FREQUENCY-TEMPERATURE CHARACTERISTIC ANALYSIS OF PIEZOELECTRIC RESONATORS USING FINITE ELEMENT MODELING

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ABSTRACT

The resonators made of piezoelectric crystals such as a quartz crystal are widely used. Their frequency-temperature characteristics are of primary importance for their applications to the frequency control devices. The characteristics estimation is useful for determining their design parameters. In the present paper, several types of resonators are numerically analyzed. The numerical solutions are made using 3-D Finite Element Modeling, and the results are compared with the theoretical values whenever they are available. To demonstrate the validity of the present numerical approach, the application is made to the analysis of the plates with some well-established cutting angles. For the resonator stable with temperature change, the cutting angle is important in which the temperature coefficient of the first order is chosen to be zero. The rotated Y-cut plates in thickness-shear mode are considered. The equivalent circuit representation is often used for describing the characteristics at the electrical terminals which enables the circuit analysis including the effect of temperature change by using the circuit simulators. The equivalent circuit parameters are obtained by fitting the admittance-frequency curve from the finite element analysis.

1 INTRODUCTION

The resonators made of piezoelectric crystals are widely used for the frequency control devices. In such applications, the frequency-temperature characteristics of the resonators are primarily important. In order to control the frequency-temperature characteristics, various cutting angles are devised for the crystal. Proper cutting angles have historically been developed experimentally for some simple modes of vibration. The temperature effect however depends on the shape of the resonators, which should be examined by the numerical method such as the finite element modeling.

In this paper, the frequency-temperature characteristics of a thickness-shear mode resonator made of quartz crystal are examined by using three-dimensional finite element modeling. The equivalent circuit parameters are also determined for the mode of interest. Thus the resonator can easily be incorporated in the electric circuit analysis.

It should be noted that the effect of the temperature change in the resonant frequencies for the crystal plate resonators was considered by means of the finite element method as early as in 1981[1], where a square crystal plate in plane motion was analysed in the two-dimensional modelling.

2 MODELING

Three-dimensional finite element modeling is used for numerical simulations. The formulation is made for the isoparametric cubic elements with eight nodes. The discretized equation of vibration including piezoelectric effect is given by

$$\begin{bmatrix} (1+j\frac{1}{Q_m})-\omega^2[M] & [\Gamma] \\ [\Gamma]^T & -[G] \end{bmatrix} \begin{bmatrix} \{u\} \\ \{\phi\} \end{bmatrix} = \begin{bmatrix} \{f\} \\ \{q\} \end{bmatrix} \tag{1}$$

where $[K]$, $[M]$, $[G]$ and $[\Gamma]$ are stiffness, mass, capacitance and electro-mechanical coupling matrices, $\{u\}$, $\{\phi\}$, $\{f\}$ and $\{q\}$ are displacement, electric potential, force and electric charge vectors. Q_m is the mechanical quality factor of the plate.

2.1 Temperature Dependency

The piezoelectric equations of e form are expressed as

$$\{T\} = \lceil c^E \rceil \{S\} - [e]^T \{E\} \tag{2}$$

$$\{D\} = [e] \{S\} + \lceil \varepsilon^S \rceil \{E\} \tag{3}$$

$\{T\}$, $\{D\}$, $\{S\}$, $\{E\}$, $\lceil c^E \rceil$, $[e]$ and $\lceil \varepsilon^S \rceil$ are stress, electric flux, strain, electric field, stiffness, electro-mechanical coupling constants and permittivity respectively. The effect of the temperature change on the parameters is the result of the changes of some physical constants due to the temperature change. Though the values of $\lceil c^E \rceil$, $[e]$ and $\lceil \varepsilon^S \rceil$ may change with the temperature, only $\lceil c^E \rceil$ among others is chosen to be of interest. In addition, the structural deformation and the change of mass density, caused by the thermal expansion $[L]$, are included. Each component of both $\lceil c^E \rceil$ and $[L]$ is expanded in the third order polynomials, which are expressed as follows

$$\chi = \chi_0 + \alpha_\chi \Delta t + \beta_\chi \Delta t^2 + \gamma_\chi \Delta t^3 \tag{4}$$

where χ_0 refers to the value at the reference temperature, and α_χ, β_χ and γ_χ are the first, second and third order temperature constants, which are generally measured with respect to the main crystal coordinate axes.

Since thermal expansion in quartz crystal is anisotropic, resultant deformation depends on the cutting angle. Thus the thermal expansion matrix $[L]$ as well as other physical constants must be converted into the orientation so that

$$[L'] = [l] [L] [l]^T \tag{5}$$

where $[L']$ and $[L]$ are the converted and original thermal expansion matrix and $[l]$ is the rotation matrix, which consists of directional cosines. Note that converted thermal expansion matrix is not diagonal while the original thermal expansion matrix is diagonal.

Mass density ρ also changes by thermal expansion. It is simply expressed using the reciprocal of volume expansion

$$\rho = \rho_0 \Big/ \prod_{i=1}^{3} L_{ii} \tag{6}$$

where ρ_0 is mass density at the reference temperature. L_{ii} is coefficients of the thermal expansion defined by

$$L_{ii} = \frac{x_i}{x_{i0}} \tag{7}$$

Table 1: Material constants of quartz

$c^E 11$	$c^E 12$	$c^E 13$	$c^E 14$	$c^E 33$
0.86474	0.0699	0.1191	−0.1791	1.072
$c^E 44$	$c^E 66$		$\varepsilon^S_{11}/\varepsilon_0$	$\varepsilon^S_{33}/\varepsilon_0$
0.5794	0.3988 [$\times 10^{11}$N/m^2]		4.43	4.63
e_{11}	e_{25}		ρ	
0.171	0.0403 [C/m^2]		2650 [kg/m^3]	

Table 2: Temperature coefficients

	α_χ [$\times 10^{-6}$]	β_χ [$\times 10^{-9}$]	γ_χ [$\times 10^{-12}$]
$c^E 11$	−48.5	−107	−70
$c^E 12$	−3000	−3050	−1260
$c^E 13$	−550	−1150	−750
$c^E 14$	101	−48	−590
$c^E 33$	−160	−275	−250
$c^E 44$	−177	−216	−216
$c^E 66$	178	118	21
L_{11}	13.71	6.5	−1.9
L_{33}	7.48	2.9	−1.5

where x_{i0} and x_i are the lengths in i direction at the reference temperature and after the expansion, respectively.

3 NUMERICAL DEMONSTRATION

A thickness-shear mode resonator made of rotated Y-cut quartz crystal plate is solved for the temperature characteristics. The material constants of the quartz and their temperature coefficients used for the analysis are shown in Tables 1 and 2, which are taken from the reference, R.Bechmann *et al* [2].

3.1 Comparison with the Analytical Solutions for Infinite Plate Model

The analytical value of the resonant frequency f_r of the fundamental thickness-shear mode, for an infinite plate, is given by

$$f_r = \frac{1}{2y} \sqrt{\frac{c_{66}^{E\,\prime}}{\rho}} \tag{8}$$

where y and ρ are the plate thickness and mass density respectively. $c_{66}^{E\,\prime}$ is a component of the stiffness of the rotated Y-cut plate, depending on cutting angle, which is

$$c_{66}^{E\prime} = l_{22}^2 c_{66}^E + l_{32}^2 c_{44}^E + 2\, l_{22}\, l_{32}\, c_{14}^E \tag{9}$$

where l_{22} and l_{32} are the components of the rotation matrix $[\,l\,]$, which appear in equation(5). They are expressed for the rotation angle θ about x axis,

$$\begin{cases} l_{22} = \cos\theta \\ l_{23} = \sin\theta \end{cases} \tag{10}$$

Thickness y of the plate under the thermal deformation is given as follows

$$y = y_0 \sqrt{\frac{L_{22}^2\, L_{33}^2}{l_{22}^2\, L_{33}^2 + l_{32}^2\, L_{22}^2}} \tag{11}$$

where y_0 is the thickness at the reference temperature.

The configuration and finite element model with element division for the infinite plate model is shown in Fig. 1. Proper boundary conditions make this model equivalent to an infinite plate.

The frequency-temperature curve for the 35.1°-rotated Y-cut plate is shown in Fig. 2. FEM(a) is the case in which the deformation by thermal expansion depends on equation(5). FEM(b) is the case in which the deformation by thermal expansion is restricted only to the direction of thickness. This means that the thickness is determined by equation(11), same value used for the analytical solution. The values of the analytical and FEM(a) solution agree each other. However, the value of the FEM(b) solution is slightly shifted. This is because as the temperature increses from the reference temperature, the thermal expansion may cause the shear deformation as well as volume deformation, which may effect on the vibrational mode.

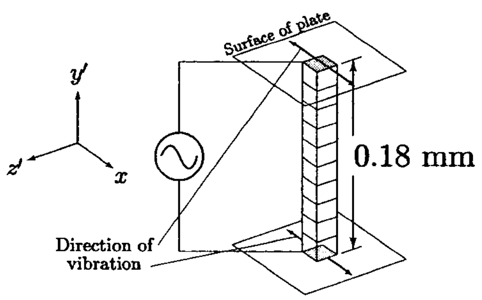

Fig. 1: The finite element model with element division for an infinite plate model in thickness shear mode

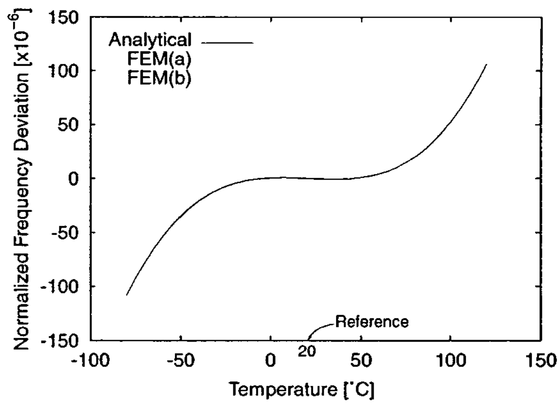

Fig. 2: Frequency-temperature dependency of a 35.1°-rotated Y-cut infinite plate model by FEM and analytical results

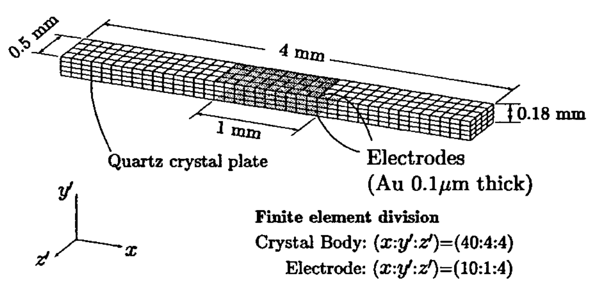

Fig. 3: A quartz crystal plate, configuration and finite element division

3.2 Three-Dimensional Model for a plate of finite dimension

The plate, its configuration and the finite element division, is shown in Fig. 3. The fundamental thickness-shear mode is shown in Fig. 4 with the electric potential distribution. The vibration is trapped in the electroded region.

The frequency-temperature characteristics are examined for various cutting angles from 34.9° to 35.2°, which are shown in Fig. 5 including the solution for the infinite plate model. It is found that the freqency of the three-dimensional model tends to be lower than that of the infinite plate model at the reference temperature. The first order frequency-temperature coefficient is responsible for that. The three-dimensional model shows that the cutting angle with which the first order coefficient becomes zero is smaller than that of AT-cut plate($\theta = 35.25°$).

Fig. 6 shows the first, second and third order frequency-temperature coefficients, which are determined by fitting the equation(4) to the frequency-temperature curve. α_f is zero for the cutting angle about 34.7°, which is smaller by 0.55° than that of the AT-cut infinite plate. At that cutting angle, the second and the third order temperature coefficients β_f and γ_f are 1.5×10^{-9} and 115.6×10^{-12} respectively, whose values roughly agree with the known values 1.2×10^{-9} and 100×10^{-12}, given in reference [3].

3.3 Equivalent Circuit Representation

The characteristics of piezoelectric resonators at their electrical terminals are often represented by the equivalent circuit as shown in Fig. 7. The damped capacitance C_0 is directly solved by static finite element analysis, while L_1, C_1 and R_1 are obtained by fitting the admittance-frequency curve of the circuit to that of the finite element solution, as shown in Fig. 8.

The equivalent circuit parameters and their temperature coefficients of the resonator made of 34.7° rotated Y-cut plate are shown in Table 3. Note that the first and the second order coefficients of L_1 and C_1 are complementary.

Table 3: Equivalent circuit parameters and their temperature coefficients ($\theta = 34.7°$)

		α_X $[\times 10^{-6}]$	β_X $[\times 10^{-9}]$	γ_X $[\times 10^{-12}]$
C_0	$1.25 \times 10^{-13}[F]$	9.8	4.4	-4.4
L_1	$0.23[H]$	-69	-32	6.5
C_1	$1.2 \times 10^{-15}[F]$	69	32	-233
R_1	$136[\Omega]$	-69	-28	128

4 CONCLUSION

The frequency-temperature characteristics of a quartz crystal plate resonator are solved by three-dimensional finite element modeling.

The finite element solutions for the infinite plate model are compared with the analytical solutions of the one-dimensional model. When the anisotropic thermal deformation is included, the numerical solutions are slightly different from the analytical solution. When the plate thickness is only assumed to change due to thermal expansion, the FEM solution agrees with the analytical solution. This means that the one-dimensional

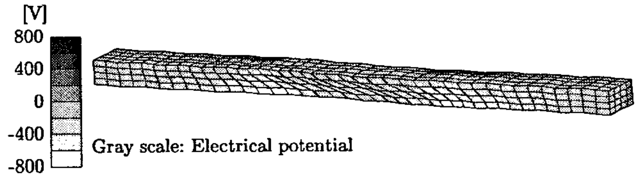

Fig. 4: Deformation and electric potential distribution for the fundamental thickness-shear mode, obtained by 3-D FEM

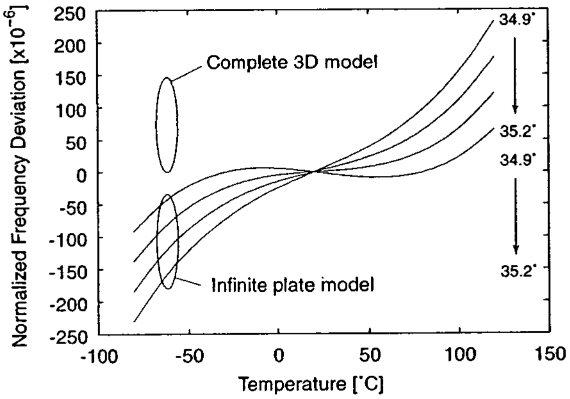

Fig. 5: Frequency-temperature dependency of a rotated Y-cut plate (3-D FEM)

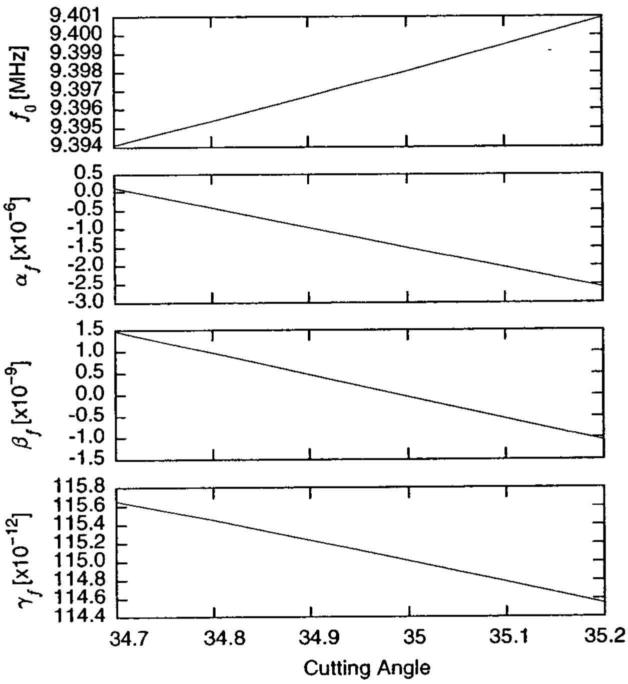

Fig. 6: Changes of resonant frequency and its temperature coefficients against the cutting angle

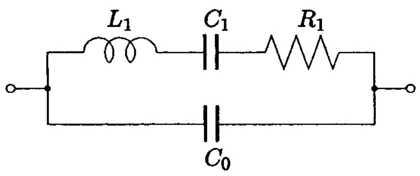

Fig. 7: Equivalent circuit of the resonator

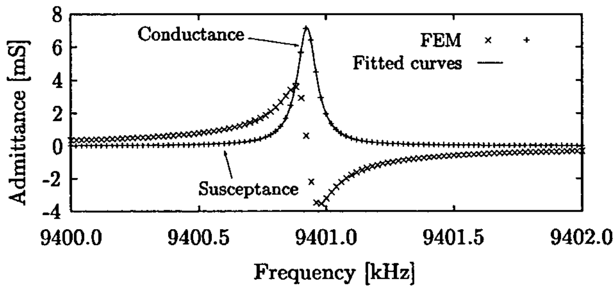

Fig. 8: Admittance-frequency curve

analysis is not proper for the temperature characteristics evaluation. The effect of the plate dimension must be included.

The frequency-temperature characteristics are then solved for the three-dimensional model. The resonant frequency and the equivalent circuit parameters are obtained by fitting the admittance-frequency curve of the circuit to the finite element solutions. Their temperature coefficients are also obtained. They may now be incorporated with the electronic circuit, suitable for the analysis by a circuit simulator such as SPICE.

REFERENCES

[1] Y.Kagawa, H.Maeda and M.Nakazawa, "Finite Element Approach to Frequency-Temperature Characteristic Prediction of Rotated Quartz Crystal Plate Resonators," IEEE Transactions on Sonics and Ultrasonics, Vol. SU-28, No. 4, Jul. 1981

[2] R.Bechmann, A.Ballato and T.J.Lukaszek, "Higher Order Temperature Coefficients of the Elastic Stiffnesses and Compliances of Alpha-Quartz," Proceedings IRE, Vol. 50, pp1812-1822, Aug. 1962

[3] Committee of Ultrasonic Handbook, "Ultrasonic Handbook"(in Japanese), Maruzen, Tokyo, 1999

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