NUMERICAL ANALYSIS OF DOUBLY ROTATED* CUT SAW DEVICES

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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-wt) 0 to 30° 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 waves (SAW) on doubly rotated cuts of alpha quartz are presented.

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. 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.

The most straightforward method for calculating the frequency-temperature characteristics of a SAW device is the Finite Difference method. The Rayleigh wave velocities are calculated for different temperatures, yielding the values V(Ti), i=1,2,....., n. This is done by first calculating the fundamental constants at the temperature Ti of interest. These constants are then rotated into the coordinate system of interest. An iterative procedure is used to calculate the velocity V(T) 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 have provided a computer program to calculate the first order TCD using a perturbation approach. The constants used in this program are derived from the original experimental data of Bechmann, Ballato, and Lukaszek, 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 latter method to be more accurate, and angular orientations of the zero TCF surfaces calculated by the two programs differ by as much as three 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 (XY-wt) PHI/THETA/PSI for quartz were used throughout the investigation. Using the Finite Difference approach with the available crystal constants, the calculated results show that the zero TCF surfaces do not intersect with the zero TCF surfaces, based on the interpolated results of the 10° x 10° x 10° resolution. It is not likely that a higher 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 ≤ PHI ≤ 30°, 0 ≤ PSI ≤ 180°, and -90° ≤ THETA ≤ 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. 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 found, 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.

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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,\textsuperscript{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\textsuperscript{(1)} calculated by Sinha and Tiersten approach, with TCF\textsuperscript{(2)} and TCF\textsuperscript{(3)} calculated using the Finite Difference approach. These areas are chosen because of zero TCF\textsuperscript{(1)} and low TCF\textsuperscript{(2)}. TCF\textsuperscript{(3)} can be mostly cancelled out by TCF\textsuperscript{(1)} if the propagation direction is slightly rotated away from the zero TCF\textsuperscript{(1)} direction, so that the TCF\textsuperscript{(2)} 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>ANGLES OF ZTCF\textsuperscript{(1)}, DEGREES (S AND T'S PROGRAM)</th>
<th>VELOCITY (MSEC)</th>
<th>$k^2$</th>
<th>POWER FLOW ANGLE (DEGREES)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PHI</td>
<td>THETA</td>
<td>PSI</td>
<td>TCF\textsuperscript{(2)}=c\textsuperscript{2} (X10\textsuperscript{-8})</td>
</tr>
<tr>
<td>6 26 136.31</td>
<td>-1.4</td>
<td>-0.3</td>
<td>6 27 136.93</td>
</tr>
<tr>
<td>6 27 135.93</td>
<td>-1.3</td>
<td>0.57</td>
<td>6 28 135.59</td>
</tr>
<tr>
<td>7 26 135.99</td>
<td>-1.5</td>
<td>0.65</td>
<td>7 27 135.64</td>
</tr>
<tr>
<td>7 28 135.27</td>
<td>-1.3</td>
<td>0.67</td>
<td>8 26 135.74</td>
</tr>
<tr>
<td>8 27 135.36</td>
<td>-1.4</td>
<td>0.67</td>
<td>8 28 134.97</td>
</tr>
<tr>
<td>1 26 137.78</td>
<td>-1.2</td>
<td>0.68</td>
<td>1 27 137.48</td>
</tr>
<tr>
<td>1 28 137.17</td>
<td>-1.1</td>
<td>0.68</td>
<td>0 26 138.07</td>
</tr>
<tr>
<td>0 27 137.78</td>
<td>-1.1</td>
<td>0.68</td>
<td>0 28 137.49</td>
</tr>
<tr>
<td>-1 26 138.37</td>
<td>-1.2</td>
<td>0.80</td>
<td>-1 27 138.09</td>
</tr>
<tr>
<td>-1 28 137.80</td>
<td>-1.1</td>
<td>0.73</td>
<td>14 39 40.195</td>
</tr>
<tr>
<td>14 40 40.415</td>
<td>-1.0</td>
<td>0.66</td>
<td>14 41 40.64</td>
</tr>
<tr>
<td>15 39 40.195</td>
<td>-1.0</td>
<td>0.66</td>
<td>15 40 40.415</td>
</tr>
<tr>
<td>15 41 40.64</td>
<td>-1.0</td>
<td>0.68</td>
<td>16 39 39.79</td>
</tr>
<tr>
<td>16 40 39.505</td>
<td>-1.0</td>
<td>0.68</td>
<td>16 41 39.825</td>
</tr>
</tbody>
</table>

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 $f_0$ were calculated and compared with SAW. The polar plots of the inverse velocities for a (YX wlt) 0/27/137.8 and 7/27/135.5 are shown in Figure 1 and Figure 2, respectively. The inverse surface wave velocity for 0/27/137.8 is 3.06 x 10\textsuperscript{-4}, that for 7/27/137.8 is 3.03 x 10\textsuperscript{-4}. These values are larger than the minimum (1/vbulk) 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).
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 velocity, power flow angle, \( \Delta \nu \), 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 TCF'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), 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 \( \frac{\partial TCF(1)}{\partial \phi} \). The large values of \( \frac{\partial TCF(1)}{\partial \phi} \) impose strict fabrication tolerances on the SAW cuts and mask alignment. Fabrication accuracy to within 5 minutes is required to keep the total temperature variation due to TCF(1) within 45 ppm over the temperature range -50°C to 100°C.

Table 3. \( \frac{\partial TCF(1)}{\partial \phi} \) for Selected Cuts

<table>
<thead>
<tr>
<th>PHI</th>
<th>THETA</th>
<th>PSI</th>
<th>( \frac{\partial TCF(1)}{\partial \phi} )</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>
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<td>+2.7</td>
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<tr>
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<td>27</td>
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<td>+2.7</td>
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<tr>
<td>8</td>
<td>26</td>
<td>135.74</td>
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<td>27</td>
<td>135.36</td>
<td>+2.7</td>
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<tr>
<td>8</td>
<td>28</td>
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<td>+2.8</td>
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<tr>
<td>1</td>
<td>28</td>
<td>137.17</td>
<td>+2.8</td>
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<tr>
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<td>26</td>
<td>136.07</td>
<td>+3.0</td>
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<td>0</td>
<td>27</td>
<td>137.78</td>
<td>+3.0</td>
</tr>
<tr>
<td>0</td>
<td>28</td>
<td>137.49</td>
<td>+3.0</td>
</tr>
<tr>
<td>-1</td>
<td>26</td>
<td>138.37</td>
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</tr>
<tr>
<td>-1</td>
<td>28</td>
<td>137.80</td>
<td>+3.0</td>
</tr>
<tr>
<td>14</td>
<td>39</td>
<td>40.195</td>
<td>-3.5</td>
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<td>14</td>
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<td>16</td>
<td>41</td>
<td>39.825</td>
<td>-3.7</td>
</tr>
</tbody>
</table>

Table 4. \( \frac{\partial TCF(1)}{\partial \theta} \) and \( \frac{\partial TCF(1)}{\partial \psi} \) for Selected Cuts

<table>
<thead>
<tr>
<th>PHI</th>
<th>THETA</th>
<th>PSI</th>
<th>( \frac{\partial TCF(1)}{\partial \theta} )</th>
<th>( \frac{\partial TCF(1)}{\partial \psi} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>27</td>
<td>135.64</td>
<td>-0.7 (PPM/C°)/DEGREE</td>
<td>-0.5 (PPM/C°)/DEGREE</td>
</tr>
<tr>
<td>0</td>
<td>27</td>
<td>137.78</td>
<td>-0.6</td>
<td>-0.8</td>
</tr>
<tr>
<td>15</td>
<td>40</td>
<td>40.00</td>
<td>-1.5</td>
<td>0.7</td>
</tr>
</tbody>
</table>

**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, \( \phi \) and \( \theta \) are known to be within ±4 minutes. \( \psi \) 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.
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.

The linear term in temperature is virtually absent in the device fabricated at (YX wlt) 0/42.75/0 (figure 4). 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 calculations, appreciably affect TCF(2). Both devices have a calculated second order TCF(2) of about $-0.15 \times 10^{-7}$, 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 $-0.16 \times 10^{-7}$. These results are summarized in Table 5.
Table 5. Comparison of Experimental and Calculated Results

<table>
<thead>
<tr>
<th>Angles</th>
<th>Calculated</th>
<th>Measured</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phi</td>
<td>Thet</td>
<td>Psi</td>
</tr>
<tr>
<td>0</td>
<td>42.75</td>
<td>0</td>
</tr>
<tr>
<td>8.05</td>
<td>25.9</td>
<td>135.7</td>
</tr>
<tr>
<td>6.57</td>
<td>26.88</td>
<td>134.9</td>
</tr>
</tbody>
</table>

†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 x 10⁻⁷ (see Table 1) but does not include the effects of coordinate axis skewing 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 and a Perturbation technique developed by Sinha and Tiersten 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

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