

An Efficient Numerical Method in Calculating the Electrical Impedance Different Modes of AT-Cut Quartz Crystal Resonator

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Abstract—Lee and Brebbia in 1978 presented a finite element analysis (FEA) of AT-cut quartz crystal resonator by including the thickness-shear branches in the length-width directions and the flexural branch in the thickness direction based on Mindlin's 2-D elastic equations. The formulation was pure elastic and electrical impedance of different modes could not be calculated since piezoelectric effect and damping were not included. In the years after, many FEA-based studies were conducted using either the full-blown 3-D elastic-piezoelectric model or the simplified Mindlin's 2-D elastic-piezoelectric model. Such formulations are quite complicated and numerically time-consuming in computation. Furthermore, one experienced tremendous difficulty in resolving the many eigenmodes in the 3-D analysis.

In this paper, we first solve for the eigenmodes of the AT-cut quartz crystal resonator without piezoelectric effect using Lee-Brebbia's FEA method based on Mindlin's 2-D elastic equations. By assuming weak piezoelectric coupling, we rearrange the electrical potential to the right hand side of the elastic-piezoelectric equations of motion. These terms become the forcing terms of the pure elastic equations of motion. We also consider the constant damping terms in the equations of motion. Then we use the mode superposition method to calculate the weight of each eigenmode. The elastic displacement field with electrical potential effect can then be calculated as the weighting sum of each eigenmode. The electrical charges on the quartz crystal resonator can be obtained from the elastic displacement and electrical potential field at each node point. Finally, we can calculate the electrical impedance from the electrical charges and the potential. This method is considered much more efficient than the full-blown 3-D elastic-piezoelectric analysis or the simplified Mindlin's 2-D elastic-piezoelectric analysis.

Keywords- AT-cut quartz resonator; electrical impedance; finite element analysis; mode superposition method

I. INTRODUCTION

Because of its high Q and high temperature stability, AT-cut quartz is widely used in oscillators as the heart of the circuit. Along with the personal mobile telecommunication process, the miniaturization of circuit components, including resonators and oscillators, is inevitable. As the size of quartz resonators becomes smaller and smaller, the bonding, beveling and electrode effects are much more important than that in the bigger size device in the past. The mode coupling and

temperature stability problems are also more complex in smaller package size. If an engineer still only uses some simple experience formulae or trial and error to design resonators, it is time-consuming and therefore expensive. And it is more difficult to induce empirical formulae by trial and error. Because of the demand of more precise design tool, some commercial finite element analysis (FEA) software can be used to simulate piezoelectric resonators. But AT-cut quartz resonators are strip or round plates and the diameter (or length) to thickness ratio is typical 50 to 100, so it is very hard to take both thickness direction resolution and element aspect ratio into consideration as meshing the quartz plate. However, how to build the model for the electrode and beveling chip is also a challenge in commercial FEA tool. Besides precision, efficiency is also very important for a design engineer. If it spends tens of hours to several days to simulate only one case, the design cycle will be too long and impractical. Because of these reasons, we develop an efficient numerical method and use FORTRAN program to calculate the electrical impedance of different modes of AT-cut quartz crystal resonator. This method can simulate not only pure mechanical vibration behavior but also electrical impedance response, and is both precise enough and efficient for design engineers.

II. THEORY OF PIEZOELECTRIC FINITE ELEMENT

According to Mindlin's two-dimensional plate equations [1] and neglecting the coupling with extensional motions by setting $\bar{c}_{14} = \bar{c}_{34} = c_{56} = 0$, we obtain:

$$Q_{1,1} + Q_{3,3} = 2b\rho\ddot{u}_2 \quad (1a)$$

$$M_{1,1} + M_{5,3} - Q_1 = \frac{2}{3}b^3\rho\ddot{\psi}_1 \quad (1b)$$

$$M_{5,1} + M_{3,3} - Q_3 = \frac{2}{3}b^3\rho\ddot{\psi}_3 \quad (1c)$$

where M_1 and M_3 are bending moment; M_5 is twist moment; Q is shear force; b is half thickness; ρ is density of quartz; ψ_1 and ψ_3 are the rotating angle along axis x_3 and x_1 .

For strip quartz plate, we use the nine-node quadratic element as the FEA elements.

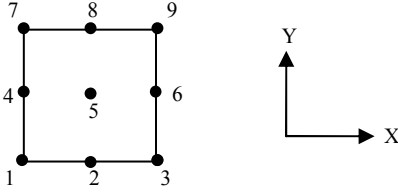


Figure 1. Nine-node quadratic element

Then for an element with dimension W and L along x and y directions, respectively, the interpolation functions are [2]:

$$\phi = \begin{bmatrix} \phi_1 & \phi_4 & \phi_7 \\ \phi_2 & \phi_5 & \phi_8 \\ \phi_3 & \phi_6 & \phi_9 \end{bmatrix} \quad (2)$$

where

$$\begin{aligned} \phi_1 &= \left(1 - \frac{2x}{W}\right) \left(1 - \frac{x}{W}\right) \left(1 - \frac{2y}{L}\right) \left(1 - \frac{y}{L}\right) \\ \phi_2 &= \frac{4x}{W} \left(1 - \frac{x}{W}\right) \left(1 - \frac{2y}{L}\right) \left(1 - \frac{y}{L}\right) \\ \phi_3 &= \frac{x}{W} \left(\frac{2x}{W} - 1\right) \left(1 - \frac{x}{W}\right) \left(1 - \frac{2y}{L}\right) \left(1 - \frac{y}{L}\right) \\ \phi_4 &= \left(1 - \frac{2x}{W}\right) \left(1 - \frac{x}{W}\right) \frac{4y}{L} \left(1 - \frac{y}{L}\right) & \phi_5 &= \frac{4x}{W} \left(1 - \frac{x}{W}\right) \frac{4y}{L} \left(1 - \frac{y}{L}\right) \\ \phi_6 &= \frac{x}{W} \left(\frac{2x}{W} - 1\right) \frac{4y}{L} \left(1 - \frac{y}{L}\right) & \phi_7 &= \left(1 - \frac{2x}{W}\right) \left(1 - \frac{x}{W}\right) \frac{y}{L} \left(\frac{2y}{L} - 1\right) \\ \phi_8 &= \frac{4x}{W} \left(1 - \frac{x}{W}\right) \frac{y}{L} \left(\frac{2y}{L} - 1\right) & \phi_9 &= \frac{x}{W} \left(\frac{2x}{W} - 1\right) \frac{y}{L} \left(\frac{2y}{L} - 1\right) \end{aligned} \quad (2a)$$

Based on the Mindlin's 2D model, there are three degrees of freedom for each node in the element (one displacement and two rotating angle), so the interpolation function of one element is:

$$\phi = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix}_{3 \times 27} \quad (3)$$

where

$$\begin{aligned} \phi_1 &= [\phi_1 \ 0 \ 0 \ \phi_2 \ 0 \ 0 \ \phi_3 \ 0 \ 0 \ \dots \ \phi_9 \ 0 \ 0]_{1 \times 27} \\ \phi_2 &= [0 \ \phi_1 \ 0 \ 0 \ \phi_2 \ 0 \ 0 \ \phi_3 \ 0 \ \dots \ 0 \ \phi_9 \ 0]_{1 \times 27} \\ \phi_3 &= [0 \ 0 \ \phi_1 \ 0 \ 0 \ \phi_2 \ 0 \ 0 \ \phi_3 \ \dots \ 0 \ 0 \ \phi_9]_{1 \times 27} \end{aligned} \quad (3a)$$

By the finite element displacement method for Mindlin's 2D model developed by P.C.Y. Lee et al. [3], the displacement-nodal displacement relationship is:

$$\{U\} = \begin{Bmatrix} u_2 \\ \psi_1 \\ \psi_3 \end{Bmatrix} \quad (4)$$

The displacement vector at i^{th} node of an element is:

$$u^i = \begin{Bmatrix} u_2^i \\ \psi_1^i \\ \psi_3^i \end{Bmatrix} \quad (5)$$

So, the element nodal displacement U^e is:

$$\{U^e\} = \begin{Bmatrix} u^1 \\ u^2 \\ \vdots \\ u^9 \end{Bmatrix}_{27 \times 1} \quad (6)$$

Then, the displacement field, U , within the element is

$$U = [\phi] \{U^e\} \quad (7)$$

The equation of motion for an element (pure mechanical vibration, without damping):

$$[M^e] \{\ddot{U}^e\} + [K^e] \{U^e\} = \{0\} \quad (8)$$

where

$$\begin{aligned} [M^e] &= \int_A [\phi]^T [m] [\phi] dA \\ [m] &= \begin{bmatrix} 2b\rho(1+R) & 0 & 0 \\ 0 & \frac{2}{3}b^3\rho(1+3R) & 0 \\ 0 & 0 & \frac{2}{3}b^3\rho(1+3R) \end{bmatrix} \end{aligned} \quad (8a)$$

$R = 2\rho'b'/\rho b$ is the ratio of the mass of electrodes to the mass of the plate per unit area (if no electrodes, $R=0$)

and

$$\begin{aligned} [K^e] &= \int_A \left([B_b]^T [D_b] [B_b] + [B_t]^T [D_t] [B_t] \right) dA \\ [B_b] &= \begin{bmatrix} \phi_{2,1} \\ \phi_{3,3} \\ \phi_{3,1} + \phi_{2,3} \end{bmatrix}_{3 \times 27} & [B_t] &= \begin{bmatrix} \phi_{1,1} + \phi_2 \\ \phi_{1,3} + \phi_3 \end{bmatrix}_{2 \times 27} \\ [D_t] &= 2b \begin{bmatrix} k_1^2 c_{66} & 0 \\ 0 & \bar{k}_3^2 \bar{c}_{44} \end{bmatrix} \\ [D_b] &= \frac{2}{3} b^3 \begin{bmatrix} \hat{c}_{11} & \hat{c}_{13} & 0 \\ \hat{c}_{13} & \hat{c}_{33} & 0 \\ 0 & 0 & \hat{c}_{55} \end{bmatrix} \end{aligned} \quad (8b)$$

$$k_1^2 = \pi^2(1+3R)/12(1+R)^2$$

$$\bar{k}_3^2 = k_3^2(1+3R)/(1 + \frac{12}{\pi^2} k_3^2 R)^2$$

$$k_3^2 = \pi^2 \left\{ c_{22} + c_{44} - [(c_{22} - c_{44})^2 + 4c_{24}^2]^{1/2} \right\} / 24\bar{c}_{44}$$

$$\bar{c}_{pq} = c_{pq} - c_{2p}c_{q2} / c_{22}$$

$$\hat{c}_{pq} = \bar{c}_{pq} - \bar{c}_{4p}\bar{c}_{q4} / \bar{c}_{44}, \quad \hat{c}_{55} = c_{55} - c_{56}^2 / c_{66}$$

For the piezoelectric effect, we need to extend the pure mechanical equations of motion to include piezoelectric term [4]. The constitutive equations of piezoelectric media in matrix form are:

$$\{T\} = [c^E]\{S\} - [e]\{E\} \quad (9a)$$

$$\{D\} = [e]^T\{S\} - [\epsilon^S]\{E\} \quad (9b)$$

where

- T mechanical stress
- S mechanical strain
- E electric field
- D dielectric displacement
- c^E mechanical stiffness matrix for constant E
- ϵ^S permittivity matrix for constant S
- e piezoelectric stress constant matrix

The electric field E can be expressed by the electrical potential V:

$$E = -\nabla V \quad (10)$$

and the mechanical strain S to the mechanical displacement u by:

$$S = Bu \quad (11)$$

where in the Cartesian coordinates:

$$B = \begin{bmatrix} \partial/\partial x & 0 & 0 & 0 & \partial/\partial z & \partial/\partial y \\ 0 & \partial/\partial y & 0 & \partial/\partial z & 0 & \partial/\partial x \\ 0 & 0 & \partial/\partial z & \partial/\partial y & \partial/\partial x & 0 \end{bmatrix}^T \quad (11a)$$

By Newton's 2nd Law

$$\nabla T = \rho \partial^2 u / \partial t^2 \quad (12)$$

where ρ is the density of the piezoelectric medium. By Maxwell's equation (no free volume charge in the piezoelectric medium):

$$\nabla D = 0 \quad (13)$$

Now, each node has four degrees of freedom: one displacement, two rotating angle, and one electrical potential. By equations (9)-(13), we can obtain the governing equations for piezoelectric medium. The equation of motion for one element:

$$\begin{bmatrix} M^e & 0 \\ 0 & 0 \end{bmatrix} \begin{Bmatrix} \ddot{U}^e \\ \ddot{V}^e \end{Bmatrix} + \begin{bmatrix} K^e & K_{uV}^e \\ K_{uV}^{eT} & K_{VV}^e \end{bmatrix} \begin{Bmatrix} U^e \\ V^e \end{Bmatrix} = \begin{Bmatrix} F^e \\ Q^e \end{Bmatrix} \quad (14)$$

where

$$V = \{V_1 \ V_2 \ V_3 \ \dots \ V_9\}^T \quad \text{electrical potential of each node}$$

$$K_{uV}^e = \int_A B_u^T e^T B_V dA$$

$$B_u = B\phi$$

$$B_V = \begin{Bmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{Bmatrix} \begin{Bmatrix} \varphi_1 & \varphi_2 & \varphi_3 & \dots & \varphi_9 \end{Bmatrix} \quad (14a)$$

$$K_{VV}^e = \int_A B_V^T \epsilon^S B_V dA$$

F^e external force on each node

Q^e electrical charge on each node

in the first term of left hand side, there are zeros in this matrix (no mass for electrical potential), so choosing a suitable method to solve this problem is very important. We do not intend to solve these equations directly, but introduce the "weak coupling" character of quartz to solve the pure mechanical vibration and electrical potential separately.

III. SOLVING THE EQUATIONS OF MOTION WITH PIEZOELECTRIC EFFECT

After assembling the whole elements, we can get the equations of motion in matrix form of the quartz plate:

$$\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{Bmatrix} \ddot{U} \\ \ddot{V} \end{Bmatrix} + \begin{bmatrix} K & K_{uV} \\ K_{uV}^T & K_{VV} \end{bmatrix} \begin{Bmatrix} U \\ V \end{Bmatrix} = \begin{Bmatrix} F \\ Q \end{Bmatrix} \quad (15)$$

symbols in (15) without superscript e means for the whole finite element model. In our model, we consider no external force, so $\{F\} = 0$; nodes of elements with electrodes (plated): $\{V\} = \text{constant}$; nodes of elements without electrodes (unplated): $\{V\} = 0$; $\{Q\}$ is unknown to be solved.

Based on weak piezoelectric coupling, we solve the mechanical and electrical potential parts separately. First we solve the pure mechanical vibration as an eigenmode problem.

$$[M]\{\ddot{U}\} + [K]\{U\} = \{0\} \quad (16)$$

the eigenfunctions

$$\omega_f^2 [M]\{U\} + [K]\{U\} = \{0\} \quad (17)$$

where ω_f is the angular frequency of the quartz plate. By solving (17), we can get the eigenmodes (no external force), $U_1, U_2, U_1, \dots, U_n$, and the eigenvalues, $\omega_{f1}, \omega_{f2}, \omega_{f3}, \dots, \omega_{fn}$. Finishing the pure mechanical vibration analysis, we can get only natural frequencies and shapes in free vibration, but no response amplitude. Many numerical modes even do not exist in the measured results.

To get the electrical potential, we rearrange the electrical potential to the right hand side of the elastic-piezoelectric equations of motion. These terms become the forcing terms of the pure elastic equations of motion:

$$[K_{uV}]\{V(\omega)\} = \{F_e(\omega)\} \quad (18)$$

in (18), we consider the applied electrical potential V is sinusoidal $V(\omega)$; the subscript e in F means the applied force by electrical potential. Add the forcing and damping term into the equations of motion:

$$\omega^2 [M] \{U_{pie}\} + j\omega[\eta] \{U_{pie}\} + [K] \{U_{pie}\} = \{F_e(\omega)\} \quad (19)$$

the subscript pie means the displacement U with piezoelectric effect. In this paper, we consider the damping is constant. Using the mode superposition method [5] to solve U_{pie} :

$$U_{pie} = \alpha_i U_i + \alpha_{i+1} U_{i+1} + \alpha_{i+2} U_{i+2} + \dots + \alpha_k U_k \quad (20)$$

where $U_i, U_{i+1}, U_{i+2}, \dots, U_k$ are the free vibration eigenmodes we choose to superpose; $\alpha_i, \alpha_{i+1}, \alpha_{i+2}, \dots, \alpha_k$ are weights.

We use eigen-expansion to decouple (19) to get decoupled ODEs for the weight of each eigenmode. The elastic displacement field with electrical potential effect, U_{pie} , can then be calculated as the weighting sum of each eigenmode. The electrical charges on the quartz crystal resonator can be obtained from the elastic displacement and electrical potential field at each node point:

$$\begin{bmatrix} K_{uv}^T & K_{vV} \end{bmatrix} \begin{Bmatrix} U_{pie} \\ V \end{Bmatrix} = \begin{Bmatrix} Q(\omega) \end{Bmatrix}$$

IV. SIMULATION RESULTS

By this method, we develop a FORTRAN program to calculate the finite element simulation. The case we present in this paper is a 26 MHz ($3.5 \times 1.86 \text{ mm}^2$) quartz crystal resonator. Its electrode dimension is $1.55 \times 1.2 \text{ mm}^2$ and it is bonded on its two short edges. Because of the symmetry in geometric, we can only model the quarter plate to save memory and enhance the efficiency.

A. Convergence Test

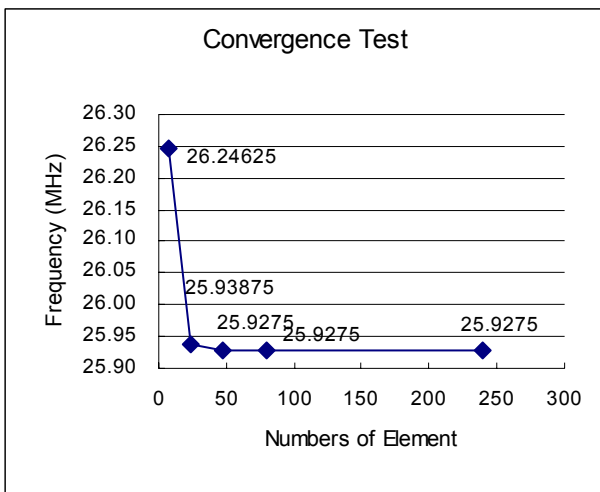


Figure 2. Convergence test for the program in this 26MHz case

The convergence test shows that as the element number over 50, the major vibration mode (thickness shear) frequency will converge to 25.9275 MHz.

B. Comparison Between Simulation and Test Results

Figure 3 is the test results of the 26 MHz resonator measured by Agilent E5100A. It shows that the major vibration frequency is 25.987 MHz, and there are two strong spurious in 26.33817 MHz and 26.745195 MHz

Figure 4 is the simulation results. The major vibration frequency is 25.93875 MHz, and there are also two strong spurious. The two spurs are in 26.31375 MHz and 26.83500 MHz respectively. This simulation results coincide with the test one.

Figure 5a is the legend of Figures 5b-5d. It shows the quarter model of the strip quartz plate.

Figures 5b-5d show the mode shapes of these three resonance frequency. The major vibration in 25.93875 MHz is thickness shear mode; the second, 26.31375 MHz, is flexure mode; and the third, 26.83500 MHz, is thickness twist mode. The program can obtain the electrical potential response but also the vibration mode shape with piezoelectric effect.

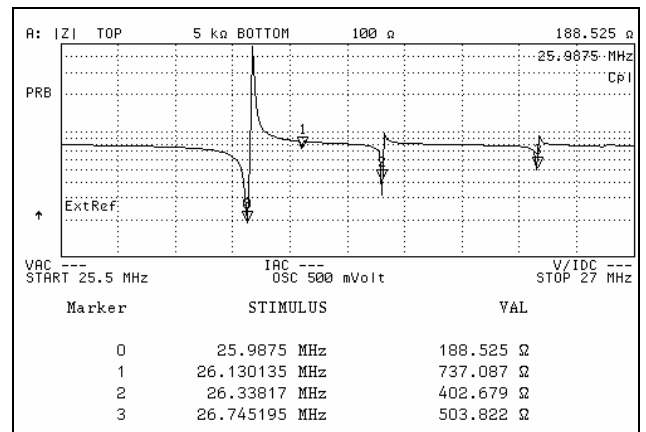


Figure 3. Test results of the 26MHz strip quartz resonator

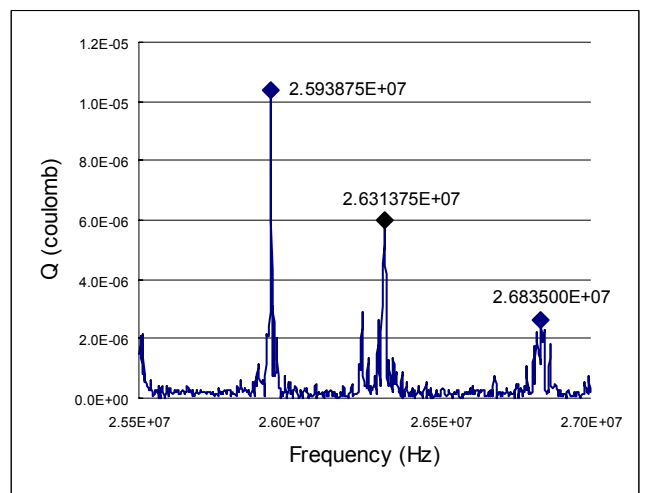


Figure 4. Simulation results of the 26MHz strip quartz resonator

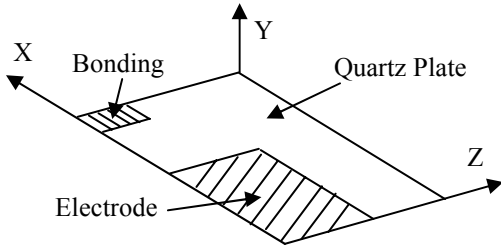


Figure 5a. The legend of the mode shape charts

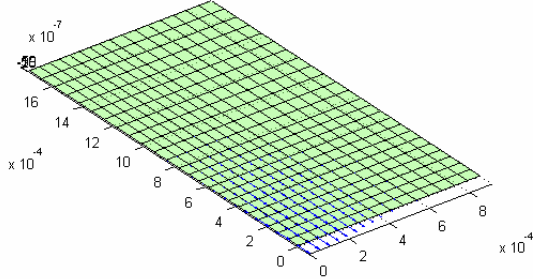


Figure 5b. The mode shape of the major vibration- thickness shear, 25.93875 MHz. The displacement field is concentrated in the plated area, and the displacements are all in the same X direction.

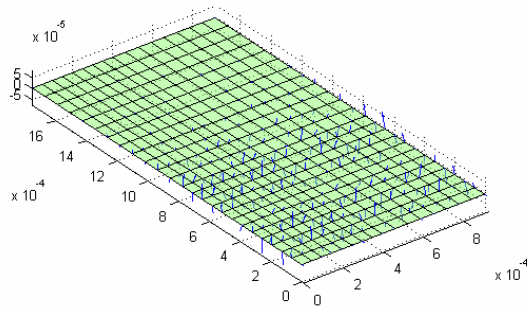


Figure 5c. The mode shape of the second resonance point- flexure, 26.31375 MHz. The displacements are in the out of plane Y direction.

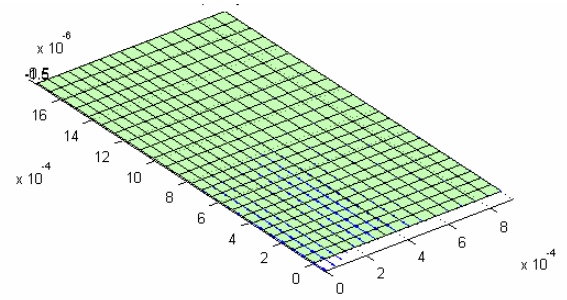


Figure 5d. The mode shape of the third resonance point- thickness twist, 26.83500 MHz. The displacement field is concentrated in the plated area, but the displacements are in different +X and -X direction.

V. CONCLUSION

Based on Mindlin 2-D elastic-piezoelectric model and weak piezoelectric coupling assumption, we separate the pure mechanical vibration and electrical potential effect to develop an efficient numerical method to analyze the AT-cut quartz resonator. First, we solve the free vibration eigenmodes without piezoelectric effect. Second, rearrange the electrical potential and treat them as forcing terms, and then use the mode superposition method to solve the weak coupling vibration mode shape. By the displacement field, we can get charges on the quartz crystal resonator and the electrical impedance. According to the simulation and test results, this method can analyze AT-cut quartz resonator response with piezoelectric effect and electrode very well. In the future, it can be applied to analyze beveling blanks. It is both precise and efficient enough for design engineers.

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