Novel Quartz Crystal Cuts for SAW Substrates with Cubic Frequency-temperature Relations

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***Abstract*—This study focused on the searching of new cuts for SAW substrates of triply-rotated quartz with cubic frequency-temperature (f-T) relationship by solving the equations of the first and second derivatives of the f-T function. First we established the f-T function of SAW, which was presented in matrix form and was based on the thermal incremental field theory. Next the wave velocity was obtained by the golden search method. Then the first two derivatives of the f-T function were calculated by multi-point finite difference formula. Finally, solving the nonlinear equations of the first two derivatives in the whole range of triply-rotated quartz, we obtained some new cuts with high inflection temperature T_i about 85℃.**

Keywords—SAW, quartz, crystal, frequency, temperature, rotation

I. Introduction

For bulk acoustic wave (BAW) resonators, the frequency-temperature function of AT-cut quartz crystal is a cubic function while the BT-cut is parabolic function. Since the cubic f-T function is more stable, AT-cut is much more widely used in resonators than BT-cut although whose frequency constants are higher. Just like the BT-cut in BAW, the corresponding cut with parabolic function in surface acoustic wave resonators (SAW) is the ST-cut. However, crystal cuts like AT-cut with cubic f-T function are not found in SAW except 33°Y-cut which was fabricated with some special technology on electrodes [1]. A lot of efforts are made in finding the temperature insensitive cuts [2], but it seems that a systematic searching for triply-rotated quartz crystal without the consideration of electrodes have not been tried until now.

In an earlier study [3], we introduced a general method by solving the equations of the first two derivatives of the f-T function to find optimal cuts with cubic f-T functions in BAW. Using this method in doubly-rotated quartz, we obtained some f-T curves that run through the existed cuts like AT-, FC-, IT-, SC- cuts and their inflection temperatures. Now we are extending this method to the triply-rotated quartz crystal for SAW resonators.

II. An Description of Methods

A. Rotation angles in SAW

In this study, we use the so-called "BAW angles" that can be expressed by standard IRE 49 [4] notation as $(yxwlw)\phi,\theta,\psi$. It can be transformed into Eulerian angles (λ,μ,θ) easily which is familiar to SAW researchers [2].

B. The method to find cuts with cubic f-T function

The frequency f is propotional to the surface wave velocity c , and the c can be calculated through the characteristic equation which is the function of rotation angles ϕ,θ,ψ and temperature T of the quartz crystal substrate. So it is possible to obtain the function $f(\phi,\theta,\psi,T)$ in an implicit form that it can be only calculated numerically.

We can expand $f(\phi,\theta,\psi,T)$ vs. T at reference temperature T_0 as

$$f(\phi,\theta,\psi,T)=f_0(\phi,\theta,\psi,T_0)+f'(\phi,\theta,\psi,T_0)(T-T_0)+f''(\phi,\theta,\psi,T_0)(T-T_0)^2+f'''(\phi,\theta,\psi,T_0)(T-T_0)^3. \quad (1)$$

The high-order terms are neglected since they are very small, and the first derivative are defined as

$$f'(\phi,\theta,\psi,T_0)=\left.\frac{\partial f}{\partial T}\right|_{T=T_0}. \quad (2)$$

In fact, we are concerned with the relative shift of frequency $\frac{\Delta f}{f}(\phi,\theta,\psi,T)$ vs. the change of temperature $(T-T_0)$ as

$$\frac{\Delta f}{f}(\phi,\theta,\psi,T)=T_f^{(1)}(\phi,\theta,\psi,T_0)(T-T_0)+T_f^{(2)}(\phi,\theta,\psi,T_0)(T-T_0)^2+T_f^{(3)}(\phi,\theta,\psi,T_0)(T-T_0)^3, \quad (3)$$

where $T_f^{(1)},T_f^{(2)},T_f^{(3)}$ are the first-, second- and third-order temperature coefficients of frequency respectively

$$\frac{\Delta f}{f}(\phi,\theta,\psi,T)=\frac{f(\phi,\theta,\psi,T)-f_0(\phi,\theta,\psi,T_0)}{f_0(\phi,\theta,\psi,T_0)}, \quad (4)$$

$$T_f^{(1)}(\phi,\theta,\psi,T_0)=\frac{f'(\phi,\theta,\psi,T_0)}{f_0(\phi,\theta,\psi,T_0)}, \quad (5)$$

$$T_f^{(2)}(\phi,\theta,\psi,T_0)=\frac{f''(\phi,\theta,\psi,T_0)}{f_0(\phi,\theta,\psi,T_0)}, \quad (6)$$

$$T_f^{(3)}(\phi,\theta,\psi,T_0)=\frac{f'''(\phi,\theta,\psi,T_0)}{f_0(\phi,\theta,\psi,T_0)}. \quad (7)$$

In (3), we set

$$\begin{cases}T_f^{(1)}(\phi,\theta,\psi,T_0)=0\\ T_f^{(2)}(\phi,\theta,\psi,T_0)=0\end{cases}. \quad (8)$$

The roots of (8) are denoted as $(\phi_i,\theta_i,\psi_i,T_i)$ in earlier papers where i denotes the inflection point whose second derivative is zero. However, it is saddle point since the first two derivatives are both zero actually.

Then (3) becomes

$$\frac{\Delta f}{f}(\phi_i,\theta_i,\psi_i,T) = T_f^{(3)}(\phi_i,\theta_i,\psi_i,T_i)(T-T_i)^3. \quad (9)$$

We call (9) the ideal cubic f-T function to distinguish it from a general cubic function. In (9), $T_f^{(3)}(\phi_i,\theta_i,\psi_i,T_i)$ is quite small, so (9) varies slowly with temperature near the inflection point which is used to be the reference temperature in practical applications.

The cut (ϕ_i,θ_i,ψ_i) we are searching for will have the ideal cubic f-T function if the reference temperature is the inflection point temperature T_i. Furthermore, because there are four variables in two equations in (8), the roots $(\phi_i,\theta_i,\psi_i,T_i)$ cannot be independent and they constitute surfaces in a four-dimensional space.

C. *Frequency-temperature function of SAW*

The derivation of f-T function of SAW are based on the incremental thermal field theory of piezoelectricity, and the detailed derivation can be referred to the earlier papers [3, 5-7]. Here we give the equations in the matrix form directly which can be rewritten from linear equations easily. Meanwhile, the third coordinate x_3 in Fig.1 is neglected because of the feature of the propagation of surface waves.

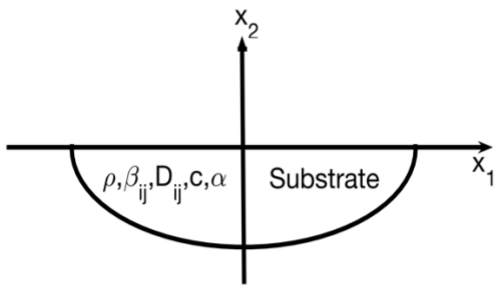

Fig. 1. The analytical model of a semi-infinite substrate

Firstly, we have the strain-displacement relation,

$$\boldsymbol{S} = \boldsymbol{ABu}, \quad (10)$$

where $\boldsymbol{S}$ and $\boldsymbol{u}$ are tensors of strain and displacements respectively, and

$$\boldsymbol{S} = [S_1 \quad S_2 \quad S_4 \quad S_5 \quad S_6]^T, \quad (11)$$

$$\boldsymbol{u} = [u_1 \quad u_2 \quad u_3]^T, \quad (12)$$

$$\boldsymbol{A} = \begin{bmatrix} \beta_{11} & \beta_{21} & \beta_{31} & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta_{12} & \beta_{22} & \beta_{32} \\ 0 & 0 & 0 & \beta_{13} & \beta_{23} & \beta_{33} \\ \beta_{13} & \beta_{23} & \beta_{33} & 0 & 0 & 0 \\ \beta_{11} & \beta_{22} & \beta_{32} & 0 & 0 & 0 \end{bmatrix}, \quad (13)$$

$$\boldsymbol{B} = \begin{bmatrix} \partial_{x_1} & 0 & 0 \\ 0 & \partial_{x_1} & 0 \\ 0 & 0 & \partial_{x_1} \\ \partial_{x_2} & 0 & 0 \\ 0 & \partial_{x_2} & 0 \\ 0 & 0 & \partial_{x_2} \end{bmatrix}, \quad (14)$$

where β_{ij} is the thermal expansion coefficients which can be found in Ref. [3], and

$$\partial_{x_1} = \frac{\partial}{\partial x_1}, \partial_{x_2} = \frac{\partial}{\partial x_2}. \quad (15)$$

Secondly, the stress-strain relations are

$$\boldsymbol{T} = \boldsymbol{CS}, \quad (16)$$

$$\boldsymbol{T_B} = \boldsymbol{FS}, \quad (17)$$

where $\boldsymbol{T}$ and $\boldsymbol{T_B}$ are the stress tensors,

$$\boldsymbol{T} = [T_1 \quad T_2 \quad T_4 \quad T_5 \quad T_6]^T, \quad (18)$$

$$\boldsymbol{T_B} = [T_2 \quad T_4 \quad T_6]^T, \quad (19)$$

$$\boldsymbol{C} = \begin{bmatrix} D_{11} & D_{12} & D_{13} & D_{14} & D_{15} & D_{16} \\ D_{21} & D_{22} & D_{23} & D_{24} & D_{25} & D_{26} \\ D_{41} & D_{42} & D_{43} & D_{44} & D_{45} & D_{46} \\ D_{51} & D_{52} & D_{53} & D_{45} & D_{55} & D_{56} \\ D_{61} & D_{62} & D_{63} & D_{64} & D_{65} & D_{66} \end{bmatrix}, \quad (20)$$

$$\boldsymbol{F} = \begin{bmatrix} D_{21} & D_{22} & D_{23} & D_{24} & D_{25} & D_{26} \\ D_{41} & D_{42} & D_{43} & D_{44} & D_{45} & D_{46} \\ D_{61} & D_{62} & D_{63} & D_{64} & D_{65} & D_{66} \end{bmatrix}, \quad (21)$$

where D_{ij} is the thermal elastic constants which can be found in Ref. [3].

Thirdly, the equations of motion are

$$\rho\ddot{\boldsymbol{u}} = \boldsymbol{DET}, \quad (22)$$

where ρ is the density, and

$$\boldsymbol{D} = \begin{bmatrix} \beta_{11} & \beta_{12} & \beta_{13} & \beta_{13} & \beta_{12} & \beta_{11} \\ \beta_{21} & \beta_{22} & \beta_{23} & \beta_{23} & \beta_{22} & \beta_{21} \\ \beta_{31} & \beta_{32} & \beta_{33} & \beta_{33} & \beta_{32} & \beta_{31} \end{bmatrix}, \quad (23)$$

$$\boldsymbol{E} = \begin{bmatrix} \partial_{x_2} & 0 & 0 & 0 & 0 \\ 0 & \partial_{x_2} & 0 & 0 & 0 \\ 0 & 0 & \partial_{x_2} & 0 & 0 \\ 0 & 0 & 0 & \partial_{x_1} & 0 \\ 0 & 0 & 0 & 0 & \partial_{x_1} \\ 0 & 0 & 0 & 0 & \partial_{x_2} \end{bmatrix}. \quad (24)$$

Finally, substituting (10) and (16) into (22), we have

$$\rho\ddot{\boldsymbol{u}} = \boldsymbol{DECABu}. \quad (25)$$

The displacements function of surface waves are

$$\boldsymbol{u} = \boldsymbol{a}e^{-k\alpha x_2}e^{\mathrm{i}k(x_1-ct)}, \quad (26)$$

where k is the wavenumber, α is the decaying index, c is the wave velocity, and $\boldsymbol{a} = [a_1 \quad a_2 \quad a_3]^T$ is the vector of amplitudes.

Substituting (26) into (25) and using the following transformation

$$\partial_{x_1} \to \mathrm{i}, \qquad \partial_{x_2} \to -\alpha, \quad (27)$$

we have

$$(\boldsymbol{DECAB} + \rho c^2\boldsymbol{I})\boldsymbol{a} = \boldsymbol{0}, \quad (28)$$

where $\boldsymbol{I} = \mathrm{diag}(1,1,1)$. There are nontrivial solution of $\boldsymbol{a}$ in (28) that is equivalent to

$$\det(\boldsymbol{DECAB} + \rho c^2\boldsymbol{I}) = 0. \quad (29)$$

The equivalent characteristic polynomial of α always have three decaying roots whose real parts are positive [8]. Selecting those three roots and substituting them into (28), we have three eigenvectors $\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{a_3}$ and they form a matrix $\boldsymbol{b} = [\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{a_3}]$. They can span a general solution,

$$\boldsymbol{u} = c_1 \boldsymbol{a_1} e^{-k\alpha x_2} e^{\mathrm{i}k(x_1 - ct)} + c_2 \boldsymbol{a_2} e^{-k\alpha x_2} e^{\mathrm{i}k(x_1 - ct)} + c_3 \boldsymbol{a_3} e^{-k\alpha x_2} e^{\mathrm{i}k(x_1 - ct)}. \tag{30}$$

Substituting the general solution (30) into the boundary condition

$$\boldsymbol{T_B} = \boldsymbol{FABu} = \boldsymbol{0}, \qquad x_2 = 0, \tag{31}$$

Meanwhile, we define $\boldsymbol{B_1}$, $\boldsymbol{B_2}$, $\boldsymbol{B_3}$ when ∂_{x_2} in $\boldsymbol{B}$ is substituted by $\alpha_1, \alpha_2, \alpha_3$ respectively. Finally, we have

$$\boldsymbol{T_B} = [\boldsymbol{FAB_1a_1} \quad \boldsymbol{FAB_2a_2} \quad \boldsymbol{FAB_3a_3}] \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \boldsymbol{0}, \tag{32}$$

or

$$\det([\boldsymbol{FAB_1a_1} \quad \boldsymbol{FAB_2a_2} \quad \boldsymbol{FAB_3a_3}]) = 0. \tag{33}$$

The left handside in (33) is a function of $(\phi, \theta, \psi, T, c)$, and the solution can be expressed as

$$c = c(\phi, \theta, \psi, T), \tag{34}$$

and frequency f is proportional to the wave velocity c, so we have the frequency-temperature function

$$f = f(\phi, \theta, \psi, T). \tag{35}$$

D. *Numerical Examples*

The f-T function $f(\phi, \theta, \psi, T)$ is an implicit function by solving Eq. (33) that is in complex domain so it cannot be solved by using bisection method. However, it can be transformed to an absolute value equation

$$|\det([\boldsymbol{FAB_1a_1} \quad \boldsymbol{FAB_2a_2} \quad \boldsymbol{FAB_3a_3}])| = 0 \tag{36}$$

which can be solved by golden section search method.

Eq. (8) are nonlinear equations, it can be transformed to an extreme problem and the local minimum can be found by the minimization method. When the local minimum are found, it is easy to check if the conditions are satisfied.

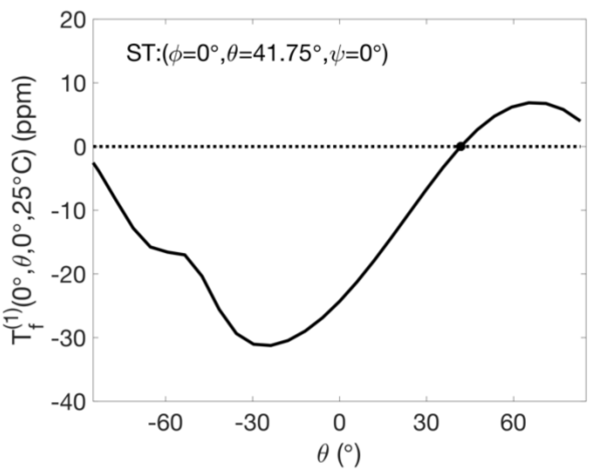

Fig. 2. The first derivatives vs. singly-rotated angle of Y-cut quartz. The intersection is the ST-cut whose angle is 41.75℃ that smaller than 42.75℃ [2, 9].

III. RESULTS & DISCUSSION

With a formulation based on the frequency-temperature relation of the surface acoustic waves in a quartz crystal blank of three rotations, we can look for cuts with good thermal behavior from the known f-T function.

First of all, we use the known popular cuts with good f-T properties to validate the formulation. With just one rotation, we obtained an f-T curve at constant temperature 25℃ as shown in Fig. 2. It is clear that we have a cut of $\theta = 41.75$℃, which is close to known ST-cut [2, 9]. Further comparison of f-T curves of two cuts is presented in Fig. 3. It is clear that the formulation can confirm the known results [10], giving the confidence to search novel cuts with certain requirements.

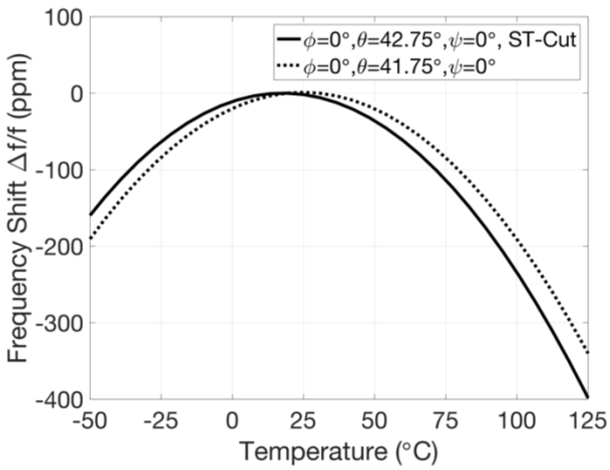

Fig. 3. The f-T curves of $\theta = 41.75°$ and $\theta = 42.75°$.

To find better cuts with the ideal cubic f-T curves, we now adopt the searching criteria by setting the first and second derivatives of the frequency function to zeroes, which can find cuts from two to three rotations. After extensive calculations, with two rotation angles we have results shown in Figs. 4 and 5. It reveals that there are two cuts with cubic f-T curves. However, the inflection temperatures are relatively high than room temperature for most resonators, and the applications should be for some special cases to take the advantage. The details of the f-T relations are shown in Fig. 6, demonstrating a rare thermal property never known in SAW resonators before.

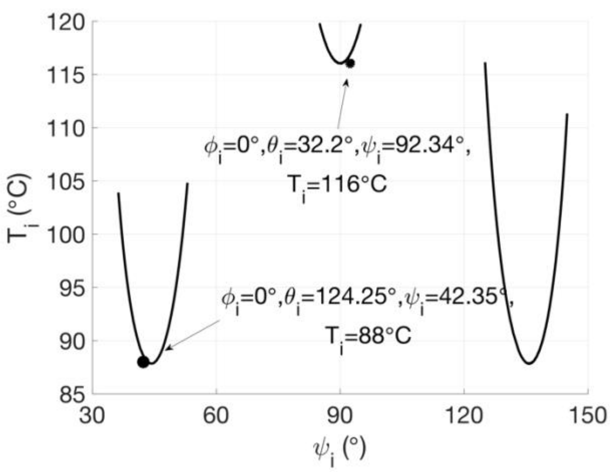

Fig. 4. Front view of curve of novel cuts of doubly-rotated Y-cut quartz.

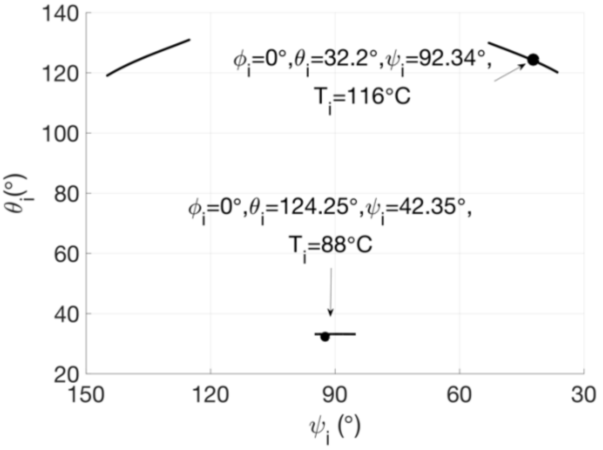

Fig. 5. Top view of curve of novel cuts of doubly-rotated Y-cut quartz.

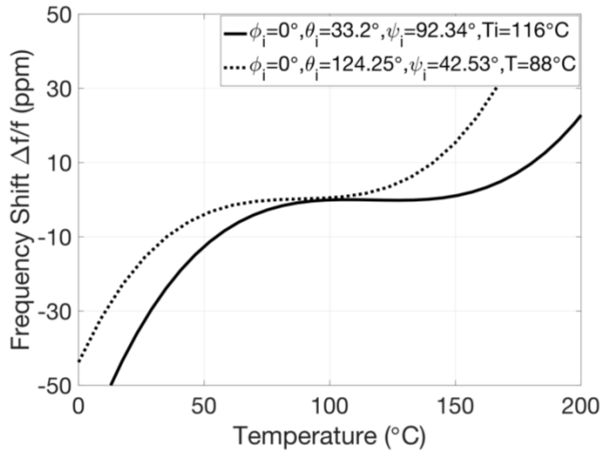

Fig. 6. Frequency-temperature curve of novel cuts.

IV. Conclusions

A complete formulation of the frequency-temperature relation of SAW in quartz crystal is presented with the consideration of rotation angles and the incremental thermal theory. By utilizing the f-T function from the formulation, cuts with better f-T properties are confirmed and found. The formulation is validated with known results, and it can be extended for quartz crystal and other materials for ideal cuts to meet SAW resonator development requirements.

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