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 misorientation than comparable AT- or BT-cuts. We have arbitrarily designated these crystals as the AK-cut. We report experimental data for seven orientations, ϕ-angle variations between 30-46° and θ-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 (ϕ, θ) where ϕ and θ are rotations around the z- and x-axis, respectively. In this nomenclature, ϕ-angle limits are $0° < \phi < 60°$ and θ-angle rotations are $0° < \theta < 90°$. The angular rotations associated with the AK-cuts are approximately between $\phi = 30°$ and $\phi = 47°$, and between $\theta = 17°$ and $\theta = 30°$. For example, one specific (ϕ, θ) combination is (40.9, 21.0)°. In another commonly used notation, this rotation is on the "negative theta" side and is designated as (19.1, -21.0)°.

Figure 2 shows the calculated (ϕ, θ) loci for selected turnover temperatures between 75°C and 160°C of AK-cut c-mode vibrations, The temperature coefficients of the elastic constants are valid between -200°C and +200°C. For AT-cut crystals, $\phi = 0°$, the turnover temperatures throughout this temperature range are single value functions of the θ-angle, and are obtained at θ-angles slightly larger than 35.25°. In the 50°C to 100°C range, the AT-cut T_{to} shifts by 2.6°C per minute of arc. The AT-cut angle equivalent to T_{to} = 200°C is $\theta = 36.70°$. For AK-cut crystals, the lowest possible T_{to}, based on BBL(1963) LSF parameters, is approximately 75°C, and for a specified ϕ-angle there are two θ-angles which give identical T_{to}. For a selected T_{to}, the (ϕ, θ) loci exhibit concentric quasi-elliptical characteristics, with the angular boundaries increasing with T_{to}. The distortions in the T_{to} = 140°C and T_{to} = 160°C curves at the higher ϕ-angles and upper θ-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 (ϕ, θ) 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 (ϕ, θ), is implicit in the curves shown in Fig. 2. For example, at $\phi = 37°$ the tolerance on the θ-angle for the T_{to} to be between 75°C and 85°C is $\Delta\theta = \pm 1.9°$. In contrast, for the same T_{to} range, the tolerance for the AT-cut is $\Delta\theta = \pm 2'$, approximately 60 times more sensitive. The T_{to} position of the b-mode BT-cut ($\phi = 60°$) is less sensitive to θ-angle changes than the AT-cut, and the comparable angular tolerance is $\Delta\theta = \pm 14'$.

Figure 3 shows a comparison of the (ϕ, θ) loci for T_{to} = 90°C 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 (ϕ, θ), 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 (ϕ, θ) orientations. Their applicability to a particular crystallographic region may depend on the (ϕ,θ) distribution of the original data set. To the best of our knowledge, data points from the (ϕ, θ) 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 (ϕ, θ) 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 (ϕ, θ) orientations. Figure 4 shows the (ϕ, θ) positions of the selected cuts, and the Miller indices of the lattice planes associated with this crystallographic region. The primary (ϕ, θ) selection criterion was ease of orientation and fabrication. Three rotations, (30, 24.44)°, (36.58, 28.45)°, and (46.10, 23.59)° are low index lattice planes, [111], [323], and [312], respectively. Another three rotations, (40.9, 21.0)°, (40.9, 23.59)°, and (40.9, 27.0)° are situated along the [211] and [212] planes, and the seventh (36.0, 24.44)°, 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 π-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 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 $(f_{meas} - f_0)/f_0$, 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_{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_{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_{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 (ϕ, θ) combination, the fundamental and the 3rd overtone T_{to} agree within 2°C. As shown in Table 1, this is not the case for other (ϕ, θ) orientations. For (30.0, 24.44)°, the 3rd overtone T_{to} is 27°C higher, and for (36.58, 28.45)° and (46.1, 23.50)° the fundamental mode T_{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.

Orientation ϕ	θ	measured T_{to}	temperature coefficients a_1 /°C	a_2 /°C^2	a_3 /°C^3	standard deviations	ΔF (see text)
Fundamental mode							
30.00°	24.44°	145°C	4.35×10^{-6}	-22.3×10^{-9}	22.6×10^{-12}	1.0×10^{-7}	14.2×10^{-9}
36.00°	24.44°	84	3.58	-29.2	-11.9	0.8	31.3
36.58°	28.45°	101	4.50	-27.8	-14.8	0.8	31.2
40.90°	21.00°	129	7.31	-30.6	-33.9	3.7	41.0
40.90°	23.59°	113	6.48	-30.8	-47.7	4.5	43.4
40.90°	27.00°	107	6.18	-32.0	-42.5	2.3	42.6
46.10°	23.59°	154	11.90	-31.8	-72.3	3.7	60.0
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

$$\Delta F = |\Delta f/f_0(T = T_{to}\pm1) - \Delta f/f_0(T = T_{to})|,$$

the difference between the calculated normalized frequency at T_{to} and T_{to} ±1°C. This quantity is a measure of the "flatness" of the frequency-temperature curve at T_{to}. The values range from 14×10^{-9} to 60×10^{-9}, and there seems to be some correlation between these values and the ϕ-angles. Comparative values for AT-cut range from $\Delta F = 21.5\times10^{-9}$ for T_{to} = 85°C to $\Delta F = 40.0\times10^{-9}$ for T_{to} = 160°C.

Figure 6 shows the mode spectrum for the fabricated resonators vibrating in the fundamental b- and c-modes measured at room temperature. All (ϕ, θ) pairs show similar patterns. The amplitude of the lowest c-mode resonance is very large, and we designate this frequency, for each respective (ϕ, θ), 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

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

ϕ	θ	$(f_b - f_c)/f_b$ calculated	experimental
30.0°	24.44°	14.6%	13.4%
36.0	24.44	11.6	11.1
36.58	28.45	5.7	5.5
40.9	21.0	14.3	14.7
40.9	23.59	10.4	10.1
40.9	27.0	5.1	5.2
46.1	23.59	7.2	6.9

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 $3f_0$ positions, and the spectra are aligned at $3f_0$. For several orientations, there are a large number of strong resonances below $3f_0$, and there is no one dominant resonance that can be designated as the equivalent to f_0. 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 $3f_0$? For some resonators we have measured f(T) for several modes, and in some cases we do find considerable differences in their T_{to}. 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 1.5×10^6, 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_{to} 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_{to}. 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 ΔF between T_{to} and $T_{to} \pm 1°$ as a function of ϕ-angles for the BBL(1963) LSF T_{to} = 90°C curve shown in Fig. 3. The ΔF values are not exactly symmetric around the 90°C turnover temperatures and we have calculated ΔF 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 θ-angle. The ΔF values range from approximately 22×10^{-9} at the lower ϕ-angles to 42×10^{-9} at the upper ϕ-angles, with ΔF for the lower θ-angle always less, by $2\text{-}3 \times 10^{-9}$, than for the upper one. This is also consistent with the experimental ΔF increase with the ϕ-angles, shown in Table 1.

For low ΔF values, one would select low ϕ-angles and the lower θ-angle. The corresponding ΔF value, at T_{to} = 90°C, for the AT-cut is 22.8×10^{-9} and for the BT-cut 62.2×10^{-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 ΔF values for both the AT- and BT-cuts increase with T_{to}, whereas for some AK-cut (ϕ, θ) combinations ΔF 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 ϕ for T_{to} = 90°C. Data for the lower θ-angle is drawn with a solid line and for the upper θ-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 θ-angle k_c becomes equal to k_b at ϕ = 38°. At the higher ϕ-angles k_c continues to increase while k_b decreases. For the upper θ-angles, k_b is stronger than k_c up to approximately ϕ = 40°.

Figure 11 shows the relative frequency separations, in percent, between the b- and c-modes as a function of ϕ-angle for T_{to} = 90°C. The curve corresponding of the upper θ-angle starts approximately at 11%, dips to 6% and increases to 8% at the high ϕ-angle. In contrast, the curve corresponding to the lower θ-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)°, 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 θ-angle and to ϕ-angles from ϕ = 37° to ϕ = 40.8°. The ΔF value in this ϕ-angle range increases from 30.7×10^{-9} to 41.7×10^{-9}. In addition, the frequency separation criterion will completely eliminate the upper θ-angle for practical resonators. For a given T_{to}, the optimum resonator design will then be a compromise between fabrication tolerances on the ϕ- and θ-angles, and the constraints imposed by k_b, k_c, and the b- to c-mode frequency separation.

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FIGURE CAPTIONS

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

Figure 2. Calculated (ϕ, θ) 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 (ϕ, θ) loci for T_{to} = 90°C, based on three sets of 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.

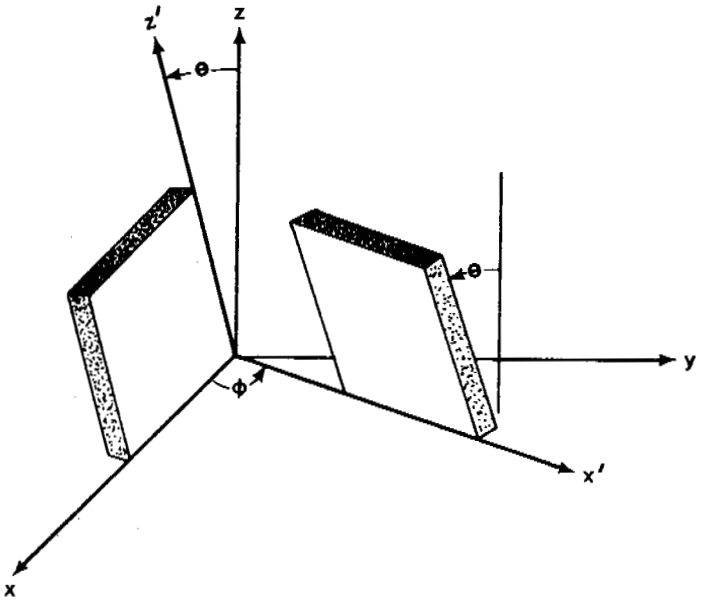
Figure 7. 3rd overtone c-mode spectra measured for six AK-cuts.

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

Figure 9. Calculated frequency offsets between T_{to} = 90°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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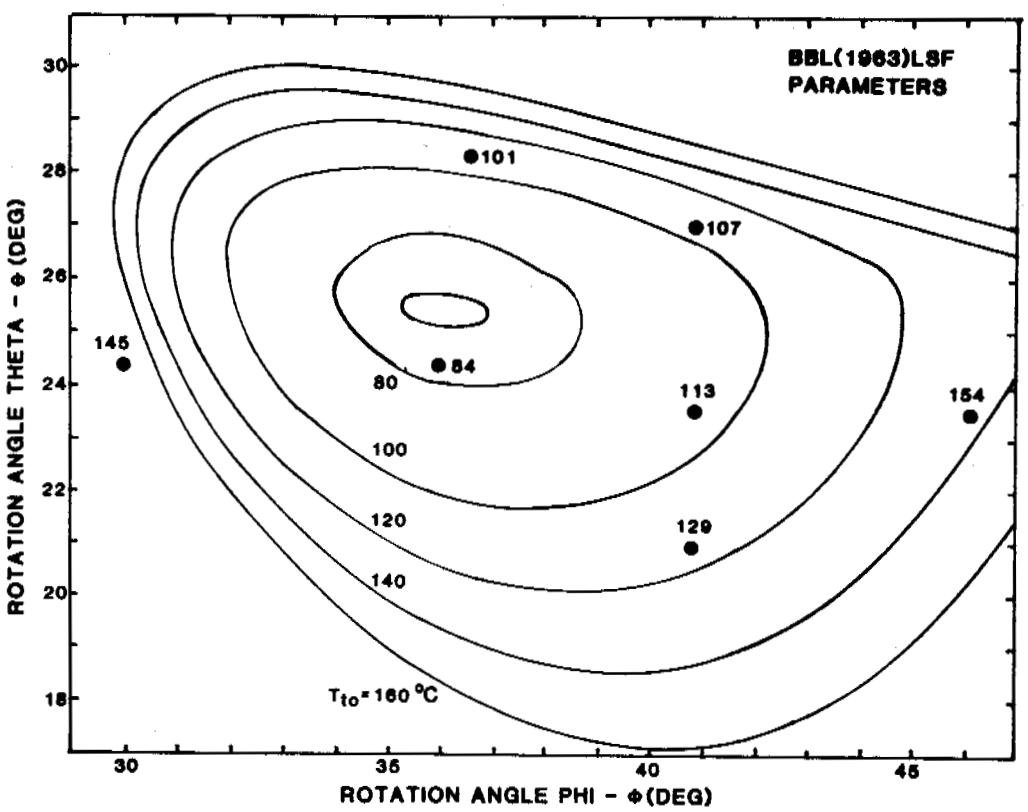

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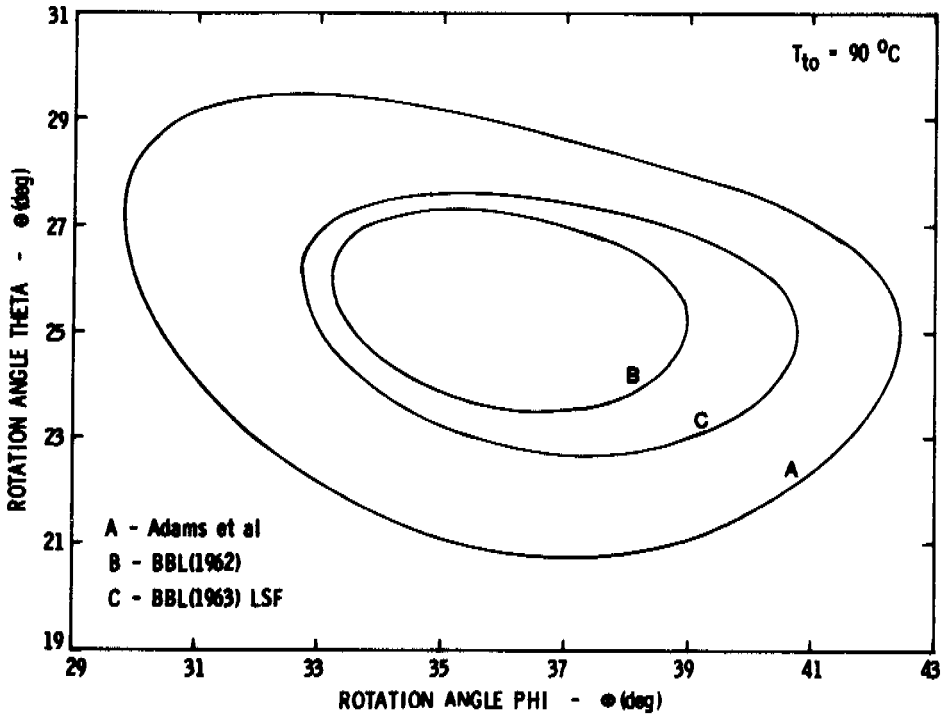

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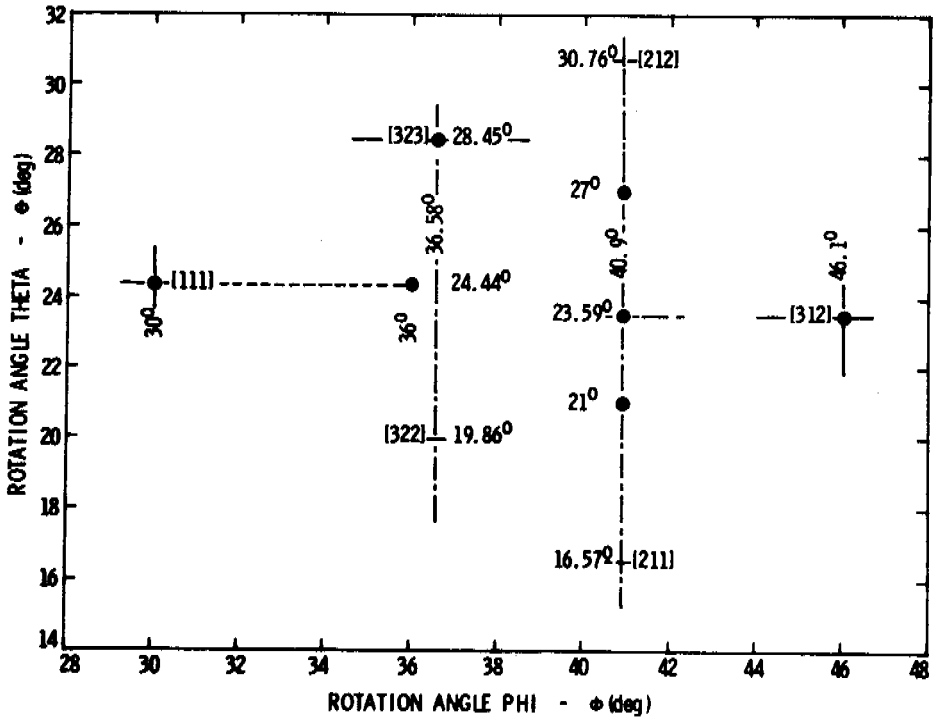

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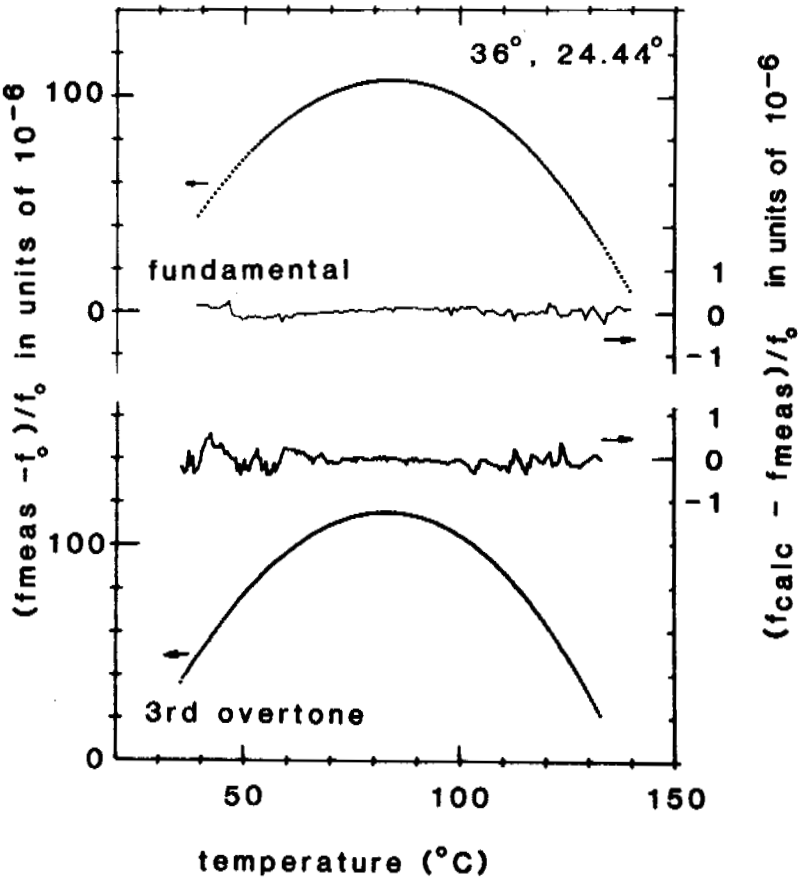

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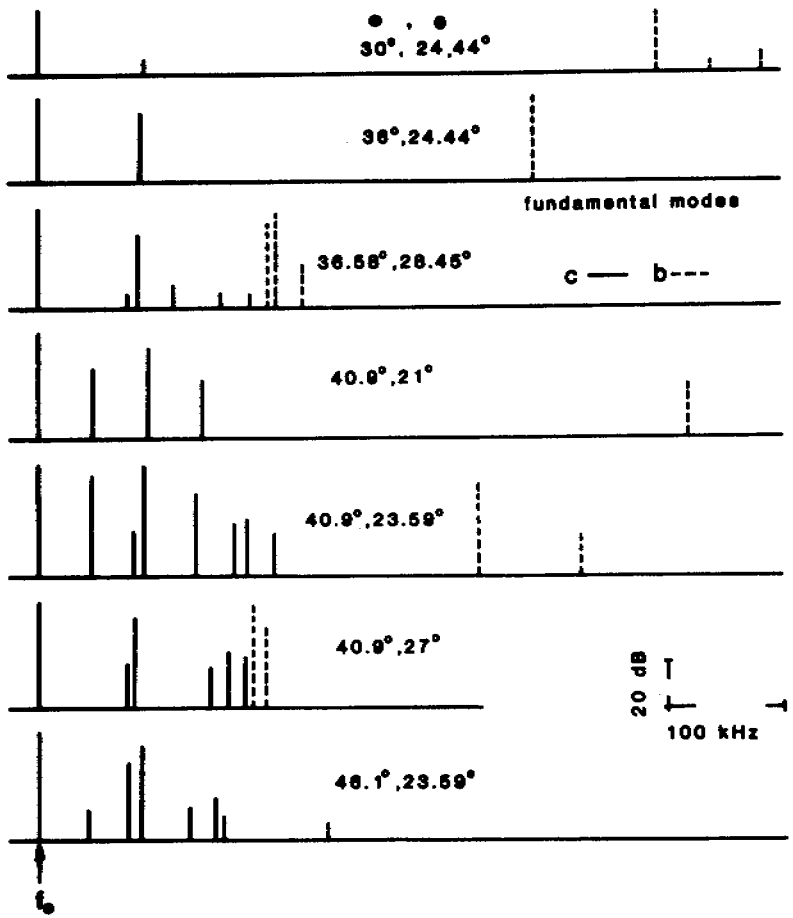

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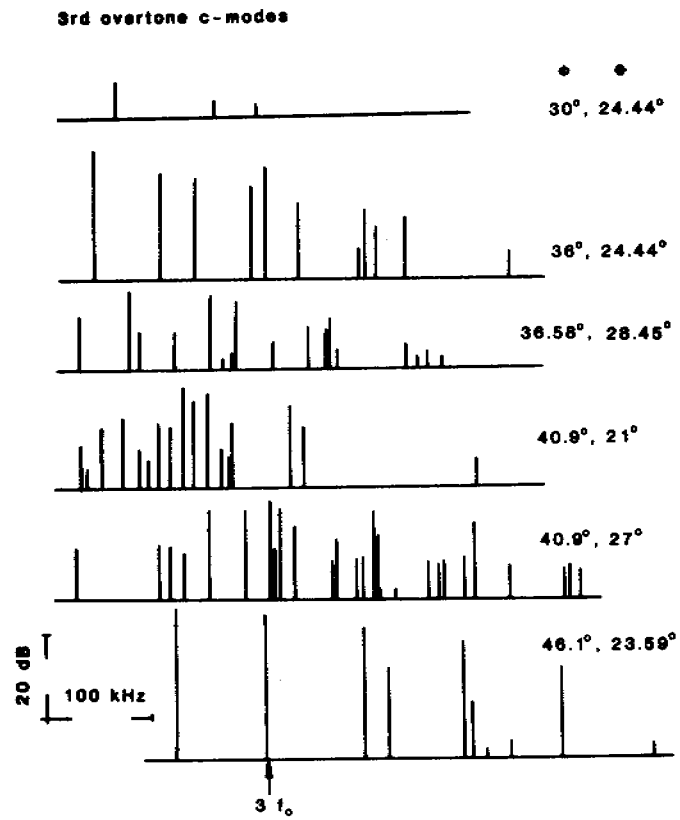

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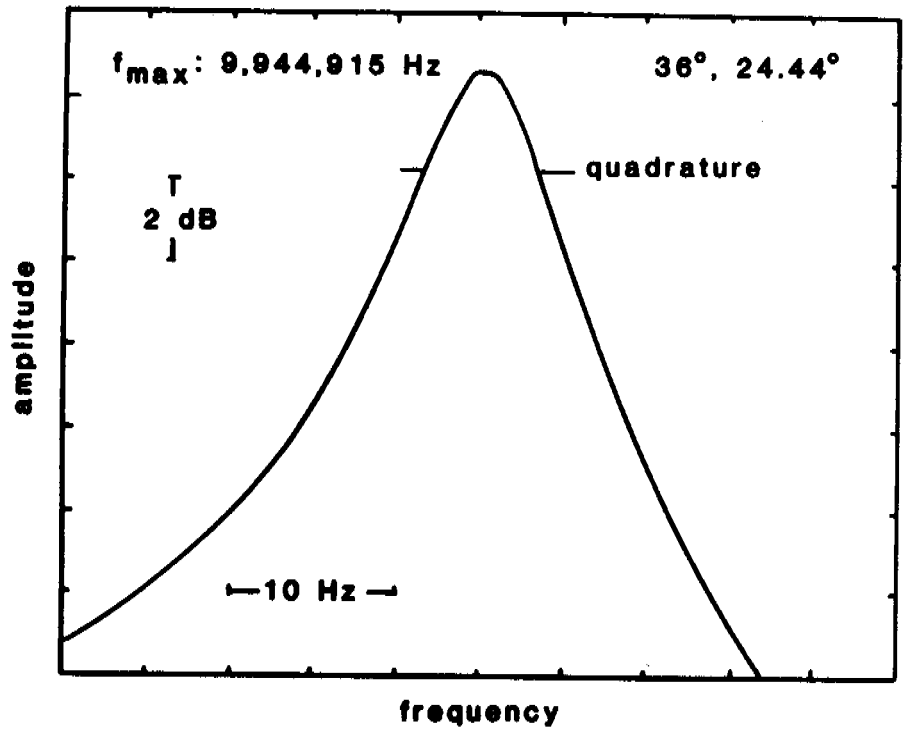

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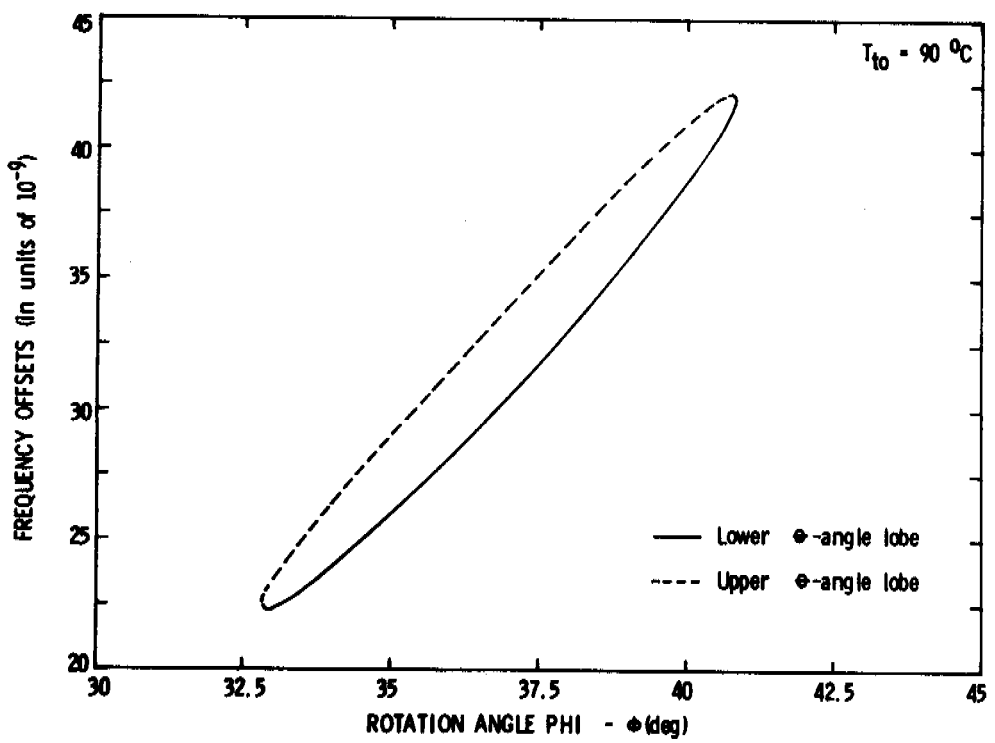

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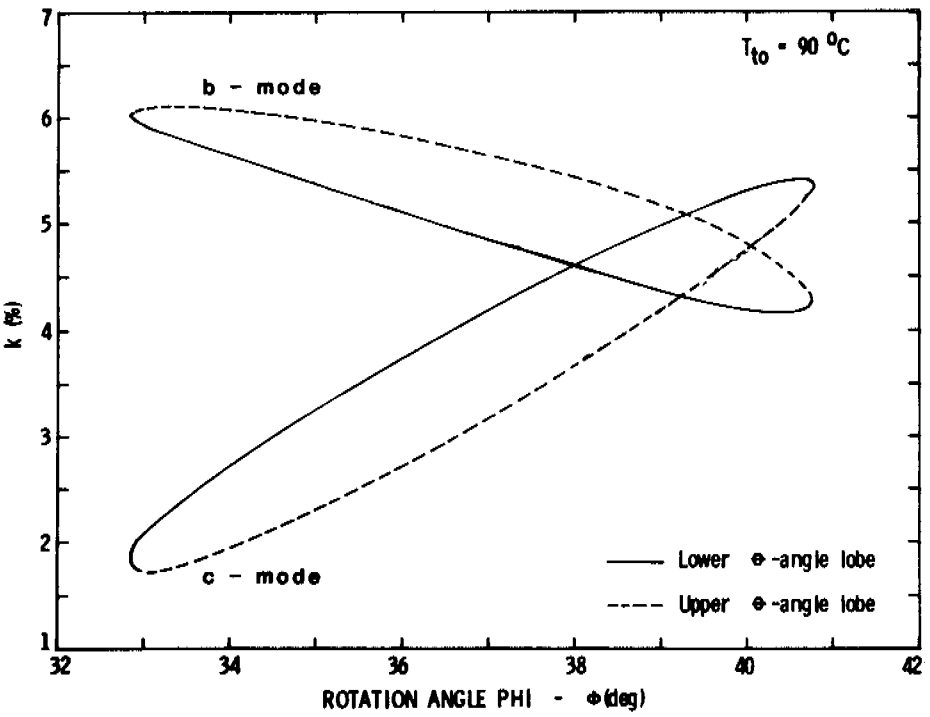

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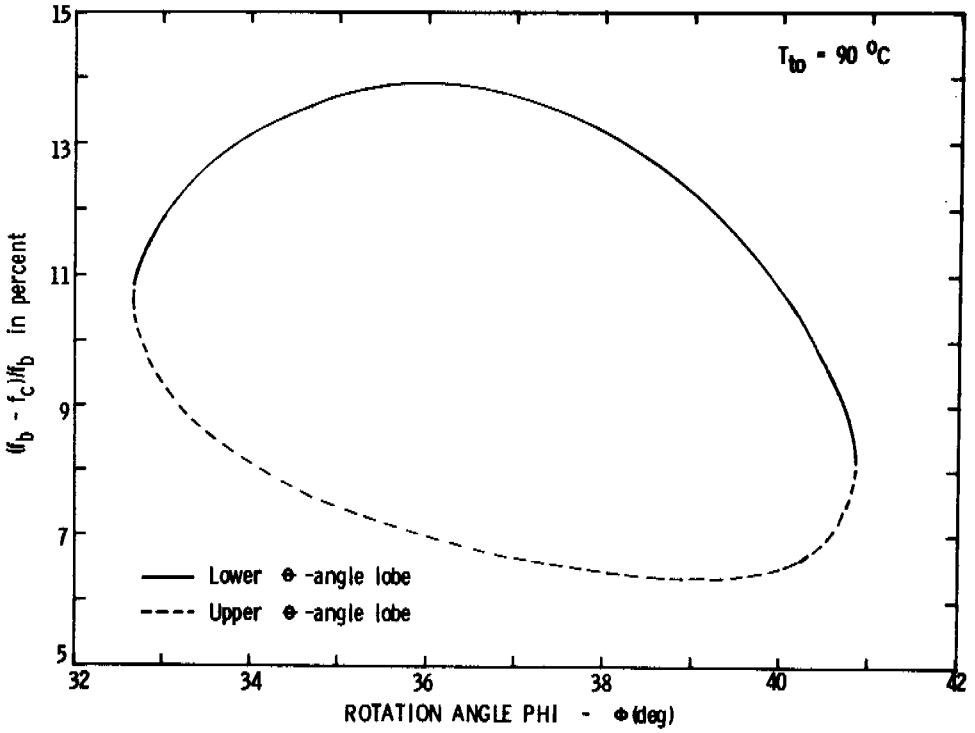

Figure 11. Calculated b-mode to c-mode frequency separation for AK-cuts with turnover at 90°C.

QUESTIONS AND ANSWERS

None for Paper #29