



## 2017 ICU Honolulu

### *Sixth International Congress on Ultrasonics*

Honolulu, Hawaii, USA

18-20 December 2017

### Physical Acoustics: Paper ICU2017 - 51

## Optimal orientations of quartz crystals for bulk acoustic wave resonators with the consideration of thermal properties

**Ji Wang, LiangMeng Zhang, ShaoyunWang, LongTao Xie, Bin Huang, TingFeng Ma and JianKe Du**

*Piezoelectric Device Laboratory, Ningbo University, Ningbo, Zhejiang, 315211, CHINA;  
wangji@nbu.edu.cn, 1002101047@qq.com, wangshaoyun88@163.com, xielongtao@nbu.edu.cn,  
huangbin@nbu.edu.cn, matingfeng@nbu.edu.cn, dujianke@nbu.edu.cn*

**Min-Chiang Chao and JuLian Shen**

*TXC (Ningbo) Corporation, Ningbo, Zhejiang, 315800, CHINA; chaomk@txc.com.tw; obi-wan@txc.com.tw*

**RongXing Wu**

*Department of Civil Engineering, Ningbo Polytechnic, 1069 Xinda Road, Belun, 315800, CHINA;  
wurongxing98@163.com*

**HaiFeng Zhang**

*Department of Mechanical and Energy Engineering, University of North Texas, Denton, 76210, TX;  
Haifeng.Zhang@unt.edu*

Piezoelectric crystals are widely used for acoustic wave resonators of different functioning modes and types including BAW and SAW. It is well-known that only some special orientations of crystals will exhibit desirable properties such as mode couplings, thermal stability, acceleration sensitivity, and others that are important in design and applications of resonators. With extensive studies on physical properties in last decades and increasing industrial needs of novel products, it is necessary to comb the known knowledge of quartz crystal material for novel orientations and better products. With known elastic, piezoelectric, dielectric, and thermal constants, we can establish the relationships between vibrations and bias fields such as temperature to ensure a resonator immunizing from excessive response to changes causing significant degradation of resonator properties and performances. Since the theoretical framework of wave propagation in piezoelectric solids is known, we need to use the existing data and results for the validation of current orientations in actual products. Through rotations, we calculated physical properties as functions of angles and bias fields, enabling the calculation of resonator properties for the identification of optimal cuts.



## 1. INTRODUCTION

The study on the relationship between the frequency and temperature of a resonator has a long history. Shortly after the invention of resonator in the 1920s, Koga set the first-order derivative of the frequency-temperature relationship ( $T_f^{(1)}$ ) to zero for a singly-rotated crystal plate at 25°C, discovered the AT- and BT-cut crystal resonators<sup>1-3</sup>. In 1962, Bechmann solved the equation of the first derivative of the frequency to temperature of the doubly-rotated crystal at 25°C systematically and obtained the curves of the two angles<sup>4</sup>. However, AT- and SC- cut resonators which are widely used have the so-called cubic temperature behavior<sup>5</sup>, which also need the second derivative of the frequency-temperature relationship ( $T_f^{(2)}$ ) to be zero. In this paper, we established the frequency temperature relation  $f(\theta, \phi, T)$  of doubly-rotated crystal based on thermal incremental field theory<sup>6</sup>, then we set  $T_f^{(1)} = T_f^{(2)} = 0$  and obtained curves corresponding to two angles and reference temperature ( $T_f$ ) near which the frequency of resonators varied very slowly with temperature.

## 2. THEORY

### A. BASIC EQUATIONS OF QUARTZ CRYSTAL IN A THERMAL FIELD

Temperature affects crystal vibrations in two ways. On one hand, the free object will expand when the temperature rises and the thermal stress will be generated when the object is bounded. On the other hand, the elastic constants change as the temperature changes. With the consideration of those two factors, Lee established the thermal incremental field equations which are linearized from the nonlinear equations based on a Lagrangian description<sup>6</sup>.

The strains with thermal consideration are

$$e_{ij} = \frac{1}{2}(\beta_{ki}u_{k,j} + \beta_{kj}u_{k,i}), \quad (1)$$

where  $u_i$ ,  $e_{ij}$ ,  $\beta_{ij}$  are the components of incremental displacement, strain and thermal expansion coefficients, respectively, and

$$\beta_{ik} = \delta_{ij} + \alpha_{ij}^{(1)}(T - T_0) + \alpha_{ij}^{(2)}(T - T_0)^2 + \alpha_{ij}^{(3)}(T - T_0)^3, \quad (2)$$

where  $\delta_{ij}$  is Kronecker symbol,  $T$  is the actual temperature,  $T_0$  is room temperature of 25°C,  $\alpha_{ij}^{(k)}$ , ( $k = 1, 2, 3$ ) is the  $k$ th-order expansion coefficient, and the values are chosen from Lee<sup>6</sup>.

The thermal stress-strain relations are

$$t_{ij} = D_{ijkl}e_{kl}, \quad (3)$$

where  $t_{ij}$  and  $D_{ijkl}$  are stress and thermal elastic constants, and

$$D_{ijkl} = C_{ijkl} + D_{ijkl}^{(1)}(T - T_0) + D_{ijkl}^{(2)}(T - T_0)^2 + D_{ijkl}^{(3)}(T - T_0)^3, \quad (4)$$

where  $C_{ijkl}$  and  $D_{ijkl}^{(m)}$ , ( $m = 1, 2, 3$ ) are the elastic constants, the  $m$ th-order thermal elastic constants whose values are chosen from Lee<sup>6</sup>.

The stress equations of motion are

$$\beta_{ik}t_{jk,j} = \rho\ddot{u}_i \quad \text{in } V, \quad (5)$$

and the traction-stress relations in boundary are

$$p_i = n_j(\beta_{ik}t_{jk}) \quad \text{in } S. \quad (6)$$

where  $t_{ij}$ ,  $p_i$ ,  $n_j$  are the stress tensor, traction vector and the surface normal, respectively.

### B. EQUATIONS OF AN INFINITE PLATE IN AN INCREMENTAL THERMAL FIELD

As we know, the vibration of plates is extremely complicated, but quartz resonators work in thickness-shear mode which is relatively simple and can be derived from the model of an infinite plate. Although many factors can affect the frequency, previous studies show the piezoelectricity and the effect

of electrode can be neglected<sup>7-8</sup> and our results won't change significantly while the ratio of length and thickness is greater than 50<sup>6,8</sup>.

For infinite plates, the length and width coordinates are ignored and only the thickness coordinates are left. In this case, the displacement function can be written as<sup>9</sup>

$$u_i = u_i(x_2, t), \quad (7)$$

and the boundary conditions of the plate can be expressed as

$$T_2 = T_4 = T_6 = 0, \quad x_2 = \pm b. \quad (8)$$

Now we rewrite the tensor form of Eqs. (1) - (6) in matrix form by using infinite plates assumption as the gradient equations

$$\begin{bmatrix} S_6 \\ S_2 \\ S_4 \end{bmatrix} = \begin{bmatrix} \beta_{11} & \beta_{12} & \beta_{13} \\ \beta_{12} & \beta_{22} & \beta_{23} \\ \beta_{13} & \beta_{23} & \beta_{33} \end{bmatrix} \begin{bmatrix} u_{1,2} \\ u_{2,2} \\ u_{3,2} \end{bmatrix}, \quad (9)$$

constitutive equations

$$\begin{bmatrix} T_6 \\ T_2 \\ T_4 \end{bmatrix} = \begin{bmatrix} D_{66} & D_{26} & D_{46} \\ D_{26} & D_{22} & D_{24} \\ D_{46} & D_{24} & D_{44} \end{bmatrix} \begin{bmatrix} S_6 \\ S_2 \\ S_4 \end{bmatrix}, \quad (10)$$

equations of motion

$$\rho \begin{bmatrix} \ddot{u}_1 \\ \ddot{u}_2 \\ \ddot{u}_3 \end{bmatrix} = \begin{bmatrix} \beta_{11} & \beta_{12} & \beta_{13} \\ \beta_{12} & \beta_{22} & \beta_{23} \\ \beta_{13} & \beta_{23} & \beta_{33} \end{bmatrix} \begin{bmatrix} T_{6,2} \\ T_{2,2} \\ T_{4,2} \end{bmatrix}. \quad (11)$$

By substituting Eq. (9) into the Eq. (10), and then into Eq. (11) resulting the following matrix equation

$$\rho \begin{bmatrix} \ddot{u}_1 \\ \ddot{u}_2 \\ \ddot{u}_3 \end{bmatrix} = \mathbf{K} \begin{bmatrix} u_{1,2} \\ u_{2,2} \\ u_{3,2} \end{bmatrix}, \quad (12)$$

where

$$\mathbf{K} = \begin{bmatrix} \beta_{11} & \beta_{12} & \beta_{13} \\ \beta_{12} & \beta_{22} & \beta_{23} \\ \beta_{13} & \beta_{23} & \beta_{33} \end{bmatrix} \begin{bmatrix} D_{66} & D_{26} & D_{46} \\ D_{26} & D_{22} & D_{24} \\ D_{46} & D_{24} & D_{44} \end{bmatrix} \begin{bmatrix} \beta_{11} & \beta_{12} & \beta_{13} \\ \beta_{12} & \beta_{22} & \beta_{23} \\ \beta_{13} & \beta_{23} & \beta_{33} \end{bmatrix}. \quad (13)$$

Solving the above equation, we first assume a special solution  $u_i = A_i e^{i(\eta x_2 - \omega t)}$ , and substitute the solution into Eq. (12) to obtain the eigenvalue equation. Defining wave speed as  $c = \rho \omega^2 / \eta^2$ , we can get the following eigenvalue equation

$$\mathbf{K}\mathbf{A} = c\mathbf{A}. \quad (14)$$

Solving the above eigenvalue equation, and then substituting the general solution according to the principle of superposition to the boundary condition, we can obtain

$$f_i = \frac{n}{4b} \sqrt{\frac{c_i}{\rho}}, \quad i = 1, 2, 3, n = 1, 3, 5, 7, \dots \quad (15)$$

In the above we choose  $f_1 > f_2 > f_3$ , and their vibration modes are designated as A, B, and C mode, respectively.

### C. DERIVATIVE EQUATIONS

Having obtained the frequency formula, we need to calculate the derivatives of frequency on the temperature. Because the frequency is always positive, we write the above equation in logarithmic form in order to facilitate the calculation<sup>1</sup>,

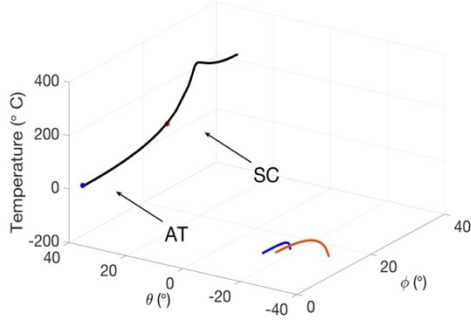
$$\ln f = \ln \frac{n}{2} - \ln b + \frac{1}{2} \ln c - \frac{1}{2} \ln \rho. \quad (16)$$

Because those equations are based on Lagrange description, the density, thickness and orientation of the crystal plate are chosen to be constant values in their natural state whose temperature is 25°C. Only the wave speed changes with temperature so that its derivative and the second derivative are zeroes, resulting in the following two equations

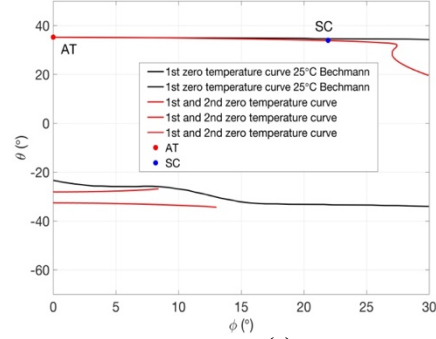
$$T_f^{(1)}(\phi, \theta, T) = \frac{d \ln f}{dT} = \frac{1}{2c} \frac{dc}{dT} = 0, \quad (17)$$

$$T_f^{(2)}(\phi, \theta, T) = \frac{dT_f^{(1)}}{dT} = -\frac{1}{2} \left( \frac{1}{c} \frac{dc}{dT} \right)^2 + \frac{1}{2c} \frac{d^2c}{dT^2} = 0. \quad (18)$$

Solving the above two equations simultaneously, we obtained curves with two angles and temperature as three independent variables.



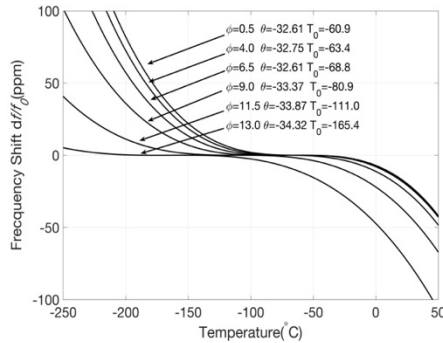
**Figure 1.** Three-dimensional curves of  $T_f^{(1)} = 0$ ,  $T_f^{(2)} = 0$  for mode C.



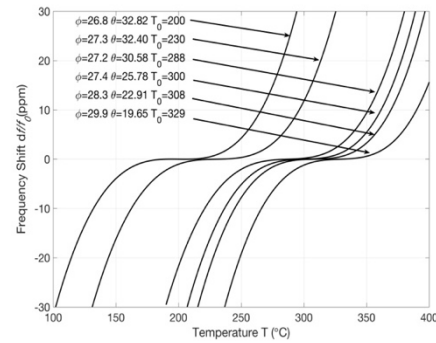
**Figure 2.** Locus of  $T_f^{(1)}(\phi, \theta, 25^\circ\text{C}) = 0$  by Bechmann and  $T_f^{(1)} = 0$ ,  $T_f^{(2)} = 0$  for mode C.

### 3. RESULTS

The quartz belongs to the 32 symmetry group, so the minimum period of  $\phi, \theta$  are  $60^\circ$  and  $180^\circ$  respectively. However, we chose the rotation angles in the range of  $\phi \in (0^\circ, 30^\circ)$  and  $\theta \in (-90^\circ, 90^\circ)$  which was same as Bechmann<sup>4</sup>, since the angle  $\phi$  of solutions are symmetric in the minimum period. The three-dimensional (3-D) curves of reference temperature and two angles are shown in Fig. 1, which are in a large temperature range of  $(-200^\circ\text{C}, 350^\circ\text{C})$ . For comparison, we superimposed the 3-D curves which were projected in plane of two angles to the Bechmann's solution curves of  $T_f^{(1)}(\phi, \theta, 25^\circ\text{C}) = 0$  in Fig. 2.



**Figure 3.** Frequency-temperature curves of different angles of black branch in  $\phi \in (0^\circ, 25^\circ)$  in Fig.1.



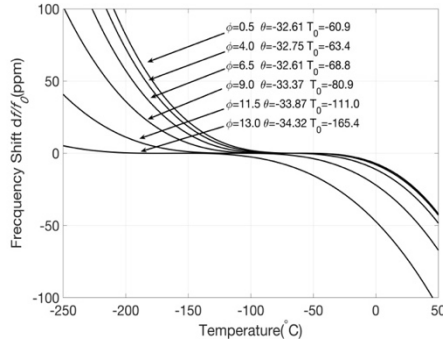
**Figure 4.** Frequency-temperature curves of different angles of black branch in  $\phi \in (25^\circ, 30^\circ)$  in Fig.1.

In order to clearly show that the points on the curves of  $T_f^{(1)} = T_f^{(2)} = 0$  do have excellent frequency-temperature performance, we selected some points evenly on the top three curves to draw their temperature-frequency curves, as shown in Figs. 3-6.

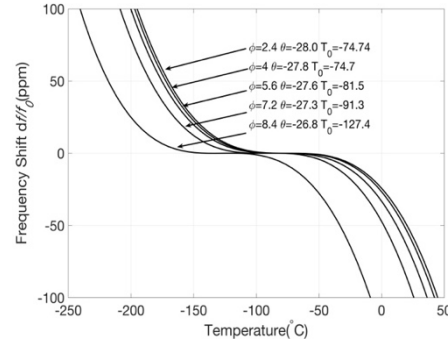
### 4. CONCLUSIONS AND DISCUSSIONS

Using the equations  $T_f^{(1)} = T_f^{(2)} = 0$ , we gained the 3-D curves of reference temperature and two angle in doubly-rotated crystal. On these curves, resonators have the cubic temperature property as the most commonly used AT- and SC-cut types. This is a general procedure to find good temperature-frequency effect, which can provide reference for the future research on the relationship between frequency and temperature of other crystal materials. We compared our curves with Bechmann's and

found that the positive branch  $\phi \in (0^\circ, 25^\circ)$  are close to each other. It accounts for the fact that the AT- and SC-cut resonators obtained through  $T_f^{(1)}(\phi, \theta, 25^\circ\text{C}) = 0$  have the property  $T_f^{(2)} = 0$ . In addition, we found that two branches of  $\phi \in (25^\circ, 30^\circ)$  and  $\theta < 0$  have very high and low second-order zero temperature coefficient points, implying the potential to create high- and low-temperature resonators.



**Figure 5. Frequency-temperature curves of different angles of blue branch in Fig.1.**



**Figure 6. Frequency-temperature curves of different angles of red branch in Fig.1.**

## ACKNOWLEDGMENTS

This research is supported in part by the National Natural Science Foundation of China (Grants 11372145, 11672142, & 11772163). Additional support is from the TXC (Ningbo) Corporation under industrial partnership program with Ningbo University. The research is also supported by the K. C. Wong Magana Fund established and administered by Ningbo University.

## REFERENCES

- <sup>1</sup> V. E. Bottom, "Introduction to quartz crystal unit design," *Van Nostrand Reinhold Company*. New York, (1982).
- <sup>2</sup> I. Koga, "Temperature coefficients of elastic constants of quartz," *JIEE Japan*. **53 (545)**, 1141, (1933).
- <sup>3</sup> A. Ballato, "Doubly rotated thickness mode plate vibrators," *Physical Acoustics*. **13 (C)**, 115-181, (1977)
- <sup>4</sup> R. Bechmann, A. D. Ballato, T. J. Lukaszek, "Higher-order temperature coefficients of the elastic stiffnesses and compliances of alpha-quartz," *Proceedings of the IRE*. **50 (8)**, 1812-1822 (1962).
- <sup>5</sup> M. Weihnacht, "Links between temperature stable BAW and SAW crystal orientations," *Proceedings - IEEE Ultrasonics Symposium*. **2**, 914-917(2005).
- <sup>6</sup> P. C. Y. Lee, Y. K. Yong, "Frequency-temperature behavior of thickness vibrations of doubly rotated quartz plates affected by plate dimensions and orientations," *Journal of Applied Physics*. **60 (7)**, 2327-2342 (1986).
- <sup>7</sup> R. X. Wu, W. J. Wang, G. J. Chen, H. Chen, T. F. Ma, J. K. Du, J. Wang, "Free and forced vibrations of SC-cut quartz crystal rectangular plates with the first-order Mindlin plate equations," *Ultrasonics*. **73**, 96-106(2017).
- <sup>8</sup> J. Wang, W. J. Wang, G. J. Chen, J. K. Du, T. F. Ma, and D. J. Huang, "Vibration analysis of SC-cut quartz crystal plates with the Mindlin and Lee plate theories," *Proceedings of the 2011 Symposium on Piezoelectricity, Acoustic Waves and Devices Applications*, 445-448, (2011).
- <sup>9</sup> R. D. Mindlin, "An introduction to the mathematical theory of vibrations of elastic plates," edited by J. S. Yang, *World Scientific*, 23-34, New Jersey (2006).