An Integrated Analysis of Vibrations of Quartz Crystal Plates with the Mindlin Plate Theory for Resonator Design and Optimization

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Abstract

The high frequency vibrations of quartz crystal plates have been extensively studied for the design and optimization of resonators which work at the thickness-shear vibration mode with relatively high frequency in the RF range. Earlier research work started from the development of special plate equations required for the high frequency vibrations of quartz crystal plates by Mindlin, known as the Mindlin plate theory which is one of the few innovative theory and methods specifically targeted for the bulk acoustic wave (BAW) resonators. By using the Mindlin plate theory with selected vibrations modes, or carrying out analysis in the specified frequency range, we can design quartz crystal resonators, which have the thickness-shear mode that strongly couples to flexural, face-shear, and other modes, with precise knowledge on the effect of mode coupling for separation of vibration modes to enhance the dominance of thickness-shear vibrations. The Mindlin plate theory has been effective and also serves as the only tool for such analysis and design of quartz crystal resonators in this interdisciplinary subject pursued by both electrical and mechanical engineers in the development of this mechanical device used as one of essential electronic circuit components. The core development of the Mindlin plate theory has been efforts of a close group dedicated to the research of wave propagation in finite piezoelectric solids active in the electronic engineering community. Important knowledge and methods include the thermal and acceleration effects which are vital in the design of high precision quartz crystal resonators. Such theories have been utilized in many ways, like approximations in the early stage and the finite element and other numerical implementation lately, to increase the accuracy of analysis in the design evaluation. Experimental verifications of analyses have been made in connection with device development, and design tools have been created by many engineers and groups without publicizing details and functions. As we look back to the theoretical studies, we feel it is necessary to have some basic results checked and validated in conjunction with empirical design methods. In the meantime, it is also necessary to analyze the performance parameters such as the vibration frequency, mode coupling, quality factor, thermal effect, and electrical circuit parameters of quartz crystal resonators with given design parameters. As an effort to establish design method and process based on computational modeling, we draw a roadmap of analyses needed in the product design, and identified needed theoretical formulation and solution strategy. Of course, all the analyses have to be validated with experimental data by our manufacturing process. In addition to the known verification, we are also in the process to develop a computational model for circuit parameters. The final tools based our objective will have the initial design completed with predicted performance and circuit parameters for engineering realization. Such a design process based on wave propagation in finite piezoelectric structures can also be adopted in other acoustic weave devices such as surface acoustic wave (SAW) resonators.

1. Introduction

The quartz crystal resonators for frequency control and detection applications have been widely known with extensive research efforts on the high frequency vibration analysis aimed at, among others, the exact vibration frequency, mode coupling, and frequency stability under bias fields such as the temperature variation and acceleration [1-7]. Earlier studies, as focused on the theoretical formulation and analytical solutions, were presented as solutions from simplified equations and simplest models to guide the improvement of actual designs based on experiences and promising prototypes. Such analyses have been made, in most times, with the tailored equations of vibrations of plates with specialized configurations like beveling and electrodes to focus on the thickness-shear (TSh) vibrations and effects of shape variations [5, 7]. The usefulness of such analyses have been proven theoretically or experimentally and by the fact that many engineers have turned to the analytical theory and methods for the determination of design parameters and improvement of initial designs. Such studies started from universities with pioneering activities on the core issues of vibrations of piezoelectric crystal plates and extensive connections with the frequency control industry, namely Columbia University by Mindlin [1-2, 8-9], University of Tokyo by Koga [10], Rensselaer by Tiersten [3], Princeton by Lee [4-5, 11], Rutgers by Yong [6], and lately Nebraska – Lincoln by Yang [1, 7, 12] and others [7, 13-17, 18]. The outcomes of these studies are presented as papers in journals, proceedings, and books and utilization of these results are usually not revealed explicitly because many of the research works are done as sponsored programs by governments, which do not need specific applications, or the industry, which do not show details of the calculation and validation in detail. As a result, engineers or enterprises need to go through the theoretical formulation, mathematical programming, and experimental procedure independently for the necessary applications in the design process. It is understandable that details of such implementation are not publicized to outsiders, and the commercialization of such results is not an option due to the relatively small market and heavy dependence on empirical knowledge in the design and manufacturing of quartz crystal resonators.

In the course of the technology sophistications in the period of almost a century, analytical techniques of quartz crystal resonators have been aided by many major scientific and technological breakthroughs including the Mindlin plate theory which is considered one of great achievements in improving the classical plate theory in certain applications such as the thickness-shear vibrations of crystal resonators, and the effects of bias fields on the vibrations of elastic solids with the piezoelectric solids as one of most important applications [4, 7]. Besides, many advanced technology such as finite element method and supercomputers have been utilized in the analysis of mechanical vibrations at the RF range [6, 11, 14, 19]. Such efforts have yielded reliable results for product analysis and design, and the follow up efforts by major producers of quartz crystal resonators have shown that the traditional products and industry can be transformed by the digital technology for the revolution in the design and manufacturing processes. One caution of such approach is that the software development, data interpretation, and process integration may take a lot of efforts and technical know-how, and many small- and medium-business in the acoustic wave device industry may not be able to afford the investments of technology and expertise.

Having witnessed the power and efficiency of supercomputing and finite element method for the analysis of high frequency vibrations of quartz crystal resonators and conducted extensive studies on the simplified formulation and analysis with plate theory for the same problem, the validation experiences by others and ourselves in the past decades have indicated that the methods and solutions based on the plate theory have produced reliable results with adequate precision for product development. What is missing in the past is that the required validation procedures and results have not been reported and the user side is required to provide additional validation. Besides, the user side, usually a quartz crystal resonator producer, should commit to the systematic implementation and necessary collaboration between process engineers and design engineers. Fortunately, such interests are on the rising in some emerging industrial leaders due to limited accumulation on product development expertise and systematic mastering of the fundamental theory of analysis. Clearly, an systematic exposure to the theory for the analysis of quartz crystal plates and integration of the analytical methods, as demonstrated by Tiersten [3], would establish the firm foundation for the design and development of products based on the theoretical analysis and digital technology as emphasized as one of the technical trends in the transformation of traditional products of the manufacturing business. This can be done as we have been working on the theoretical analysis on the broader issues of quartz crystal resonators and familiar with latest technology and computing resources in both hardware and software. More importantly, we have established industrial partnership for the advances of design technology to improve the industry through advanced technology and collaboration with academic resources.

In this paper, we shall review the accomplishments of extensive studies on the theory and solutions based on the high frequency vibrations of quartz crystal plates, and summarize up the available methods, software components, and verified results and data for architecting the design software for the initial design with the integration of analytical results, empirical data, and best practice. Further analysis with advanced tools and resources based on the finite element analysis will be introduced for the completion of the design process.

2. Fundamental Theory and Approximate Methods for the Analysis of Quartz Crystal Resonators

The fundamental theory for the high frequency vibrations of quartz crystal plates starts from the inclusion of the thickness-shear vibration mode and the unusual configuration (beveled plate) and free boundary conditions [1-3, 5, 8]. Of course, electrodes on the plate substrate, piezoelectric effect, and the anisotropic material properties have also been considered in the formulation [8, 12-13]. The theory of plate vibrations is known as the Mindlin plate theory with focused applications in quartz crystal resonators. The analytical results of such equations, in most cases, are given in one-dimensional solutions which can only accommodate partial boundary conditions [1-3]. The accuracy, however, is adequate for resonator analysis and design because many measurements have confirmed the one-dimensional results and late analysis by the finite element method shows that the deformation in the direction perpendicular the propagation is almost uniform and the assumption of straight-crested waves is valid in the vicinity of the thickness-shear resonance. Again, it implies that the analytical solutions can be and should be utilized to establish a resonator design procedure with necessary verification and revision.

To recapitulate the analytical methods and results, we start from the fundamental theory and some approximations to check into details of equations and some basic physical phenomena for analysis.

1) Mindlin equations for the coupled thickness-shear vibrations of plates

It is essential to analyze high frequency vibrations, which implies the vibration modes are different from the usual flexural vibrations discussed in textbooks on plate vibrations for quartz crystal resonators. The thickness-shear vibrations, which have frequency dependence on the thickness of plates, have to be studied by the Mindlin plate theory, which was established by Mindlin to handle the analysis of quartz crystal resonators and lately used in other problems of structural vibrations in broad engineering fields [1, 2, 9]. The essence of the Mindlin plate theory is that the displacements are expanded in power series of the thickness coordinate, thus presenting the thickness-shear displacement associated with the linear term of thickness coordinate as an independent variable meeting the requirements of analysis. This makes it is possible to analyze the vibrations of finite plates because earlier methods for the vibrations of thickness-shear mode can only be one-dimensional and thickness dependent. The Mindlin plate theory has been revolutionary to the overlooked acoustic wave resonator analysis, because a brand new theory has been established for this seemingly trivial problem neglected for so many years for various reasons. The accomplishment of Mindlin is multifold, but the Mindlin plate theory has been well accepted because of its important applications and innovative assumptions in solving the complex problem. For a plate with two major faces, a systematic derivation of the Mindlin plate equations starts from the displacement expansion [1, 2, 6]

$$u_j(x_1,x_2,x_3,t)=\sum_{n=0}^{\infty}u_j^{(n)}(x_1,x_3,t)x_2^n\,,j=1,2,3,(1)$$

where $u_j, u_j^{(n)}$, x_i, and t are displacements, nth-order displacements, coordinates, and time, respectively. Further derivation of the Mindlin plate equations can be found in the monograph by Mindlin [1].

Although the Mindlin equations have been created for the analysis of vibrations of quartz crystal plates with finite size, the mathematical solutions satisfying the boundary conditions, with the major faces handled through the integration over the thickness already, at the length and width sides are also impossible to obtain for free edges. As a result, the effects of the plate width on the vibrations have been neglected with the assumption that the wave mode only varies along the direction of wave propagation. This assumption has been employed without further explanation, but our recent finite element analysis has been shown that for most plates, the deformation, or the displacements, along the width direction is indeed small and the negligence is justifiable and acceptable. Of course, the vibration frequency has been accurate with the straight-crested wave assumptions. Except a few special cases, most analytical solutions based on the Mindlin plate equations with multiple modes and piezoelectric considerations are obtained based on the straight-crested wave assumptions. The analytical foundation of our planed software tool will be based on the assumption too, with the consideration of major vibration modes like the thickness-shear (TSh), flexural (FL), face-shear (FS), and electrical potentials as the framework [1, 2, 5, 8, 15].

2) Effects of electrodes on the vibrations

As one of the core elements of a quartz crystal resonator, extensive studies on the effects of electrodes have never been enough to meet the needs of product development and improvements [3, 7, 12, 13, 16]. The basic reasons include the fact that the driving of resonator has to be enabled by the electrodes and the frequency and electrical parameters are also directly affected by the material, size, and location of the resonator. Another known phenomenon, energy trapping, is also the direct property of electrodes on the quartz crystal plate. Clearly, we need to invest effects on the studying of electrodes in vibration analysis, optimal shape and size, and the manufacturing techniques to obtain best performance of resonators. Indeed, all these issues have been studied in the course of resonator production, and there are important findings such as the optimal shapes and sizes and techniques on the electrodes process. Later studies on the effective calculation of the precise frequency effect of electrodes will be important in the estimation of frequency with electrodes and crystal blank information for the initial selection of design parameters [12-13]. In the future addition of the analytical capability, it is also important to have the optimal electrode shape considered from earlier studies as the initial design with next to the best parameters to improve the accuracy.

3) Frequency-temperature relations of quartz crystal plates

The frequency-temperature relations, or the thermal effect, of quartz crystal resonators are important in applications due to the stringent requirement on the frequency stability in modern electronics in a thinly sliced frequency band and high frequency. The analysis has to be made with the consideration of thermal fields in the vibrations of quartz crystal plates under the general theory of elasticity under bias fields [4-6, 14]. However, the high precision requirements of the analysis demand thermal elastic properties of quartz crystals, a material which is not widely used and tested in mechanical engineering, to be measured specifically for the analytical framework. Not surprisingly, such a task has been undertaken by many researchers, and the material properties have been gathered to facilitate the establishment of nonlinear thermal equations of vibrations of quartz crystal plates. As a result, the widely known cubic relations of the thickness-shear vibration and the temperature has been proven with the thermal equations, and the accuracy has also been proven through more reliable data from the finite element analysis [6, 14]. The thermal equations, as one can expect, also have been implemented with the Mindlin plate equations and the results based on the straight-crested wave solutions have been effective for the frequency-temperature solutions. With the considerations of the electrodes, beveling, the analysis of frequency-temperature relations has been closer to the actual resonators with reliable predictions for the improvement of design.

4) Electrical parameters of quartz crystal resonators

As an electronic component for circuits, the usual requirements of quartz crystal resonators are specified as electrical parameters such as the resistance, capacitance, inductance, and quality factors for the analysis of the oscillating circuits. This clearly shows a gap between the analysis of resonators with the plate theory and vibrations, because the solutions we can obtain are usually given in vibration frequency, displacements, and mode couplings which are almost useless to electrical engineers. For this reason, it is always an expected objective that the electrical properties of a quartz crystal can be extracted from the vibration solutions for circuit analysis and direct applications and comparisons with product testing and measurement. This, of course, is possible if the mechanism related to circuit parameters is incorporated into the formulation of vibrations. It turns out that the major parameters can be calculated with the consideration of material viscosity which is related to the resistance and quality factor through the energy loss in the vibrations. Other electrical parameters can be calculated and derived from the resistance. The material viscosity of quartz crystals is known through earlier measurements [20], and a formulation of the major parameters have been given, paving the path for the formulation of electrical parameters with the Mindlin plate theory [17]. The results show that the parameters from the theoretical calculation with material viscosity are much smaller than the actual measurements, and it is suspected that the viscosity from the bonding process of the electrodes and other factors are not considered but significant. Consequently, it is believed that the introduction of more viscosity parameters will improve the calculations and it is still expected the electrical parameter can be calculated to enrich the current analysis from mechanical vibrations to the electrical considerations to enable the collaborative design with application circuits.

3. Design Parameters and Procedure Specification

With the analytical methods and capabilities outlined above, we are ready to specify the initial design parameters and needed analyses based on the procedure for the optimal choices. With the analyses relying on the mechanical vibrations of an ideal quartz crystal resonator, we can conclude that the best design can be made with the vibration results and the electrical parameters by combining the results through stages and integration.

First, the initial parameters of a quartz crystal resonator include the nominal frequency, which will roughly determine the thickness of the crystal blank through the known relationship between the frequency and crystal thickness at the usual thickness-shear vibration mode. Then, through the known manufacturing process, we can determine the feasible electrodes including the material (usually gold, silver, or aluminum) and thickness. All these information will give the exact thickness of the crystal blank. The choice of package of the resonator will also give the size of crystal blank for consideration as the initial guess. Also the electrode size can be used as the optimal shape with known results from earlier studies.

With the estimated structural parameters of the crystal blank and electrodes, analysis of vibrations of the ideal resonator can be made for the precise thickness-shear vibration frequency and displacements, or deformation, and the mode couplings. Such results will reveal the frequency dependence on the aspect ratios, and provide guidelines for the optimal choice of size of the crystal blank based on the separation of the thickness-shear mode and the spurious modes, which are considered harmful and should be avoided as much as possible at the functioning frequency. This is usually done with the frequency spectra of a crystal blank from one-dimensional analysis based on straight-crested wave assumptions. Since the frequency-size relation is periodic, we can select the parameters which are most close to the package size.

The next important analysis after the determination of structural parameters is the frequency-temperature relations to avoid the frequency variation due to the change of mode coupling with temperature fluctuation. This is one of common problems frequently encountered in quartz crystal resonators and the remedy is usually on the popper choices of structural parameters such as the size and shape of the crystal blank and electrodes to minimize the effect of mode coupling on the frequency variation. This, certainly, requires a detailed and accurate analysis of quartz crystal vibrations in the required temperature range, which is about -40℃ to 100℃. Again, the analysis is usually done with the one-dimensional solutions and the thermal properties of electrodes have very small effect on the results. The results can be used to adjust structural parameters to reduce the coupling so a better frequency-temperature relation can be obtained. Apparently, there is an iterative and repeating process with the earlier step.

When the optimal structural parameters are determined, we are ready to calculate the electrical parameters of quartz crystal resonator as the final check of properties needed in the design. The major properties include the quality factor, resistance, and others. It is important to point out that the parameters are controlled by the viscosity of the bonding, and reasonable value can only be obtained from empirical knowledge of the process, which is different from production lines and companies. The accurate estimation will be used for the adjustment of structural parameters, and the procedure, again, has to be repeated with new parameters from the beginning.

Even with the optimal parameters satisfying production needs obtained through the above iterations, further calculations are needed for other factors which cannot be considered in the procedures above. One typical and important factor is the mounting through welding for the quartz crystal blanks. It is known that the crystal blanks has to be free from any restrictions, but it is impossible in actual product. As a result, the mounting structure has been minimized as two welding spot with small sizes to reduce the effect on the frequency and electrical parameters. The effect can be significant because common sense tells us that the small change of boundary condition can have major effect and they should be carefully examined before the production. There have been many examples that the designed products have to be revised to make acceptable resonators. Unfortunately, such an analysis of the mounting cannot be done with the plate theory, and the finite element analysis has to be employed to see the changes of the thickness-shear mode to enhance or retain required energy trapping.

4. Conclusions

An examination of the available analytical methods with accepted results have been made, and a procedure of quartz crystal resonator design based on the analytical procedure has been suggested. Since the analytical procedures have been familiar to engineers and some of the results have been validated, we believe that the integration of the analytical procedures will result in a complete design procedure for quartz crystal resonators with the advantage of reliable simulation to reduce the time and cost of prototyping. The procedure is familiar with us, and the suggested integration process has been the product of discussion with engineers and researchers on the theoretical analysis for quartz crystal resonators. The final design will be checked by reliable finite element analysis with well-known software tools to guarantee the reliability but also avoid high time and resource costs with three-dimensional analysis. Since the systematic design procedure has been openly studied before, our approach will be used to train engineers with limited practical experiences and companies with limited development know-hows. The design procedure will serve as a foundation to integrate both the theoretical results and practical experiences and data.

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