The Simulation of Resonant Mode and Effective Electromechanical Coupling Coefficient of Lithium Niobate Crystal with Different Orientations

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Abstract. At present, the proportion and role of thin film bulk acoustic wave (FBAR) filters in mobile communication products are becoming more and more obvious due to its higher work frequency and smaller size. As a commonly used piezoelectric material, aluminum nitride (AlN) limits the bandwidth of the FBAR filter because of its small electromechanical coupling coefficient ($k_r^2$) of ~6.5%. On contrast, lithium niobate (LiNbO$_3$, LN) crystals with some certain specific orientations have much better acoustic properties, making this type of material the promising candidate for FBAR applications. In this work, the acoustic resonant mode in LN crystal is analyzed by FEM simulations. In order to obtain the optimal orientations with good longitudinal wave property, Euler angle (EA) method is used to simulate the resonant modes and calculate the corresponding $k_r^2$ of different orientations. Besides, the correctness of EA method has been demonstrated in this work by comparing the displacement change under electrostatic field with the traditional matrix transformation operation depending on the piezoelectric effect. The simulations show that the 43°Y-cut LiNbO$_3$ has a high $k_r^2$ and a pure longitudinal wave vibration mode simultaneously, making this orientation the most proper candidate for FBAR filters application with large bandwidth.

1. Introduction

Along with the increasingly request for the high data transmission efficient and portable mobile terminal, wireless communication is rapidly developing. In the communication system, the RF front end, is responsible for receiving and transmitting RF signals. In the RF front end module, the filter mainly plays the role of effectively filtering the signals, realizing the effective signal transmission in a specific frequency band, and filtering out the signal outside the desired band. Currently, surface acoustic wave resonators (SAW) [1] and thin film bulk acoustic waveresonators (FBAR) [2] have been applied in the filter fabrication. The former techique usually can only fulfill the requirements of those bands below 2.5 GHz due to the limit of downscaling the interdigital width [3], while the latter one is undoubtedly much more popular for higher frequency bands.

At present, aluminium nitride has been widely investigated and applied in FBAR filters [4, 5]. However, its electromechanical coupling coefficient ($k_r^2$) is usually less than 6.5% [6]. Although it can reach ~12% after Scandium doping, it is usually at the expense of lifetime [7]. The low $k_r^2$ of AlN limits the bandwidth of the current FBAR filters.

Lithium niobate (LiNbO$_3$, LN) is widely studied in various applications due to its typical anisotropic characteristics. For example, Z-cut LN is researched for optical waveguide for its good electro-optical characteristics [8]. 128 Y-cut and X-cut LN have been studied in SAW devices in some works [9, 10] for its shear wave vibrational mode. Moreover, LN is potentially useful for FBAR...
applications due to its high $k^2$ of longitudinal wave vibrational mode in some specific orientations [11, 12]. In general, the combination of measurement and calculation [13, 14] is used to obtain various physical constants more accurately, such as relative permittivity matrix $[\varepsilon_i]$, compliance matrix $[s_i]$, and piezoelectric coupling matrix $[d_{ij}]$ and so on. Then the $k^2$ can be calculated by the formula of

$$k^2_f = \frac{d_{33}^2}{\varepsilon_{33} \times \varepsilon_{33}} \times \frac{1}{\varepsilon_{33} \times \varepsilon_{33}}.$$ 

In addition, the physical parameter matrices can also be obtained by the coordinate transformation calculation of referred matrixs, and is further to calculate the corresponding $k^2$. Both methods above mentioned require complex calculations, which is prone to increase the probability of error. At the same time, although the orientation of LN with a large electromechanical coupling coefficient can be obtained, the resonant mode of which is disable to be visually observed.

The present work proposed a method to obtain the $k^2$ of different orientations conveniently and quickly, and can also visually observe each resonance mode. This method mainly adopts the Euler angle to define the rotation of the coordinate system, rather than the transformation of the matrix parameters. It is worth noting that the transformation of the matrix parameters with the cut angles is inverse to the rotation of the coordinate system. The finite element simulation is used in combination with the established three-dimensional structure to simulate the piezoelectric field, and finally the resonance modes of different orientations are obtained. Besides, the corresponding $k^2$ can be calculated.

2. The Proposal and Verification of the EA Method

Crystal symmetry is not only shown in geometry, but also in physical constants, therefore, the physical properties of crystal strongly depends on its orientation. For anisotropic piezoelectric single crystals, the referred matrixes of the physical constants are based on a normal coordinate system and generally correspond to c-axis oriented crystals. However, the actual applied crystal usually has a rotary cut type, and its coordinate selection does not coincide with the normal crystal coordinate system. Therefore, the physical constant tensors must be transformed from the c-axis orientation to the rotated one. Generally speaking, the physical parameters of a specific orientation can be calculated by the coordinate transformation, which correspondingly rotates a certain angle by the referenced parameter under the c-axis orientation.

Conventional coordinate transformation needs multiple steps of matrix conversions in order to obtain the corresponding matrixes in the new rotated coordinate system. The main purpose of the present work is to obtain the resonant mode and $k^2$ of longitudinal wave in LN crystals with different orientations. If the new parameters under each orientation require the corresponding transformation calculation, the simulation process is very complicated and difficult to carry on. In this case, the Euler angle in Euclidean space is introduced to define the relationship between two Cartesian coordinate systems before and after rotation. That can directly achieve the structure with post-rotation physical properties while avoiding the tedious calculation. In this way, a more convenient and reliable method is proposed in this work to acquire the change of physical properties based on the establishment of Euler angles, which is referred as "EA method". Combining with the finite element simulation, post-rotated three-dimensional structure consisting of new physical parameters can be achieved automatically. Therefore, building the precise consistent correlation between coordinate transformation and Euler angle can effectively and quickly obtain the physical characteristics under difference orientations.

In this section, the finite element simulations based on the matrix transformation method and EA method under a same orientation are compared. It is obtained that the simulation results of the proposed EA method are consistent with the results obtained by the matrix transformation method. Finally, the EA method is used to calculate the $k^2$ of the longitudinal wave vibration mode for different oriented LN crystal.

2.1. Matrix Transformation Method

In the matrix transformation process, the cut type is usually used to represent the wafer orientation, which is generally indicated by the symbol specified by the IRE standard. Specifically, the IRE symbol contains a set of letters and angles. For example, the cut type "(xy)/θ" is often used for piezoelectric crystal. The first two letters include x, y, and z, among which, the first letter indicates the
thickness direction of the wafer before rotation, and the second letter indicates the length direction of the wafer before rotation. The remaining letters indicate the rotation axis, which is defined by "t, l, w" and indicates rotation along with the thickness direction, the length direction, and the width direction, respectively. In addition, the final angle represents the rotated angle. If the angle value is positive, it means that the angle value is rotated counterclockwise along the rotation axis; otherwise, it is rotated clockwise along the rotation axis.

Therefore, “(yxl)θ” means that the initial thickness direction of the wafer is along the y-axis, the length direction is along the x-axis. It means that the normal direction of initial wafer is the y-axis. Besides, the angle θ is rotated counterclockwise about the length direction, i.e. the x-axis. The detailed wafer direction is shown in Fig. 1.

![Figure 1](image.png)

Figure 1. The wafer structure of cut type “(yxl)θ” before and after coordinate system rotation.

LiNbO₃ crystal follows the point group of 3m, which has a third order shaft and three symmetrical planes. Simplified physical constants remain invariable after symmetry operation so that they can be obtained in the matrixes. Using the c-axis orientated LN as a reference, the relative permittivity matrix is

\[
\varepsilon = \begin{bmatrix}
\varepsilon_{11} & 0 & 0 \\
0 & \varepsilon_{11} & 0 \\
0 & 0 & \varepsilon_{11}
\end{bmatrix} = \begin{bmatrix}
84 & 0 & 0 \\
0 & 84 & 0 \\
0 & 0 & 30
\end{bmatrix}. \tag{1}
\]

The compliance matrix is

\[
s = \begin{bmatrix}
s_{11} & s_{12} & s_{13} & s_{14} & 0 & 0 \\
s_{12} & s_{11} & s_{13} & -s_{14} & 0 & 0 \\
s_{13} & s_{11} & s_{13} & 0 & 0 & 0 \\
s_{14} & -s_{14} & 0 & s_{44} & 0 & 0 \\
0 & 0 & 0 & s_{44} & 2s_{14} & 0 \\
0 & 0 & 0 & 0 & 2s_{14} & 2(s_{11} - s_{12})
\end{bmatrix} = \begin{bmatrix}
5.78 & -1.01 & -1.47 & -1.02 & 0 & 0 \\
-1.01 & 5.78 & -1.47 & 1.02 & 0 & 0 \\
-1.47 & -1.47 & 5.02 & 0 & 0 & 0 \\
-1.02 & 1.02 & 0 & 17 & 0 & 0 \\
0 & 0 & 0 & 0 & 17 & -2.04 \\
0 & 0 & 0 & 0 & -2.04 & 13.6
\end{bmatrix} \times 10^{-12} \left[ \frac{1}{\text{Pa}} \right]. \tag{2}
\]

The piezoelectric coupling matrix is

\[
d = \begin{bmatrix}
0 & 0 & 0 & d_{15} & -2d_{22} \\
-d_{22} & d_{22} & 0 & d_{15} & 0 \\
d_{31} & d_{31} & 0 & 0 & 0
\end{bmatrix} = \begin{bmatrix}
0 & 0 & 0 & 68 & -42 \\
-21 & 21 & 0 & 68 & 0 \\
-1 & 1 & 6 & 0 & 0
\end{bmatrix} \times 10^{-12} \left[ \frac{\text{C}}{\text{N}} \right]. \tag{3}
\]

According to the matrix transformation method, an orthogonal matrix [A] and the corresponding
strain tensor transformation matrix \([N]\) are introduced to establish the relationship between rotated coordinate system and the initial coordinate system. For \(\theta\)-rotated Y-cut LN, the orthogonal matrix can be expressed as

\[
[A] = \begin{bmatrix}
1 & 0 & 0 \\
0 & \cos\theta & \sin\theta \\
0 & -\sin\theta & \cos\theta
\end{bmatrix}.
\]  

(4)

And the strain tensor transformation matrix is described as

\[
[N] = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & \cos^2\theta & \sin^2\theta & \sin\theta\cos\theta & 0 & 0 \\
0 & \sin^2\theta & \cos^2\theta & -\sin\theta\cos\theta & 0 & 0 \\
0 & -\sin2\theta & \sin2\theta & \cos^2\theta - \sin^2\theta & 0 & 0 \\
0 & 0 & 0 & 0 & \cos\theta & -\sin\theta \\
0 & 0 & 0 & 0 & \sin\theta & \cos\theta
\end{bmatrix}.
\]  

(5)

On the basis of coordinate transform of relative permittivity, the new relative permittivity of \(\theta\)-rotated Y-cut LN is

\[
\varepsilon' = [A]\varepsilon[A]^{-1}.
\]  

(6)

The new compliance matrix of \(\theta\)-rotated Y-cut LN is

\[
s' = [N]s[N]^t.
\]  

(7)

The new piezoelectric coupling matrix of \(\theta\)-rotated Y-cut LN is

\[
d' = [A]d[N]^t.
\]  

(8)

Where, \([A]^{-1}\) is the inverse matrix of \([A]\) and \([N]^t\) is the transposed matrix of \([N]\). For instance, setting the value of angle \(\theta\) as 128°, then the post-rotated relative permittivity can be calculated out:

\[
\varepsilon = \begin{bmatrix}
84 & 0 & 0 \\
0 & 50.47 & 26.20 \\
0 & 26.20 & 63.53
\end{bmatrix}.
\]  

(9)

The post-rotated compliance matrix can be acquired:

\[
s = \begin{bmatrix}
5.78 & -0.80 & -1.68 & 0.69 & 0 & 0 \\
-0.80 & 5.70 & -2.36 & 0.18 & 0 & 0 \\
-1.68 & -2.36 & 6.87 & 0.31 & 0 & 0 \\
0.69 & 0.18 & 0.31 & 13.45 & 0 & 0 \\
0 & 0 & 0 & 0 & 11.77 & 0.30 \\
0 & 0 & 0 & 0 & 0.30 & 15.83
\end{bmatrix} \cdot 10^{-12} [1/\text{Pa}].
\]  

(10)

The post-rotated piezoelectric coupling matrix can be obtained:

\[
d = \begin{bmatrix}
12.14 & 18.05 & -27.04 & -7.77 & 0 & 0 \\
17.16 & 17.66 & -37.29 & 1.09 & 0 & 0
\end{bmatrix} \cdot 10^{-12} \left[ \frac{\text{C}}{\text{m}^2} \right].
\]  

(11)

One point that needs to be mentioned is that the three-dimensional LN structure is established with the y-axis as the normal direction instead of the z-axis, and the y-axis is mainly derived from initial Y-cut structure. Then a three-dimensional y-axis oriented LN block is established and the grid is split by free tetrahedral mode. Then the post-rotated physical parameters are substituted into the model structure to replace the original reference parameters. A plane needs to be restrained to make the calculation converge. Then the simulation results are exhibited in Fig. 2, which is mainly expressed from fixed planes due to the anisotropy of LN. Fig. 2(a–c) show the displacement distributions when the xy-plane, the yz-plane and the xz-plane is fixed, respectively. The color change in the model represents the different displacement magnitude at that location. It can be seen that the displacement deformation of the three-dimensional structure in different directions under the same
The electric field structure is different.

Figure 2. The total displacement under different fix conditions based on matrix transformation method. (a) the xy-plane fixed, (b) the yz-plane fixed, (c) the zx-plane fixed.

2.2. Euler Angle (EA) Method

The rotation process of the coordinate system can be decomposed into three independent fixed-axis motions, respectively generating three angles, which are defined as the precession angle $\alpha$, the nutation angle $\beta$, and the spin angle $\gamma$, respectively. These three angles can be expressed by Euler angles in the form of $(\alpha, \beta, \gamma)$. The process of representing the rotation of the coordinate system with Euler angles can be represented by Fig. 3. If the initial coordinate system is expressed by "xyz", the coordinate system after one rotation, the second rotation and the third rotation is defined as "x'y'z'", "x''y''z''" and "XYZ", respectively. Wherein, the angles $\alpha$, $\beta$, $\gamma$ respectively indicate that the initial coordinate system is rotated $\alpha$ angle counterclockwise around the z axis, then $\beta$ angle is rotated counterclockwise around the x' axis, and the angle $\gamma$ is rotated counterclockwise around the z' axis. Thus, the finally obtained system is “XYZ” as shown in Fig 3.

Figure 3. The coordinate system before and after rotation.

It should be noted that the rotation of the wafer is opposite to the rotation of the coordinate system, i.e. when the wafer is rotated by $\theta$ counterclockwise around the x-axis, if the same wafer tangential direction is desired, it requires to rotate the coordinate system clockwise by $\theta$ around the x-axis. Taking the 128° Y-cut for example, it means that the Y-cut LN rotates counterclockwise by 128° around the x-axis. Therefore, in order to simplify the representation of Euler angles, establishing a three-dimensional model directly with the Y-axis as the normal direction is suggested instead of the reference Z-axis. At the same time, following the principle of opposite rotation, the coordinate system needs to be rotated by 128° clockwise around the x-axis. Then, the corresponding Euler angle can be
obtained of (0°, -128°, 0°), but the correctness of which is uncertain. Hence, it is further verified by substituting the Euler angle into the three-dimensional structure to conduct finite element simulation in piezoelectric effect. Concretely, the simulation results of piezoelectric effect are shown in Fig. 4, which is also expressed in three directions with fixed planes as the same as Fig. 2. By comparing with the simulation results in Fig. 3, the displacement change obtained by rotating the coordinate system by the EA method is almost identical to that obtained by the matrix transformation method. This shows that the LN structure with a specific orientation can obtain the physical properties after the rotation of Euler angle, without the calculation of corresponding physical parameters.

3. The Simulation of Resonance Mode and Longitudinal Wave Electromechanical Coupling Coefficient (K) of LN with Different Orientations
According to the proposed EA method above, the simulation and analysis of resonant modes and the $k_t^2$ of different orientation LNs are carried out. Specifically, the simulation principle follows the piezoelectric characteristic of the piezoelectric LN film. When an electrical signal is applied on the piezoelectric film, the electrical signal is converted into mechanical energy by the inverse piezoelectric effect, specifically in acoustic wave mode. Then vibratory acoustic wave would be transformed into electrical signal to transmit out by the piezoelectric effect. The acoustic wave contains shear wave and longitudinal wave. In general, both kinds of acoustic waves exist in the crystal simultaneously. The point is that which one is dominant. The bulk acoustic wave resonator mainly relies on the longitudinal wave mode. So the simulation in this work focuses on the longitudinal wave $k_t^2$ that is important to the bandwidth of FBAR filters. The longitudinal wave $k_t^2$ is achieved by the resonance characteristic of the piezoelectric film, which is defined as $k_t^2 = \frac{\pi^2 (f_p - f_s)}{4 \times f_p}$. In the formula, $f_p$ is the parallel resonance frequency and $f_s$ is the series resonance frequency. A single crystal LN piezoelectric material with a thickness of 50 μm is served as the model structure and is established by initial y-axis oriented. In the meanwhile, the rotating coordinate system represented by Euler angle is introduced into the finite element simulation. The nutation angle $\beta$ of Euler angle is set from 0° to 180°, and the increment is 5°, while maintaining the other two angles at 0°. Then the continuous parameter scanning calculation is performed. The simulated frequency range is designed to 20 MHz~115 MHz, which is mainly estimated by the formula of $f = \frac{\vartheta}{2d}$, where $f$ is the resonant frequency, $v$ is the acoustic velocity of LN, and $d$ is the LN thickness.

![Figure 4.](image)

The simulated resonant modes are obtained and exhibited in Fig. 5(a), which is expressed by the curve of “admittance vs frequency”. It can be seen that there is a vibration mode of the shear wave near the desired longitudinal wave vibration mode, which needs to be avoided in the applications of...
bulk acoustic wave. In addition, the \( f_s \) and \( f_p \) of each resonant mode can be get from Fig. 5(a) and have some offset with the angle of rotation changes. Meanwhile, the \( k_t^2 \) can be calculated through

\[
k_t^2 = \frac{\pi^2 \times (f_p - f_s)}{4 \times f_p}
\]

and the result of \( k_t^2 \) varying with different cut angles is shown in Fig. 5(b). Obviously, the \( k_t^2 \) is large in the range of 10° to 50°. In view of the \( k_t^2 \) and resonant mode, the simulation is further performed in the range of 10° to 50° with an interval of 1°.

\[
k_t^2 = \frac{\pi^2 \times (f_p - f_s)}{4 \times f_p}
\]

\( k_t^2 \) of Y-cut LN with different rotation angles.

\section*{Figure 5.} The simulated and analyzed results. (a) the simulation of resonant mode of (0°~180°)-rotated Y-cut LN; (b) the \( k_t^2 \) of Y-cut LN with different rotation angles.

In this case, the obtained curve of “admittance vs frequency” is expressed in Fig. 6(a), the resonant frequency of which is relatively concentrated. Extracted and calculated \( k_t^2 \) in Fig. 6(b) are both in good agreement with the result in Fig. 5(b), and the largest value of \( k_t^2 \) can be acquired around 27.24% when the cut angle is 30°Y-cut. However, there is still a shear wave near the wanted longitudinal wave for 30°Y-cut LN in Fig. 6(c). Observing the resonant mode of each cut-direction, it only exists pure longitudinal wave mode without the interference of shear wave when the orientation is 43°Y-cut in Fig. 6(d). In the meanwhile, the \( k_t^2 \) of 43°Y-cut LN is ~22.65%, which is also relatively high and much larger than other reported piezoelectric film [15, 16]. Therefore, the 43°Y-cut is more prospective to be chosen as the piezoelectric film for the application of FBAR devices.

\section*{Figure 6.} (a) the simulated resonant mode of (10°~50°)-rotated Y-cut LN; (b) the \( k_t^2 \) of Y-cut LN under different rotation angles; (c) the resonant mode for 30°Y-cut LN; (d) the resonant mode for 43°Y-cut LN.
4. Conclusion
The Euler angle (EA) method is used to simulate the resonant mode and calculate the \(k^2\) of LiNbO\(_3\) material with different orientations. Meanwhile, it is verified that the EA method is more advantageous over the traditional matrix transformation operation by the simulation of displacement change under electrostatic field. With this method, the resonant modes of longitudinal wave in LN crystal are obtained by rotating different angles around Y-cut LN and the corresponding \(k^2\) is calculated successfully. Finally, it is shown that 43°Y-cut LN has a high \(k^2\) and a pure longitudinal wave vibration mode simultaneously, which is potentially useful as the piezoelectric film in the FBAR device applications to get much larger filter bandwidth. In addition, this EA method is also promising to simulate other performances for anisotropic materials.

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