AK-cut Crystal Resonators

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ABSTRACT

Calculations have predicted the existence of crystallographically doubly rotated quartz orientations with turnover temperatures which are considerably less sensitive to angular mis-orientation than comparable AT- or BT-cuts. We have arbitrarily designated these crystals as the AK-cut. We report experimental data for seven orientations, \(\phi\)-angle variations between 30-46° and \(\theta\)-angle variations between 21-28°, measured on 3.3-3.4 MHz fundamental mode resonators vibrating in the thickness shear c-mode. The experimental turnover temperatures of these resonators are between 80°C and 150°C, in general agreement with calculated values. The normalized frequency change as a function of temperature has been fitted with a cubic equation.

INTRODUCTION

In a previous publication,\(^1\) the turnover temperatures, \(T_{to}\), of crystallographically doubly rotated quartz plates vibrating in the thickness shear mode were calculated. It was shown that in addition to the usual rotation angles associated with the AT-, FC-, IT-, SC-, RT-, and BT-cuts, there is another crystallographic region which yields \(T_{to}\) values in the temperature range of practical interest to temperature controlled resonators. These crystal orientations, vibrating in the thickness shear c-mode, were arbitrarily designated as AK-cuts. The frequency as a function of temperature characteristics of the AK-cuts are located between the AT- and BT-cuts, but the \(T_{to}\) values are considerably less sensitive to angular orientation than any of the other cuts. In this paper, we give additional theoretical results related to the AK-cut, and at the same time report experimental confirmation of turnover temperatures on 10 MHz, 3rd overtone, resonators fabricated from seven different crystallographic orientations.

The computations performed in this investigation are based on elastic constant values, \(c_{pq}\), of quartz published by Bechmann, Ballato, and Lukaszek,\(^2\) hereafter referred to as BBL(1962), and on a set of temperature coefficients of the elastic constants, \(T_n(c_{pq})\), derived in Ref. 3, and hereafter referred to as BBL(1963) LSF. These temperature coefficients are based on the least squares fit (LSF) of experimental data published by Bechmann, Ballato, and Lukaszek (BBL) in 1963.\(^4\) A \(T_n(c_{pq})\) set has been derived in BBL(1962) and another set has been published by Adams, Enslow, Kusters, and Ward,\(^5\) and we refer to this set as Adams et al. In Ref. 3 we compared and discussed the limitations associated with the different sets, and their AP-
plicability to predict the frequency-temperature behavior of arbitrary doubly rotated crystal orientations. This topic has also been treated in Refs. 6 and 7. For reasons outlined in these references, we find the BBL(1963) LSF set more satisfying than the one derived in BBL(1962). For the crystallographic region associated with the AK-cuts, all three sets give similar general results and predict the existence of this cut, but actual $T_{TO}$ values for a specific pair of rotation angles depend on the particular set used in the computations. In this paper, we intend to illustrate general results, and we limit the computations, with one exception, to the BBL(1963) LSF set of temperature coefficients of elastic constants.

**CALCULATED TURNOVER TEMPERATURES**

Figure 1 depicts the plate geometry and crystallographic coordinate systems used in this investigation. The orientation of the plate is described by angles $(\phi, \theta)$ where $\phi$ and $\theta$ are rotations around the $z$- and $x$-axis, respectively. In this nomenclature, $\phi$-angle limits are $0^\circ < \phi < 60^\circ$ and $\theta$-angle rotations are $0^\circ < \theta < 90^\circ$. The angular rotations associated with the AK-cuts are approximately between $\phi = 30^\circ$ and $\phi = 47^\circ$, and between $\theta = 17^\circ$ and $\theta = 30^\circ$. For example, one specific $(\phi, \theta)$ combination is $(40.9, 21.0)^\circ$. In another commonly used notation, this rotation is on the "negative theta" side and is designated as $(19.1, -21.0)^\circ$.

Figure 2 shows the calculated $(\phi, \theta)$ loci for selected turnover temperatures between $75^\circ C$ and $160^\circ C$ of AK-cut $c$-mode vibrations. The temperature coefficients of the elastic constants are valid between $-200^\circ C$ and $+200^\circ C$. For AT-cut crystals, $\phi = 0^\circ$, the turnover temperatures throughout this temperature range are single value functions of the $\theta$-angle, and are obtained at $\theta$-angles slightly larger than $35.25^\circ$. In the $50^\circ C$ to $100^\circ C$ range, the AT-cut $T_{TO}$ shifts by $2.6^\circ C$ per minute of arc. The AT-cut angle equivalent to $T_{TO} = 200^\circ C$ is $\theta = 36.70^\circ$. For AK-cut crystals, the lowest possible $T_{TO}$, based on BBL(1963) LSF parameters, is approximately $75^\circ C$, and for a specified $\phi$-angle there are two $\theta$-angles which give identical $T_{TO}$. For a selected $T_{TO}$, the $(\phi, \theta)$ loci exhibit concentric quasi-elliptical characteristics, with the angular boundaries increasing with $T_{TO}$. The distortions in the $T_{TO} = 140^\circ C$ and $T_{TO} = 160^\circ C$ curves at the higher $\phi$-angles and upper $\theta$-angle segments are due to the interference of the $T_{TO}$ branch containing the AT-type turnover temperatures. This can be deduced from Ref. 1, Fig. 9. The $(\phi, \theta)$ locations of the experimental resonators are shown in Fig. 2 by dots, with the experimental $T_{TO}$ values indicated. (These will be discussed further on.)

The primary advantage of AK-cut crystals, that is, the relative insensitivity of $T_{TO}$ to inaccuracies in $(\phi, \theta)$, is implicit in the curves shown in Fig. 2. For example, at $\phi = 37^\circ$ the tolerance on the $\theta$-angle for the $T_{TO}$ to be between $75^\circ C$ and $85^\circ C$ is $\Delta \theta = \pm 1.9^\circ$. In contrast, for the same $T_{TO}$ range, the tolerance for the AT-cut is $\Delta \theta = \pm 2^\circ$, approximately 60 times more sensitive. The $T_{TO}$ position of the $b$-mode BT-cut $(\phi = 60^\circ)$ is less sensitive to $\theta$-angle changes than the AT-cut, and the comparable angular tolerance is $\Delta \theta = \pm 14^\circ$.  

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Figure 3 shows a comparison of the $(\phi, \theta)$ loci for $T_{to} = 90^\circC$ calculated with $T_n(c_{pq})$ values based on Adams et al., BBL(1962), and BBL(1963) LSF. All three sets show the quasi-elliptical nature of the curves, but vary in detailed numerical results. For a given $(\phi, \theta)$, Adams et al. parameters yield the lowest $T_{to}$ values, the BBL(1963) LSF set predicts higher $T_{to}$, and BBL(1962) gives the highest $T_{to}$ values. A similar order is followed in calculating the lowest possible $T_{to}$ for the AK-cuts, approximately 55°C for Adams et al., 75°C for BBL(1963) LSF, and 85°C for BBL(1962). These results also point out the difficulty in comparing theoretical predictions with experimental data. The $T_n(c_{pq})$ values are derived from the first, second, and third order temperature coefficients of frequencies measured on a set of $(\phi, \theta)$ orientations. Their applicability to a particular crystallographic region may depend on the $(\phi, \theta)$ distribution of the original data set. To the best of our knowledge, data points from the $(\phi, \theta)$ region defining the AK-cut were not included in any of the three data sets. For AK-cut calculations there is then neither an a priori preference for selecting a particular $T_n(c_{pq})$ set, nor is there any confidence that the predicted $T_{to}$ values will be observed. For reliable computations, it is essential to collect experimental data weighed heavily with $(\phi, \theta)$ orientations applicable to the crystallographic region of interest, and then based on this data derive a "local" set of $c_{pq}$ and $T_n(c_{pq})$.

EXPERIMENTAL PROCEDURES AND RESULTS

The primary objective of this investigation was to confirm the existence of thickness shear c-mode vibrations yielding turnover temperatures in the 80°C to 200°C temperature range for crystallographic orientations which are unrelated to angular values usually associated with the general class of doubly rotated AT-cuts.

The initial evaluation of the AK-cut crystals comprises seven $(\phi, \theta)$ orientations. Figure 4 shows the $(\phi, \theta)$ positions of the selected cuts, and the Miller indices of the lattice planes associated with this crystallographic region. The primary $(\phi, \theta)$ selection criterion was ease of orientation and fabrication. Three rotations, $(30, 24.44)^\circ$, $(36.58, 28.45)^\circ$, and $(46.10, 23.59)^\circ$ are low index lattice planes, [111], [323], and [312], respectively. Another three rotations, $(40.9, 21.0)^\circ$, $(40.9, 23.59)^\circ$, and $(40.9, 27.0)^\circ$ are situated along the [211] and [212] planes, and the seventh $(36.0, 24.44)^\circ$, is obtained by a 6° rotation from [111]. The crystals were machined into plano-plano plates, beveled at the edges, and the disks were fabricated into 10 MHz, 3rd overtone, resonators at Frequency Electronics, Inc., using established manufacturing processes. The exact 10 MHz frequency value was not a fabrication requirement.

The resonators were placed in a heater and connected through a $\pi$-network to a network analyzer. A programmable synthesizer provided a stepwise variable frequency. Temperature was measured with a thermocouple attached to the resonator enclosure and connected to a digital thermometer. A data bus connected these components to a desktop computer and printer for automatic data recording. A programmable temperature controller provided linear ramps with adjustable rates, e.g. 0.1 or 0.2°C/minute. The control-
ling computer program called for repetitive frequency sweeping through the series resonance in 100 steps with 1 msec per step, and determined the resonance frequency as a function of temperature with temperature intervals of typically 0.5 to 1°C between data points. For mode spectra determination, the frequency was swept over several MHz in steps of 1 or 2 Hz at constant temperature.

Figure 5 shows the normalized measured frequency change \((f_{\text{meas}} - f_0)/f_0\), with \(f_0\) being the frequency at 25°C, as a function of temperature for the (36.0, 24.44)° cut in the fundamental and in the 3rd overtone modes. The turnover temperatures are 84°C and 82°C for the fundamental and 3rd overtone, respectively. At \(T_{\text{To}}\), the curves show maxima, similar to the b-mode BT-cut. Whereas, the c-mode SC-cut turnover changes from minimum to maximum as \(T_{\text{To}}\) shifts from below to above the inflection temperature, the curvature found with AK-cut crystals is unrelated to the inflection temperature. For this particular AK-cut orientation, the inflection temperature is calculated to be at -793°C, a meaningless number. The other fabricated resonators also have turnover temperatures in the fundamental mode, and their \(T_{\text{To}}\) values were indicated in Fig. 2. Some experimental points lie above, some below, and some almost coincide with predicted values. Considering the simplified mathematical formalism utilized for these computations, and the inaccuracies of the \(T_n(C_{pq})\) values, the general agreement between theory and experiment is surprising and gratifying. However, detailed comparisons of this data with calculated results based on the \(T_n(C_{pq})\) sets are not too meaningful.

The frequency as a function of temperature curves are fitted by a normalized cubic equation in the form

\[
\Delta f/f_0 = (f - f_0)/f_0 = \sum_{n=1}^{3} a_n(T - T_0)^n
\]

where \(T_0 = 25°C\) and \(f_0\) is the frequency at \(T_0 = 25°C\). The resulting coefficients \(a_n\) are listed in Table 1 together with the standard deviations of the fits which are reasonable and consistent. The normalized frequency differences between measured and calculated values based on the cubic equation are also plotted in Fig. 5. Throughout the entire measured temperature range, 25°C to 145°C, the data is equally well described by the cubic equation, and the deviations from the cubic are substantially less than \(\pm 1 \times 10^{-6}\). The frequency-temperature characteristics of the corresponding 3rd overtone curves were also fitted by the cubic equation. For this particular (\(\phi, \theta\)) combination, the fundamental and the 3rd overtone \(T_{\text{To}}\) agree within 2°C. As shown in Table 1, this is not the case for other (\(\phi, \theta\)) orientations. For (30.0, 24.44)°, the 3rd overtone \(T_{\text{To}}\) is 27°C higher, and for (36.58, 28.45)° and (46.1, 23.50)° the fundamental mode \(T_{\text{To}}\) is higher by 23°C and 41°C, respectively. These discrepancies do not necessarily imply inconsistencies in data or calculations. In the first order approximation, the frequency-temperature characteristics of fundamental and overtone modes are also related, in a complicated fashion, by the temperature coefficients of the electromechanical coupling factors. At the present time, we have not included this effect in our mathematical formalism. Our initial measurements
Table 1. Temperature Coefficients of Frequency for Experimental AK-cut Crystals.

<table>
<thead>
<tr>
<th>Orientation</th>
<th>measured temperature coefficients</th>
<th>standard deviations (see text)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( T_{to} )</td>
<td>( a_1 )</td>
</tr>
<tr>
<td>Fundamental mode</td>
<td></td>
<td>(^{/})C</td>
</tr>
<tr>
<td>30.00° 24.44°</td>
<td>145°C</td>
<td>4.35x10^{-6}</td>
</tr>
<tr>
<td>36.00° 24.44°</td>
<td>84</td>
<td>3.58</td>
</tr>
<tr>
<td>36.58° 28.45°</td>
<td>101</td>
<td>4.50</td>
</tr>
<tr>
<td>40.90° 21.00°</td>
<td>129</td>
<td>7.31</td>
</tr>
<tr>
<td>40.90° 23.59°</td>
<td>113</td>
<td>6.48</td>
</tr>
<tr>
<td>46.10° 27.00°</td>
<td>107</td>
<td>6.18</td>
</tr>
<tr>
<td>46.10° 23.59°</td>
<td>154</td>
<td>11.90</td>
</tr>
</tbody>
</table>

3rd overtone mode

| 30.00° 24.44° | 172 | 5.04 | -22.8 | 25.1 | 1.6 | 11.9 |
| 36.00° 24.44° | 82  | 3.90 | -31.2 | -28.6 | 1.5 | 36.2 |
| 36.58° 28.45° | 78  | 3.43 | -28.1 | -70.5 | 4.0 | 39.0 |
| 46.10° 23.59° | 113 | 7.77 | -36.3 | -55.9 | 4.0 | 51.2 |

Pertained to the 3rd overtone modes, and the corresponding \( T_{to} \) values were the ones indicated in Ref. 1, Fig. 14.

Table 1 also lists values for

\[
\Delta F = \left| \Delta f / f_0 (T = T_{to} \pm \Delta T) - \Delta f / f_0 (T = T_{to}) \right|,
\]

the difference between the calculated normalized frequency at \( T_{to} \) and \( T_{to} \pm 1^\circ C \). This quantity is a measure of the "flatness" of the frequency-temperature curve at \( T_{to} \). The values range from \( 14x10^{-9} \) to \( 60x10^{-9} \), and there seems to be some correlation between these values and the \( \phi \)-angles. Comparative values for AT-cut range from \( \Delta F = 21.5x10^{-9} \) for \( T_{to} = 85^\circ C \) to \( \Delta F = 40.0x10^{-9} \) for \( T_{to} = 160^\circ C \).

Figure 6 shows the mode spectrum for the fabricated resonators vibrating in the fundamental b- and c-modes measured at room temperature. All (\( \phi, \theta \)) pairs show similar patterns. The amplitude of the lowest c-mode resonance is very large, and we designate this frequency, for each respective (\( \phi, \theta \)), as \( f_0 \). The \( f_0 \) modes have been aligned in Fig. 6, but the \( f_0 \) values actually vary between 3.36 and 3.41 MHz. The \( f_0 \) mode is followed by a series of anharmonic modes of various strengths. Some anharmonic modes are as strong as \( f_0 \). The abundance of anharmonic modes is a characteristic feature of doubly rotated cuts, and no efforts were made to suppress unwanted vibrations. The vibration patterns associated with the anharmonic modes have not

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Table 2. Comparison of Fundamental b- and c-mode Frequency Separation.

<table>
<thead>
<tr>
<th>φ</th>
<th>θ</th>
<th>( (f_b - f_c)/f_b )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>calculated</td>
</tr>
<tr>
<td>30.0°</td>
<td>24.44°</td>
<td>14.6%</td>
</tr>
<tr>
<td>36.0</td>
<td>24.44</td>
<td>11.6</td>
</tr>
<tr>
<td>36.58</td>
<td>28.45</td>
<td>5.7</td>
</tr>
<tr>
<td>40.9</td>
<td>21.0</td>
<td>14.3</td>
</tr>
<tr>
<td>40.9</td>
<td>23.59</td>
<td>10.4</td>
</tr>
<tr>
<td>40.9</td>
<td>27.0</td>
<td>5.1</td>
</tr>
<tr>
<td>46.1</td>
<td>23.59</td>
<td>7.2</td>
</tr>
</tbody>
</table>

been identified. The dashed lines indicate the b-modes. Table 2 lists the b- to c-mode frequency separations for the seven orientations. There is close agreement between calculated and experimental values.

Figure 7 shows the corresponding 3rd overtone c-mode spectra, with the exception of (40.9, 23.59)°. The increased number of modes is consistent with the increased number of allowable vibrations. The arrow indicates the relative 3f₀ positions, and the spectra are aligned at 3f₀. For several orientations, there are a large number of strong resonances below 3f₀, and there is no one dominant resonance that can be designated as the equivalent to f₀. This poses a problem in evaluating the temperature characteristics f(T) of the resonators. Do we choose the lowest frequency, the strongest amplitude, or the mode closest to 3f₀? For some resonators we have measured f(T) for several modes, and in some cases we do find considerable differences in their T_{f₀}. The data listed for the 3rd overtone in Table 1 correspond to the lowest observed frequencies.

The real difficulty encountered in evaluating the 3rd overtone modes is that for the three φ = 40.9° orientations we are unable to observe turnover temperatures. The resonances are close together, vary considerably in strength with temperature, become coupled, and they are very hard to follow and identify with changes in temperature. The mode spectra data indicate that considerable work is needed to optimize disk geometry and suppress anharmonic vibration patterns. Figure 8 shows the 3rd overtone resonance for (36.0, 24.44)°. The Q-value is approximately 1.5 x 10⁶, that is of the same order of magnitude as high precision 10 MHz, 3rd overtone, AT-cut resonators.

OPTIMIZED ORIENTATIONS

The most important resonator performance characteristic is the frequency-temperature behavior. The claim for the AK-cut crystals relates to turnover temperature insensitivity to angular orientations. The large (φ, θ) choice available for specific T_{f₀} values of AK-cuts may also allow one to optimize the resonator design to some additional performance parameter. The primary concern is the temperature coefficient of frequency near T_{f₀}. A small value is desired, but constraints are imposed by the electromechanical coupling factors, and the b- to c-mode frequency separations.
Figure 9 shows a plot of the normalized frequency differences \( \Delta F \) between \( T_{to} \) and \( T_{to} \pm 10^\circ \) as a function of \( \phi \)-angles for the BBL(1963) LSF \( T_{to} = 90^\circ \) curve shown in Fig. 3. The \( \Delta F \) values are not exactly symmetric around the 90°C turnover temperatures and we have calculated \( \Delta F \) both at 89°C and at 91°C and selected the larger value. The solid line of this curve corresponds to the lower and the dashed line to the upper \( \theta \)-angle. The \( \Delta F \) values range from approximately \( 22 \times 10^{-9} \) at the lower \( \phi \)-angles to \( 42 \times 10^{-9} \) at the upper \( \phi \)-angles, with \( \Delta F \) for the lower \( \theta \)-angle always less, by \( 2-3 \times 10^{-9} \), than for the upper one. This is also consistent with the experimental \( \Delta F \) increase with the \( \phi \)-angles, shown in Table 1.

For low \( \Delta F \) values, one would select low \( \phi \)-angles and the lower \( \theta \)-angle. The corresponding \( \Delta F \) value, at \( T_{to} = 90^\circ \), for the AT-cut is \( 22.8 \times 10^{-9} \) and for the BT-cut \( 62.2 \times 10^{-9} \). Hence, the magnitude of the frequency-temperature curvature of the AK-cut is between that of the AT- and BT-cuts. For higher \( T_{to} \) values, the \( \Delta F \) values for both the AT- and BT-cuts increase with \( T_{to} \), whereas for some AK-cut (\( \phi, \theta \)) combinations \( \Delta F \) decreases with increasing \( T_{to} \).

Figure 10 shows the b- and c-mode electromechanical coupling factors, \( k_b \) and \( k_c \), as a function of \( \phi \) for \( T_{to} = 90^\circ \). Data for the lower \( \theta \)-angle is drawn with a solid line and for the upper \( \theta \)-angle with a dashed line. The AK-cut operates in the c-mode, and, ideally, a strong \( k_c \) and weak \( k_b \) is desired. However, for most angles, \( k_b \) is substantially stronger than \( k_c \). For the lower \( \theta \)-angle \( k_c \) becomes equal to \( k_b \) at \( \phi = 38^\circ \). At the higher \( \phi \)-angles \( k_c \) continues to increase while \( k_b \) decreases. For the upper \( \theta \)-angles, \( k_b \) is stronger than \( k_c \) up to approximately \( \phi = 40^\circ \).

Figure 11 shows the relative frequency separations, in percent, between the b- and c-modes as a function of \( \phi \)-angle for \( T_{to} = 90^\circ \). The curve corresponding of the upper \( \theta \)-angle starts approximately at 11%, dips to 6% and increases to 8% at the high \( \phi \)-angle. In contrast, the curve corresponding to the lower \( \theta \)-angle peaks at 14%. There is no established criterion for a minimum b- to c-mode frequency separation or relative strengths of electromechanical coupling factors. The recently developed doubly rotated SC-cut, \((21.93, 34.24)^\circ\), may be applied as a guideline for the AK-cut. For SC-cut crystals, the frequency separation is 9.1%, \( k_b = 5.0\% \), and \( k_c = 4.6\% \). This coupling factor criterion will limit the AK-cut mostly to the lower \( \theta \)-angle and to \( \phi \)-angles from \( \phi = 37^\circ \) to \( \phi = 40.8^\circ \). The \( \Delta F \) value in this \( \phi \)-angle range increases from \( 30.7 \times 10^{-9} \) to \( 41.7 \times 10^{-9} \). In addition, the frequency separation criterion will completely eliminate the upper \( \theta \)-angle for practical resonators. For a given \( T_{to} \), the optimum resonator design will then be a compromise between fabrication tolerances on the \( \phi \)- and \( \theta \)-angles, and the constraints imposed by \( k_b, k_c \), and the b- to c-mode frequency separation.

Acknowledgments. We wish to thank Robert J. Andrews and Cherrille D. Stewart for their technical assistance with measurements and curve fitting computations.
REFERENCES


FIGURE CAPTIONS

Figure 1. Singly and doubly rotated crystal plates. Coordinate system.

Figure 2. Calculated (\(\phi, \theta\)) loci of selected turnover temperatures, \(T_{to}\), for AK-cut crystals. Dots indicate the position of experimental resonators and their measured \(T_{to}\) values.

Figure 3. Calculated (\(\phi, \theta\)) loci for \(T_{to} = 90^\circ\text{C}\), based on three sets of temperature coefficients of the elastic constants.

Figure 4. Rotation angles of seven experimental AK-cut resonators, indicated by solid circles. Also shown are the Miller indices of lattice planes used for orientation.

Figure 5. Measured frequency-temperature characteristics for fundamental and 3rd overtone modes. Also shown are the differences between measured and fitted normalized frequencies.

Figure 6. Fundamental c- and b-mode spectra measured for seven AK-cuts.

Figure 7. 3rd overtone c-mode spectra measured for six AK-cuts.

Figure 8. Example of 3rd overtone AK-cut resonance curve.

Figure 9. Calculated frequency offsets between \(T_{to} = 90^\circ\text{C}\) and 91°C for AK-cuts.

Figure 10. Calculated electromechanical coupling factors \(k_b\) and \(k_c\) for AK-cuts with turnover at 90°C.

Figure 11. Calculated b-mode to c-mode frequency separation for AK-cuts with turnover at 90°C.
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QUESTIONS AND ANSWERS

None for Paper #29