE 16.4690 ( 20 MIN)
BETA1 = 4,14557 ( 9 MIN)
G PLUS G PRIME=EXIT ANGLE 45.6526 ( 39 MIN)
INTENSITY FACTOR1,620445 INTENSITY1,000000
LAUE ANGLES DEFINED SUCH THAT ALPHA = ANGLE FROM BEAM,
BETA = ROTATION CLOCKWISE FROM P1; DIST TO CRYSTAL = 10,000
MILLER INDICES: 0 = 1 1 LAUE SPOT ANGLES: ALPHA = 25,3180 RETA = 30.0427 X = 2.00704 Y = 1.255
MILLER INDICES: 0 = 2 1 LAUE SPOT ANGLES: ALPHA = 16,8680 RETA = 30.3295 X = 2.34222 Y = 1.92075

LAUE ANGLES DEFINED SUCH THAT ALPHA = ANGLE FROM BEAM,
BETA = ROTATION CLOCKWISE FROM P1.
FOR ROTATIONS E(1) = 0.000000 E(2) = 0.000000 E(3) = 0.000000 ACTUAL ANGLES ARE
(THELT)0.000000 (60 MIN,)/27.0000 (60 MIN,)/0.000000 ( 0 MIN,)

FOR ROTATIONS E(1) = 0.000000 E(2) = 0.000000 E(3) = 0.000000 ACTUAL ANGLES ARE
(THELT)0.000000 (60 MIN,)/27.5011 (60 MIN,)/11.7251 ( 7 MIN,)

*STOP* NORMAL
DATA INFORMATION IGNORED
APPENDIX G

X-RAY PROGRAM

The following is the FORTRAN computer program used to calculate X-ray diffraction angles for a
doubly rotated cut of quartz.
SUBROUTINE CLEAR
COMMON/CLEAN/N
COMMON /ANGLE/A1,A2,A3
N=0
WRITE(10,10)
10 FORMAT(" INPUT THE THREE ANGLES PHI,THETA,PSI")
READ(10,30)A1,A2,A3
WRITE(30)
30 FORMAT(3G16.8)
WRITE(10,20)A1,HI(A1),A2,HI(A2),A3,HI(A3)
20 FORMAT(1X,85=,ANGLES AND"
40 FORMAT(1X,4" (X/Y/Z)"/8E10.4 "(+/-" HI,+"/"0,"(,+","
31 FORMAT(1X," ** HI="/8E10.4)
30 RETURN
50 RETURN
90 CONTINUE
" LAUE ANGLES DEFINED SUCH THAT ALPHA = ANGLE FROM BEAN, W/.
" MTA = ROTATION CLOCKWISE FROM P1, W")

FORM W, MILLER INDICES, 3(T, K, 0), " LAUE SPOT ANGLES; ALPHA; W
" MTA, W. X, W, Y, W, Z.

RETURN

SUBMIT THE GOMION

INTEGER M

COMMON /INTFR/PP

COMMON /HILLER/HH,

COMMON /NORM/RH,THE

LOGICAL NO1,NO2,NO3,NO4

DIMENSION RN(3)

DATA PHI/3,1415026658/4,5,6/0

IF(A8(RN(3)).LT.0,9)RETURN

IF(L.GT.0)GOTO 12

IF(L.EQ.0)RETURN

IF(K.GT.0)GOTO 12

IF(K.EQ.0).AND.(H.GT.0)GOTO 12

RETURN

CONTINUE

NO1,T,TRUE.

NO2,TTRUE.

CALL SCFUN(THE, TTS, TTC)

T=2.*TT&BRA(N(1))

T=P,A,BRA(N(3))

IF(A8(T(1)).GT.1,0)NO1,FALSE.

IF(A8(T(2)).GT.1,0)NO2,FALSE.

IF(NO1)RET1B0=ABIN(11)/PHI

IF(NO2)RET2B0=ABIN(12)/PHI

IF(A8(BET1),GT,BETMAX)NO1,FALSE.

IF(A8(BET2),GT,BETMAX)NO2,FALSE.

IF(NOT,NO1,NO2)RETURN

THETA=A,BRA(N(3))/PHI

DELTP=180,ATAN(RN(1))/PHI

THETA=180,ATAN(RN(1))/PHI

THETA=180,ABIN(RN(1))/PHI

CALL SCFUN(THE, TTS, TTC)

CALL SCFUN(T, TTS, TTC)

CALL SCFUN(T, TTS, TTC)

CALL SCFUN(T, TTS, TTC)

CALL SCFUN(T, TTS, TTC)
171 154,400 T=TS/TC
172 154,400 IF(MS1.T).GT.1.0)NOZ=.FALSE.
173 154,400 IF(ND2).THETAP.EQ.0..AND.(T/PHI)
174 154,400 GIVTHETAP=DELP1
175 154,400 G2=GTHETAP*DELP2
176 154,400 G3=GTHETAP*DELT1
177 154,400 G4=GTHETAP*DELP2
178 154,400 CALL SCFUN(2,T,THETAS,TC)
179 154,400 CALL SCFUN(2,T,THETAS,TC)
180 154,400 IF(MS1.GT.TC).GT.1.0)NOZ=.FALSE.
181 154,400 IF(ND1).GPP1.EQ.0..AND.(A0B/TC)/PHI
182 154,400 CALL SCFUN(2,T,THETAS,TC)
183 154,400 IF(MS1.GT.TC).GT.1.0)NOZ=.FALSE.
184 154,400 IF(ND2).GPP21B=.A0B/TC)/PHI
185 154,400 IF(.NOT..NOT).AND..NOT,.NOT)RETURN
186 154,400 NL3=NOZ
187 154,110 NORM=NOZ
188 154,120 IF(G1.LT.0..OR. GPP1.LT.G1)NO1=.FALSE.
189 154,130 IF(G2.LT.0..OR. GPP2.LT.G2)NOZ=.FALSE.
190 154,140 IF(G3.LT.0..OR. GPP3.LT.G3)NOZ=.FALSE.
191 154,150 IF(G4.LT.0..OR. GPP4.LT.G4)NOZ=.FALSE.
192 154,160 CALL SCFUN(2,T,THETAS,TC)
193 154,170 CALL SCFUN(2,T,THETAS,TC)
194 154,180 FACT1=TS/(TS+GB)
195 154,190 FACT2=TS/(TS+GB)
196 154,200 FACT3=TS/(TS+GB)
197 154,210 CALL SCFUN(2,T,THETAS,TC)
198 154,220 CALL SCFUN(2,T,THETAS,TC)
199 154,230 CALL SCFUN(2,T,THETAS,TC)
200 154,240 FACT4=TS/(TS+GB)
201 154,250 CALL SCFUN(2,T,THETAS,TC)
202 154,260 CALL SCFUN(2,T,THETAS,TC)
203 154,270 FACT5=TS/(TS+GB)
204 154,280 IF(FACT1.LT.0..OR. FACT1.GT.1.0)NO1=.FALSE.
205 154,290 IF(FACT2.LT.0..OR. FACT2.GT.1.0)NOZ=.FALSE.
206 154,300 IF(FACT3.LT.0..OR. FACT3.GT.1.0)NOZ=.FALSE.
207 154,310 IF(FACT4.LT.0..OR. FACT4.GT.1.0)NOZ=.FALSE.
208 154,320 IF(FACT5.LT.0..OR. FACT5.GT.1.0)NOZ=.FALSE.
209 154,330 IF(.NOT..NOT).AND..NOT,.NOT,.NOT,.NOT,.NOT)RETURN
210 154,340 WRITE((16,.10))
211 154,350 10 ** FORMATS */" MULLER INDICES:*/S13/**
212 154,360 WRITE((16,.20))((1),..1),THETA
213 154,370 WRITE((16,.20))((1),..1),THETA
214 154,380 FORMAT(3G9.4,3G9.4,3G9.4,3G9.4)/* THETA*/
215 154,390 3G9.4,3G9.4,3G9.4,3G9.4)/* THETA*/
216 154,400 IF(.NOT..NOT).AND..NOT,.NOT,.NOT,.NOT,.NOT)RETURN
217 154,410 10 ** FORMATS */" PLATE IN POSITION */S11*/S"
214 = 190.000 + 12, * AXIS VERTICAL, 2 AXIS NORMAL, * /
216 - 184.000 'B' = B, G, = ('*12, * MIN.', * /',
218 - 144.000 'INTENSITY FACTOR, G, * INTENSITY', *G, *
219 + 190.000 IF(N01) WRITE(100,100)4=1
220 + 191.000 IF(N01) WRITE(100,110)G1,MI(G1),BET1,MI(BE11),GPP1,MI(GPP1),FACT1
221 + 191.500 'REPLACEFACT1
222 + 192.000 IF(N02) WRITE(100,100)2=3
223 + 193.000 IF(N02) WRITE(100,110)G2,MI(G2),BET2,MI(BET2),GPP2,MI(GPP2),FACT2
224 + 193.500 'REPLACEFACT2
225 + 194.000 IF(N03) WRITE(100,100)3=1
226 + 195.000 IF(N03) WRITE(100,110)G3,MI(G3),=RET1,MI(=BET1),GPP1,MI(GPP1),
227 + 195.500 'FACTS,REPLACEFACTS
228 + 196.000 IF(N04) WRITE(100,100)4=3
229 + 197.000 IF(N04) WRITE(100,110)G4,MI(G4),=RET2,MI(=BET2),GPP2,MI(GPP2),
230 + 197.500 'FACTS,REPLACEFACTS
231 + 198.000 RETURN
232 + 199.000 END
233 + 199.100 INTEGER FUNCTION MI(X)
234 + 199.200 REAL X,X1
235 + 199.250 X=ABS(X)
236 + 199.300 MI=INT(0.06*(X1=INT(X1))+.5)
237 + 199.400 RETURN
238 + 199.500 END
239 + 200.000 SUBROUTINE ERROR
240 + 200.000 COMMON /SRR/EA
241 + 200.000 COMMON /WR/K
242 + 200.000 DIMENSION EA(3),R(3,3),EB(3)
243 + 200.000 DATA PHI,3,1.19526546/
244 + 201.000 0 TO 10 TH1.3
245 + 210.000 CALL SCFUB(EA(1),EB(1),T)
246 + 210.000 TM=1,ER/1,R(3,1)+EB(3)*R(2,1)
247 + 210.000 T1(1,1)=EB(1)*R(3,1)+EB(3)*R(1,1)
248 + 214.000 AS490
249 + 214.000 IF(T.NE.0,3A3:180,6ATAN(T1/T1)/PHI
250 + 215.000 T=2,3:EB(1)*R(3,3)+EB(3)*R(1,3)
251 + 220.000 2A2*10,4Sin(T1/T1)/PHI
252 + 220.000 T1(3,3)=EB(2)*R(3,3)+EB(1)*R(2,3)
253 + 221.000 1=R(3,3)+EB(3)*R(3,3)+EB(3)*R(3,3)
254 + 221.000 AS490
255 + 221.000 IF(T.NE.0,3A3:180,6ATAN(T1/T1)/PHI
256 + 221.000 WRITE(100,201)T1:EA(3),I1,3):AI,MI(A1),A2,MI(A2),A3,MI(A3)
247 = 216,000 20 FORMAT(*) FOR ROTATIONS **3(**E(*,I1,*)) = **G,**
248 = 219,000 ** Actual angles are **/
249 = 219,500 ** (XVHLT)*,**G,** (**I2,** MIN**)/,**G,** (**I2,** MIN**)/,**G,** (**I2,**
250 = 219,900 ** MIN**)/,**G,**)
251 = 220,000 RETURN
252 = 221,000 END
253 = 222,000 SUBROUTINE SCF(U,DEG,C)
254 = 223,000 C 314 AND COS OF ANGLE IN DEGREES, EXACT AND AT 9,180,270,360
255 = 224,000 C
256 = 225,000 C
257 = 226,000 C
258 = 227,000 X = DEG
259 = 228,000 IF(X .LT. 0.) X = X +360.
260 = 229,000 IF(X .EQ. 0., .OR. X .EQ. 180.) GO TO 150
261 = 230,000 IF(X .EQ. 90., .OR. X .EQ. 270.) GO TO 200
262 = 231,000 MAN = X/9.857,295779
263 = 232,000 C = SIN(RAD)
264 = 233,000 C = COS(RAD)
265 = 234,000 100 RETURN
266 = 235,000 150 C =1.
267 = 236,000 360.
268 = 237,000 IF(X .EQ. 180.) C =1.
269 = 238,000 GO TO 100
270 = 239,000 200 C =1.
271 = 240,000 C =0.
272 = 241,000 IF(X .EQ. 270.) C =1.
273 = 242,000 GO TO 100
274 = 243,000 END
275 = 244,000
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