Proc. 34th Ann. Freq. Control Symposium, USAERADCOM, Ft. Monmouth, NJ 07703, May 1980

NUMERICAL ANALYSIS OF DOUBLY ROTATED* CUT SAW DEVICES

D.F. Williams and F.Y. Cho
Motorola Government Electronics Division

ABSTRACT

Results of a numerical study of the properties of surface acoustic waves (SAW) on doubly rotated cuts of alpha quartz are presented. First and second order TCF's have been calculated on a 10° x 10° x 10° grid spanning the range of angles (XY wlt) 0 to 30°/-90° to 90°/0 to 180°. The Finite Difference method was employed. SAW velocities were calculated at -50° C, 25° C, and 100° C. The corresponding frequencies were determined and curve fitted. Angular maps created from the data base by these calculations were used to identify zero first and second order TCF surfaces. Families of cuts with zero first order TCF and small second order TCF's have been identified and further explored on smaller angular grids (as small as 1.0° x 1.0° x 1.0°).

The results of Sinha and Tiersten's approach are correlated with the finite difference method and used to find cuts with zero first order TCF.

Families of cuts on alpha quartz with SAW temperature stability superior to that found on ST cut Quartz are identified. Coupling coefficients, power flow angles, phase-temperature plots and other parameters are given for selected cuts.

INTRODUCTION

Quartz is one of the most commonly used substrates 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 temperature stable SAW devices fabricated on quartz use the ST cut[1]. This cut 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 parameters 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 determined for a given cut.

The objective of this paper is to locate crystal cuts which exhibit lower SAW temperature coefficients of delay than the ST cut. The method used to characterize and calculate the temperature dependence of a crystal orientation is discussed. Use is made of computer models to investigate the temperature dependence of different cuts of crystal for SAW devices. Calculated and measured results are presented and compared. Finally, plans for future experimental work are outlined.

CALCULATION OF TEMPERATURE COEFFICIENTS

Defining τ 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 τ is constant in temperature. It has been shown that determining the temperature dependence of τ (time delay) is equivalent to determining the temperature dependence of F frequency via the relation $F \propto 1/\tau$.[2]

The most straightforward method for calculating the frequency-temperature characteristics of a SAW device is the Finite Difference method[3, 4]. The Rayleigh wave velocities are calculated for different temperatures, yielding the values $V_s(T_i)$, i=1,2,......, n. This is done by first calculating the fundamental constants at the temperature T_i of interest. These constants[4] are then rotated into the coordinate system of interest. An iterative procedure[3] is used to calculate a velocity V_s for which Christoffel's equation and the boundary conditions are satisfied simultaneously. Linear regression is used to calculate the temperature dependence of a Rayleigh wave and requires a complete solution of the problem to be performed at several temperatures.

Sinha and Tiersten[5] have provided a computer program to calculate the first order TCD using a perturbation approach. The constants used in this program were derived from the original experimental data of Bechmann, Ballato, and Lukaszek[6], and properly includes coordinate axis skewing. A comparison of results using the Finite Difference method and the first order temperature derivatives calculated by Sinha and Tiersten's program shows the later method to be more accurate[5], and angular orientations of the zero $TCF^{(1)}$ surfaces calculated by the two programs differ by as much as 3 degrees on off axis cuts. Although the program does not calculate the second and third order TCD's, it verifies and refines results for the first order TCD. Both computer programs were used extensively in this study.

ANALYTICAL APPROACH

IRE standard angle definitions (YX wlt) PHI/THETA/PSI for quartz were used throughout the investigation.[7] Using the Finite Difference approach with the available crystal constants, the calculated results show that the zero $TCF^{(1)}$ surfaces do not intersect with the zero $TCF^{(2)}$ surfaces, based on the interpolated results of the 10° x 10° x 10° resolution. It is not likely that a finer resolution will provide contrary information because $TCF^{(1)}$ and $TCF^{(2)}$ are relatively slow varying functions. A list of the crystal elastic constants and their temperature derivatives on which these calculations are based are given in reference 6. Calculations were performed on a 10° x 10° x 10° grid over the angular ranges $0 \leq$ PHI $\leq 30°$, $0 \leq$ PSI $\leq 180°$, and $-90° \leq$ THETA $\leq 90°$. These initial calculations defined the "angular volumes" of low TCF orientations. Calculations were then performed on a 2.5° x 2.5° x 2.5° 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 were generated.[8] Despite the number and density of points at which the first and second order TCF's were calculated, wherever $TCF^{(1)}$ was found to be less than or equal to zero, we found $TCF^{(2)}$ to be less than 0.

The investigative approach used has been to first locate the surfaces of zero $TCF^{(1)}$ (the most significant term) with the Finite Difference program. Near these surfaces of zero $TCF^{(1)}$, low values of $TCF^{(2)}$ are sought, using already calculated results of the Finite Difference programs. Where low values of $TCF^{(2)}$ have been found, the perturbation approach was used to more accurately locate the zero $TCF^{(1)}$ surface, this being the most significant term in the total temperature dependence. $TCF^{(3)}$'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.

*Work supported by U.S. Army Electronics Command, Fort Monmouth, N.J., under contract DAAK 20-79-C-0275

RESULTS OF THE INVESTIGATIVE APPROACH

Table 1 consists of a summary of the results of using the investigative approach described above. Out of the many areas with low TCF cuts, some of which have been identified in this program and some previously identified.[1,2,4,8,9,10] There are three where especially 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 $TCF^{(1)}$, calculated by Sinha and Tiersten approach, with $TCF^{(2)}$ and $TCF^{(3)}$ calculated using the Finite Difference approach. These areas are chosen because of zero $TCF^{(1)}$ and low $TCF^{(2)}$. $TCF^{(3)}$ can be mostly cancelled out by $TCF^{(1)}$ if the propagation direction is slightly rotated away from the zero $TCF^{(1)}$ direction, so that the $TCF^{(2)}$ term will dominate the performance characteristics. The angular resolution in these areas is 1° x 1° x 1°. The cuts potentially have one half to one third the temperature coefficients of ST-Cut quartz.

Table 1. Propagation Characteristics of Selected Orientations

ANGLES OF $ZTCF^{(1)}$ DEGREES (S AND T'S PROGRAM)			$TCF^{(2)}/°C^2$ ($\times 10^{-8}$) FINITE DIFFERENCE PROGRAM	$TCF^{(3)}/°C^3$ ($\times 10^{-10}$) FINITE DIFFERENCE PROGRAM
PHI	THETA	PSI		
6	26	136.31	-1.4	
6	27	135.93	-1.3	0.67
6	28	135.59	-1.3	0.57
7	26	135.99	-1.5	
7	27	135.64	-1.4	
7	28	135.27	-1.3	0.65
8	26	135.74	-1.4	0.65
8	27	135.36	-1.4	
8	28	134.97	-1.3	
1	26	137.78	-1.2	0.68
1	27	137.48	-1.2	0.65
1	28	137.17	-1.1	0.67
0	26	138.07	-1.2	0.67
0	27	137.78	-1.1	0.68
0	28	137.49	-1.1	0.62
-1	26	138.37	-1.2	0.60
-1	27	138.09	-1.2	0.62
-1	28	137.80	-1.1	0.73
14	39	40.195	-1.0	0.64
14	40	40.415	-1.0	0.66
14	41	40.64	-1.0	0.75
15	39	39.79	-1.0	0.63
15	40	40	-1.0	0.74
15	41	40.23	-1.0	0.73
16	39	39.4	-1.0	0.68
16	40	39.605	-1.0	0.66
16	41	39.825	-1.1	0.60

To insure the suitability of the cuts described above for SAW applications, the coupling coefficients, SAW velocity, and powerflow angles have been calculated for these cuts and are summarized in Table 2. 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_b were calculated and compared with f_{SAW}. The polar plots of the inverse velocities for a (YX wlt) 0/27/137.8 and 7/27/135.59 are shown in Figure 1 and Figure 2, respectively. The inverse surface wave velocity for 0/27/137.8 is 3.06 x 10^{-4}, that for 7/27/137.8 is 3.03 x 10^{-4}. These values are larger than the maximum $(1/v_{bulk}) \cos \theta$ ($< 2.9 \times 10^{-4}$), therefore, the analysis indicates that a leaky mode does not exist (see Table 2 for the SAW velocities).

Table 2. Propagation Characteristics of Selected Orientations

ANGLES OF $ZTCF^{(1)}$, DEGREES (S AND T'S PROGRAM)			VELOCITY (MSEC)	K^2 ($\times 10^{-3}$)	POWER FLOW ANGLE (DEGREES)
PHI	THETA	PSI			
6	26	136.31	3296.84	1.12	-0.3
6	27	135.93	3293.60	1.12	-0.2
6	28	135.59	3290.63	1.12	-0.1
7	26	135.99	3303.33	1.12	-0.5
7	27	135.64	3299.70	1.12	-0.4
7	28	135.27	3296.33	1.12	-0.3
8	26	135.74	3310.15	1.12	-0.7
8	27	135.36	3306.11	1.12	-0.6
8	28	134.97	3302.32	1.10	-0.5
1	26	137.78	3268.80	1.10	+0.7
1	27	137.48	3267.44	1.10	+0.9
1	28	137.17	3266.36	1.10	+1.0
0	26	138.07	3264.09	1.12	+0.9
0	27	137.78	3263.09	1.10	+1.1
0	28	137.49	3262.35	1.10	+1.2
-1	26	138.37	3259.65	1.10	+1.1
-1	27	138.09	3259.01	1.10	-1.3
-1	28	137.80	3258.64	1.08	+1.5
14	39	40.195	3298.60	0.96	-7.7
14	40	40.415	3306.67	0.96	-8.1
14	41	40.64	3315.19	0.94	-8.6
15	39	39.79	3301.82	0.96	-7.8
15	40	40.00	3310.14	0.94	-8.3
15	41	40.23	3319.09	0.98	-8.6
16	39	39.4	3305.38	0.96	-8.0
16	40	39.605	3314.03	0.98	-8.4

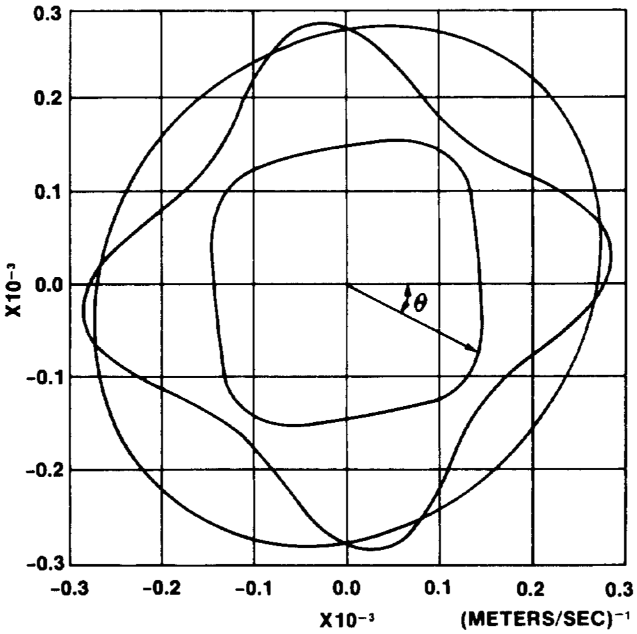

Figure 1. Polar Plots of Inverse Velocities for a (YXwlt) 0/27/137.8

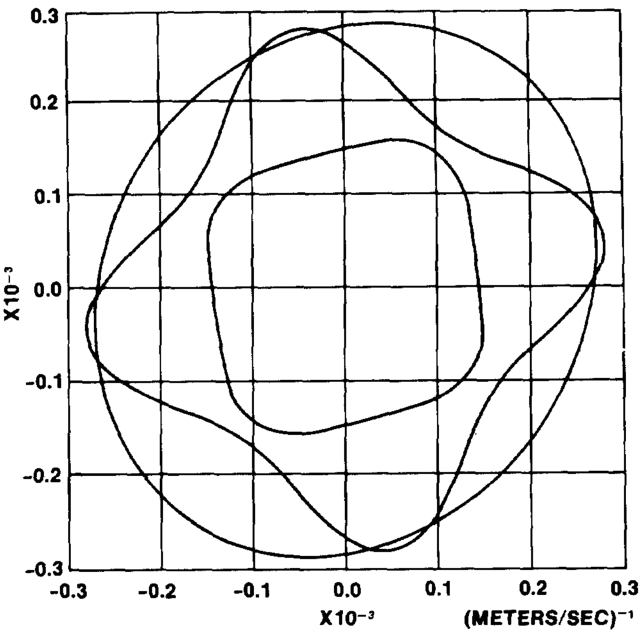

Figure 2. Polar Plots of Inverse Velocities for a (YXwlt) 7/27/135.59

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, Δ V/V, 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 earlier.

Calculation of the angular dependence on the first, second, and third order TCD's is, of course, our primary task. Of these three quantities, the first order TCF is most sensitive to angular variation. Quantities such as velocity (Table 2), power flow angles (Table 2), BAW velocities (Figures 1 and 2), coupling coefficients (Table 3), and second and third order TCF's (Table 1) do not vary quickly with angle. This is not the case for $TCF^{(1)}$. Table 3 contains a summary of $\partial\, TCF^{(1)}/\partial\psi$. The large values of $\partial\, TCF^{(1)}/\partial\psi$ 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 $TCF^{(1)}$ within 45 ppm for $\partial TCF^{(1)}/\partial\psi = 3$(PPM/° C)/degree over the temperature range -50° C to 100° C. Table 4 contains summaries of $\partial\, TCF^{(1)}/\partial\phi$ and $\partial\, TCF^{(1)}/\partial\theta$. These values impose fabrication tolerances on the rotated quartz plate angles ϕ and θ of 12 minutes to keep the total temperature variation due to $\partial\, TCF^{(1)}(15/40/40)/\partial\phi$ within 45 ppm over the temperature range -50° C to 100° C. This linear temperature variation may be compensated for by varying ψ on any particular cut if all other cut parameters vary slowly with angle.

Table 3. $\partial\, TCF^{(1)}/\partial\psi$ for Selected Cuts

ANGLES OF ZTCF$^{(1)}$, DEGREES (S AND T'S PROGRAM)			$\partial TCF^{(1)}/\partial\psi$
PHI	THETA	PSI	
6	26	136.31	+2.7 (PPM/C°)/DEGREE
6	27	135.93	+2.7
6	28	135.59	+2.7
7	26	135.99	+2.7
7	27	135.64	+2.7
7	28	135.27	+2.7
8	26	135.74	+2.7
8	27	135.36	+2.7
8	28	134.97	+2.7
1	26	137.78	+2.8
1	27	137.48	+2.8
1	28	137.17	+2.8
0	26	138.07	+3.0
0	27	137.78	+3.0
0	28	137.49	+3.0
-1	26	138.37	+3.0
-1	27	138.09	+3.0
-1	28	137.80	+3.0
14	39	40.195	-3.5
14	40	40.415	-3.5
14	41	40.64	-3.5
15	39	39.79	-3.5
15	40	40	-3.5
15	41	40.23	-3.5
16	39	39.4	-3.7
16	40	39.605	-3.7
16	41	39.825	-3.7

Table 4. $\partial\, TCF^{(1)}/\partial\phi$ and $\partial\, TCF^{(1)}/\partial\theta$ for Selected Cuts

ANGLES OF ZTCF$^{(1)}$ (S AND T'S PROGRAM), DEGREE			$\partial TCF^{(1)}/\partial\phi$	$\partial TCF^{(1)}/\partial\theta$
PHI	THETA	PSI		
7	27	135.64	-0.7(PPM/C°)/DEGREE	-0.5(PPM/C°)/DEGREE
0	27	137.78	-0.8	-0.8
15	40	40.00	+1.5	-0.7

EXPERIMENTAL VERIFICATION

Wafers with the orientation listed in Table 1 are being fabricated. Considerable care has been taken to reduce fabrication tolerances of the devices fabricated for this study. For these cuts, ϕ and θ are known to be within ±4 minutes. ψ is known to be within ±15 minutes. Two wafers with orientation (YX wlt) 8.05°/25.9°/135.7° and (YX wlt) 6.57°/26.88°/134.9° as well as a commercially supplied ST-cut wafer have been tested. A delay line oscillator was used to measure the temperature dependence of the SAW delay time. The experimental apparatus is shown in Figure 3. No coils were used to match the devices in order to eliminate inductance changes in the matching circuit over the temperature range tested. The complete experimental error is estimated to be within ±10 ppm.

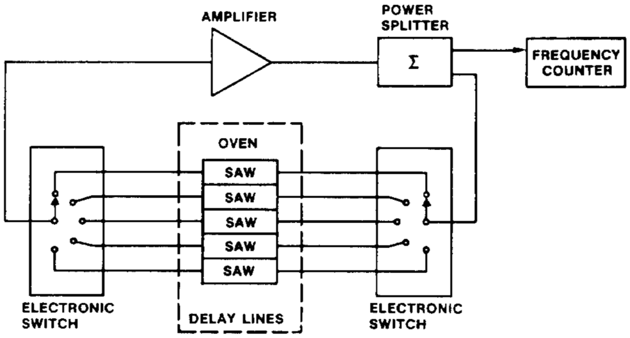

Figure 3. Measurement System

The frequency-temperature behavior of the device fabricated on the commercially supplied ST-cut wafer (YX wlt) 0/42.75/0 (angular tolerance is not known) is shown in Figure 4. Both the calculated and experimental results are plotted. Plots of the measured frequency-temperature behavior of the two devices fabricated at Motorola are shown in figure 5 and 6.

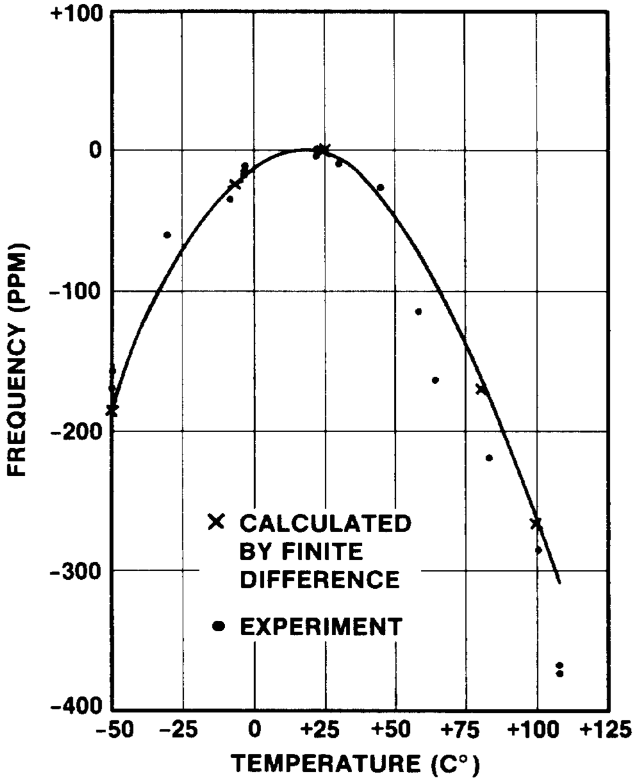

Figure 4. (YXwlt) 0/42.75/0 ST-CUT

The linear term in temperature is virtually absent in the device fabricated at (YX wlt) 6.57/26.88/134.9 (figure 5). The linear frequency term in the device fabricated at (YX wlt) 8.05/25.9/135.7 (figure 6) could be compensated for by a rotation of the mask by about 0.5 degrees. This small rotation would not, according to our calcula tions, appreciably affect $TCF^{(2)}$. Both devices have a calculated second order $TCF^{(2)}$ of about -0.15×10^{-7}, about half as large as that of ST-Cut Quartz. This result is born out by the experimental measurements, a linear regression analysis which shows a $TCF^{(2)}$ of -0.16×10^{-7}. These results are summarized in Table 5.

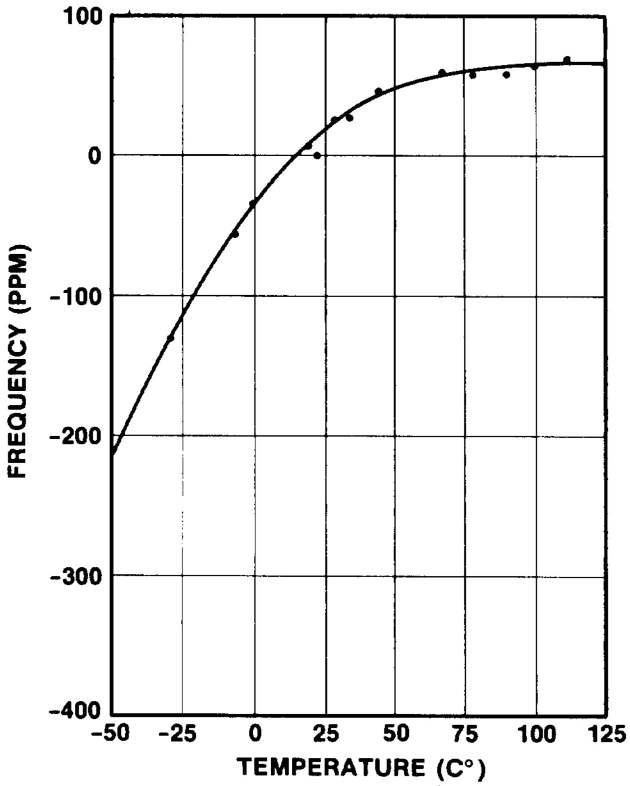

Figure 5. (YXwlt) 8.05/25.9/135.7)

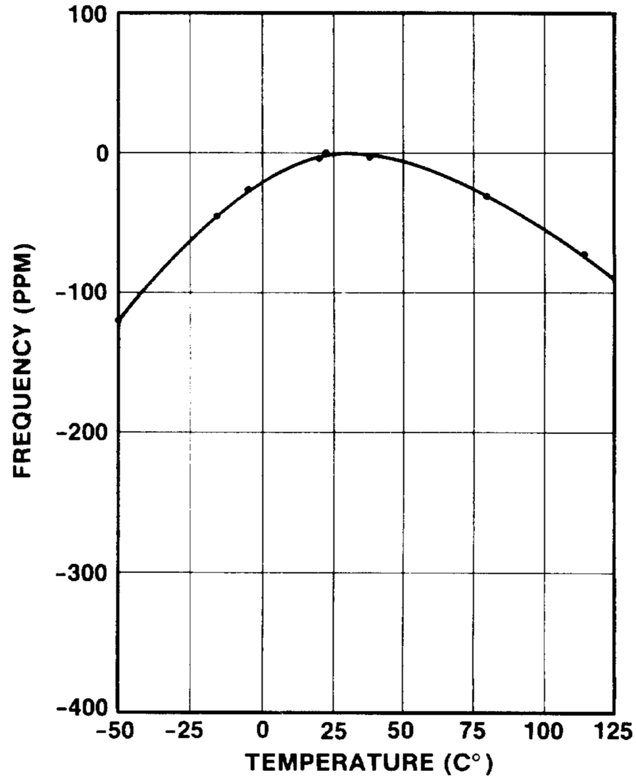

Figure 6. (YZwlt) 6.57/26.88/134.9

Table 5. Comparison of Experimental and Calculated Results

Angles			Calculated				Measured		
Phi	Thet	Psi	TCF [1] ††	TCF [1] †††	TCF [2] †††	TCF [3] †††	TCF [1]	TCF [2]	TCF [3]
0	42.75	0†	-0.07×10^{-5}	0.06×10^{-5}	-0.40×10^{-7}	0.11×10^{-10}	-0.1×10^{-5}	-0.37×10^{-7}	-0.17×10^{-10}
8.05	25.9	135.7	-0.01	0.74	-0.15	0.42	0.16	-0.16	0.58
6.57	26.88	134.9	-0.24	0.55	-0.15	0.48	0.025	-0.16	0.47

†Wafer obtained commercially. Angular tolerance is unknown.

††Calculated using Sinha and Tiersten's program.

†††Calculated using Finite Difference Approach.

The agreement between the experimental and calculated results has been excellent to date. Calculations using the Finite Difference method indicate that the doubly rotated wafers in fabrication should possess a slightly improved frequency response with $TCF^{(2)} = -0.1 \times 10^{-7}$ (see Table 1) but does not include the effects of coordinate axis skewing[5] taken into account by the Sinha and Tiersten computer program, which may become significant for these cuts which are farther off of the crystaline axes.

SUMMARY

The results of a study of the temperature coefficients of frequency on doubly rotated cuts of quartz were presented. Both a Finite Difference technique[3] and a Perturbation technique developed by Sinha and Tiersten[5] were used to select orientations with temperature stability superior to ST-Cut quartz. Experimental results are found to be in agreement with the calculations and show a two fold improvement in frequency stability over the ST-Cut.

ACKNOWLEDGEMENTS

The authors wish to thank Dr. A. Ballato for stimulating technical discussions; we wish to thank Mr. D. Green, Mr. R. Welles, Mr. J. Balacio, Mr. R. Caputo, Ms. C. Peterson and Ms. L. Fredericks in the material and fabrication areas.

REFERENCES

1"Surface Acoustic Wave Delay Lines with Small Temperature Coefficient", Schulz, Manfred B., Proc. IEEE, Sept. 1970, pp. 1361-1632.

2"Higher Order Temperature Coefficients of Quartz SAW Oscillators", D. Handen, M. Michael, J.J. Gagnepain, Frequency Control Symposium, 1978, pp. 77-86.

3"Numerical Computation of Acoustic Surface Waves in Layered Piezoelectric Media-Computer Program Descriptions", William Jones, William Smith, Donald Perry, Final Report F19628-70-C-0027, prepared for Air Force Cambridge Research Laboratories by Hughes Aircraft Company.

4"The Temperature Coefficients of Acoustic Surface Wave Velocity and Delay on Lithium Niobate, Lithium Tatalate, Quartz, and Tellerium Dioxide", Andrew Slobodnik, Report #AFCRL-72-0082, Air Force Cambridge Research Laboratories.

5"The Temperature Dependence of the Velocity of Surface Waves in Quartz", B.K. Sinha and H.F. Tiersten, IEEE, 1978, Ultrasonics Symposium, pp. 662-665.

6"Higher Order Temperature Coefficients of the Elastic Stiffnesses and Compliances of Alpha-Quartz", R. Bechmann, A. Ballato, T. Lukaszek, IRE, Aug. 1962, pp. 1812-1822.

7"Standards on Piezoelectric Crystals 1949", Pro. IRE 14, Dec. 1949, pp. 1378-1395.

8"Numerical Analysis of Doubly Rotated Cut SAW Devices", Williams and Cho, 1979 USP, IEEE Cat. No. 79CH 1482-9SU.

9"Surface and Shallow Bulk Acoustic Waves Propagating on Doubly Rotated Quartz Substrates," A. Ballato, T. Lukasek, K. Yen, R. Kagiwada, Technical Report DELET-TR-79-23, U.S. Army Electronics Technology and Devices Laboratory, Fort Monmouth, N.J.

10"A New Cut of Quartz Giving Improved Temperature Stability to SAW Oscillators", Ian Browning and Meirion Lewis, Proc. 32nd Annual Symposium on Frequency Control, 1978, pp. 87-92.