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Extraction of Modified Butterworth – Van Dyke Model of FBAR Based on FEM Analysis

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Abstract – **This paper presents a methodology for extraction of modified Butterworth-Van Dyke model (mBVD) parameters of thin-film bulk acoustic wave resonator (FBAR) using finite elements method (FEM) analysis. Simple FBAR model is developed and its frequency characteristic is obtained through FEM simulations. Then the mBVD model parameters are calculated and further optimized to fit its frequency response to those from FEM analysis with less than 1% relative error.**

Keywords – **FBAR, mBVD, FEM analysis, BAW resonator.**

I. INTRODUCTION

In last decades thin-film bulk acoustic wave resonators (FBAR) gained popularity due to its applications in RF filters and oscillators for wireless communications and the diversity of sensors applications [1]. Initially FBAR has been used in duplexers but due to their high quality factors, good temperature stability and low losses they were implemented in other communications devices. FBAR are effectively used in RF range starting from several hundreds of MHz till 2GHz but even applications at 5GHz are reported. Their other advantages are compatibility with standard CMOS process, and capability to process higher powers of the signal.

Typical FBAR architecture, shown in Fig. 1, consists of a sandwich structure with two metal electrodes and piezoelectric in between, placed over a silicon substrate [2], [3]. FBAR utilizes bulk acoustic waves propagating through the bulk structure of the piezoelectric layer. Aluminum nitride (AlN) or zinc oxide (ZnO) are used for piezoelectric layer composition, but lead zirconate titanate (PZT) is also reported as FBAR piezoelectric in some researches, while metal electrodes are made from aluminum, platinum, titanium, etc.

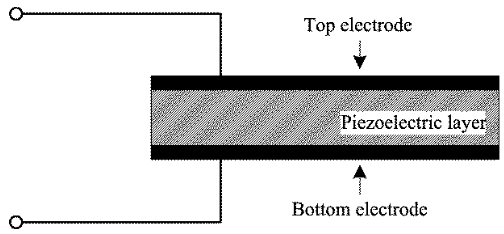

Fig. 1. FBAR cross section view.

Butterworth – Van Dyke (BVD) model is most often used for FBAR description during the design process. It is used for determining the FBAR characteristics in the schematic design and simulations as well. The equivalent BVD circuit of a classical FBAR utilize RLC acoustic arm with one capacitor in parallel. In his research in 1999 [4] Ruby introduced the modified BVD (mBVD) circuit by adding two additional resistors to the conventional BVD model describing more accurately the loss mechanisms in the resonator. The mBVD demonstrates improved accuracy between measured results and extracted model parameters.

The goal of this paper is consideration of the relationships between physical modeling of FBAR, based on finite element method analysis, and its electrical mBVD model. COMSOL Multiphysics software [5] is used for FEM analysis, aiming to characterize the current through the device in the frequency domain. The results, received from COMSOL are used for extraction of mBVD model parameters. Then the values of those parameters are refined by comparison of the frequency characteristics of the mBVD model with those, received from COMSOL.

II. mBVD CIRCUIT OF FBAR

The equivalent BVD circuit used for modeling of FBAR electrical parameters is shown in Fig. 2 (a). The standard BVD circuit contains acoustic (or motional) RLC arm and parallel capacitance C_0. The so called “motional tract” of the BVD circuit, consisting of motional capacitance C_m, resistance R_m and inductance L_m, represents the propagation of acoustic wave in the piezoelectric material and defines the acoustic properties of the resonator [2]. Static capacitance C_0 gives the equivalent electrical capacitance formed between top and bottom electrodes within the FBAR structure.

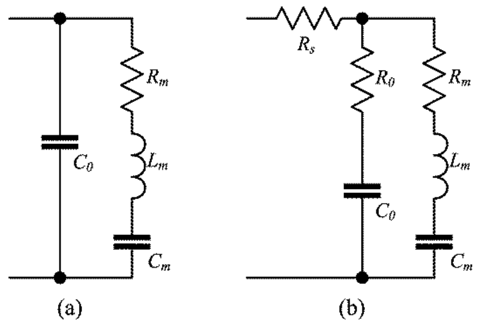

Fig. 2. (a) Equivalent Butterworth-Van Dyke circuit of FBAR; (b) the modified Butterworth-Van Dyke circuit.

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The following formulas give the relationships between BVD elements and FBAR physical parameters [6]:

$$C_m = \frac{8C_0 k_{eff}^2}{N^2\pi^2} \tag{1}$$

$$L_m = \frac{\upsilon}{64.f_s^3.\varepsilon.A.k_{eff}^2} \tag{2}$$

$$R_m = \frac{\eta.\varepsilon}{16.f_s.\rho.A.\upsilon.k_{eff}^2} \tag{3}$$

$$C_0 = \frac{\varepsilon A}{\tau} \tag{4}$$

where k^2_{eff} is the electromechanical coupling coefficient, A and τ are plate electrodes area and thickness respectively, ε is piezoelectric permittivity, η is acoustic viscosity of the wave factor k, υ is wave velocity and N shows acoustic mode number ($N = 1, 3, 5 ...$).

In comparison to the standard BVD, the modified BVD model (Fig. 2 (b)) has two additional loss resistors (R_0 and R_s) giving better fitting between frequency responses of the FBAR and the mBVD model. Both resistors depend on the specific FBAR geometry. In general R_s models the ohmic resistance of the electrodes, while R_0 helps for better description of acoustic losses when the circuit is in parallel resonance. In fact, the acoustic resistor R_m also models acoustic losses, but it affects predominately the series resonance. It has effect also in the frequency area around the parallel resonance, but it cannot define entirely the frequency behavior in this area and for this reason R_0 is introduced. The analysis of the mBVD impedance in Fig. 2(b) gives the following two formulas for FBAR impedance [6]:

$$Z = R_s + \frac{(1+s\tau_p)(s^2+s\omega_s/Q_s+\omega_s^2)}{sC_0(s^2+s\omega_p/Q_p+\omega_p^2)} \tag{5}$$

$$Z = \frac{(1+s\tau_{p0})(s^2+s\omega_{s0}/Q_{s0}+\omega_{s0}^2)}{sC_0(s^2+s\omega_{p0}/Q_{p0}+\omega_p^2)} \tag{6}$$

The resistance R_s is separated in the first formula, while in the second it is included in the general expression. The dependency of resonance frequencies ω_s and ω_p from circuit parameters are given with the expressions [3]:

$$\omega_s = \frac{1}{\sqrt{L_m C_m}};\quad \omega_p = \sqrt{\frac{C_m+C_0}{L_m C_m C_0}} = \omega_p\sqrt{1+\frac{C_m}{C_o}} \tag{7}$$

The resistance R_s changes the series resonance frequency and in the general expression (6) this frequency is marked by ω_{s0}. Both frequencies ω_s and ω_{s0} differ slightly and there is no exact formula connecting ω_{s0} with mBVD elements.

In mBVD circuit three quality factors could be defined – Q_p (quality factor of the parallel resonance), $Q_s = \omega_s L_m/R_m$ (quality factor of the series circuit $R_m L_m C_m$) and Q_{s0} (quality factor of the series resonance for the whole circuit including resistors R_0 and R_s). They are represented with the following relationships [6]:

$$Q_p = Q_s\frac{\omega_p/\omega_s}{(1+R_0/R_m)};\qquad Q_{s0} = \frac{Q_s}{(1+R_s/R_m)} \tag{8}$$

Generally, Q_s is always bigger than Q_p because ω_s/ω_p ratio varies between 1 and 1.03 while R_0/R_m is from 0.1 to 0.3. Also the effect of R_0 over the Q_{s0} is very small so it is disregarded in the expression (8).

Time constants $\tau_p = R_0C_0$ and τ_{p0} (there is no expression for it) changes the impedance magnitude by less than 2% and phase by up to 3° around the resonance frequencies [6]. The following expression for τ_p can be derived from formulas (7) and (8):

$$\tau_p = \frac{1}{\omega_p^2-\omega_s^2}\left(\frac{\omega_p}{Q_p} - \frac{\omega_s}{Q_s}\right). \tag{9}$$

III. Finite Element Method Analysis of the FBAR

For the purposes of this study an FBAR having a form of parallelepiped is investigated. Its sizes are: 2.9 µm thick AlN piezoelectric layer with length of 50 µm and width of 155µm (Fig. 3(a)). Above and below the piezoelectric layer are the Al electrodes with 0.05 µm thickness.

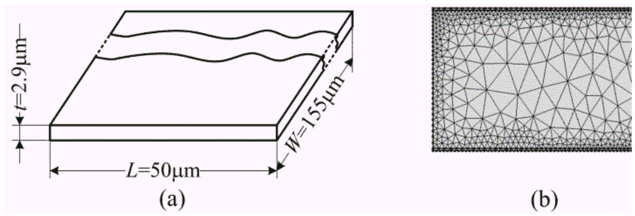

Fig. 3. (a) The sizes of the considered FBAR; (b) The mesh created by COMSOL.

Simulations of FBAR in COMSOL Multiphysics are based on FEM analysis. It is typically used to predict the behavior of complex models with complicated geometries and material properties, where the analytical approach could not lead to any solutions. FEM analysis supposes dividing of the analyzed object into elements with finite sizes forming a mesh and equalizing of the conditions at their boundaries. For the aim of the study presented here automatic division into elements created by COMSOL is used, which could be seen in Fig. 3(b). The mesh is relatively rough in the inner part of the resonator and it is finer in the boundary areas and across the piezoelectric layer-electrode interconnects, where better accuracy is required.

The goal of the FEM analysis, done here, is extraction of the harmonic response of the model when it is excited by an external signal. Current FBAR model is designed to resonate freely in all directions since there is no boundary conditions set for its outer walls. A sinusoidal voltage V_0 with 1 mV amplitude is applied between the electrodes.

The FBAR simulation with COMSOL includes frequency domain analysis of the resonator by varying the frequency of the voltage between the electrodes aiming to obtain the FBAR frequency response and from them – its series and parallel resonance frequencies. Frequency analysis is performed within the range of (1.82 – 1.9) GHz where the two resonance frequencies should appear based on preliminary approximate calculations. The frequency of the input voltage is changed with 10 kHz step – in fact this is the initial accuracy of determining of the resonance frequencies.

The complete characterization of the device supposes performing 3D analysis, which requires large computational resources. As far as the FBAR behavior is homogeneous through its width W, a 2D analysis is applied here, which allows significant reduction of the calculations. Since the third dimension of the model is not defined in the 2D simulations, all results are given as densities per unit width (per 1 m). Here the current through the FBAR is needed in order to receive its impedance. Therefore it is necessary to multiply the current density (given by COMSOL) by the real width (155 μm) of the device. Then the FBAR impedance or admittance can be calculated easily by using the Ohm low.

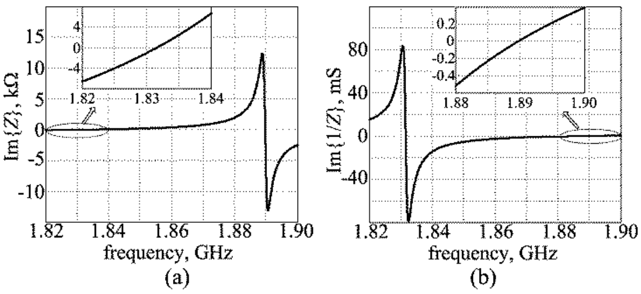

Fig. 4. Imaginary parts of FBAR impedance (a) and admittance (b).

Fig. 4(a) shows the imaginary part of the impedance received using this approach. It is more informative than the real part due to high Q-value, typical for FBAR resonators. The point, where this curve crosses the zero, gives approximately the series resonance frequency. The parallel resonance frequency can be determined from the zero-crossing point of the FBAR admittance shown in Fig. 4(b). From Fig. 4 and from numerical data the resonance frequencies are obtained: f_s = 1.83161GHz and f_p = 1.88976GHz ($f = \omega/(2\pi)$).

However these values are not the exact values of the resonance frequencies in formula (5), from which the elements of the mBVD can be calculated. There is small error due to the masking effect of the real part of the impedance.

IV. Extraction of mBVD Parameters

A. Initial Approximation of mBVD Parameters

The elements of the mBVD model can be calculated from the relationships between them and the impedance parameters ω_s, ω_p, Q_s, Q_p, τ_p, C_0 and R_s given by formulas (7) and (8). Their values will be found in two steps. First, considering the results from COMSOL, approximate values for parameters will be calculated (for resonance frequencies this was done in the previous section). Then, by comparing the frequency responses from COMSOL and the one calculated from mBVD parameters using formula (5) and minimizing the relative error between them, these values will be determined more precisely. All calculations from here on are done in MATLAB.

For frequencies much lower than resonance frequencies $Z \approx R_s + \omega_s^2/(j\omega C_0\omega_p^2)$ and for frequency much above them $Z \approx R_s + 1/(j\omega C_0)$ (the effect of τ_p is neglected). Thus the imaginary part of the admittance approximately tends to ωC_0 when $\omega \to 0$ and $\omega \to \infty$. For calculation of C_0 the FBAR frequency characteristics is simulated with COMSOL in extended frequency range from 0.5 – 4 GHz and from this simulation $\mathrm{Im}\{1/Z\}/\omega$ as function of the frequency (Fig. 5 (a)) is plotted. The approximate value of C_0 is taken as average between the values at 0.5GHz and 4GHz and it is 213.4fF.

The value of R_s can be calculated in a similar way. It follows from (5) that at very low frequencies the real part of the impedance is approximately equal to R_s. Fig. 5 (b) shows the real part of Z in the range 0.5-1GHz and from it $R_s \approx 0.09\Omega$ is determined.

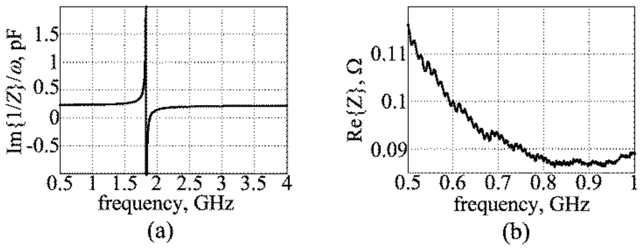

Fig. 5. Determining of C_0 and R_s: (a) The imaginary part of the admittance, divided by ω; (b) The real part of the impedance.

The Q-factors can be received by two methods. The first one is to plot the dependence $|Z(\omega)|$ using logarithmic scale for $|Z|$ (in dBOhms, relating to 1Ω). Then Q_{s0} can be calculated from ω_s and the frequencies ω_1 and ω_2, where $|Z|$ increases by 3dB from its value at ω_s: $Q_{s0} = \omega_s/(\omega_2-\omega_1)$. The quality factor Q_p can be found similarly from ω_p and the frequencies, where $|Z|$ decreases by 3dB from the value at ω_p. The second approach for determining Q_s is to use the slope of the phase characteristic of the impedance. The first approach is used in this paper. The dependence $|Z(\omega)|$ is shown in Fig. 6 and from it Q_{s0} = 1006 and Q_p = 1080 are found. There are no other arguments for determining Q_s except the relationship $Q_s > Q_p$ proved above. For this reason the initial guess for Q_s is chosen arbitrarily as Q_s = 1300 and its value will be improved later.

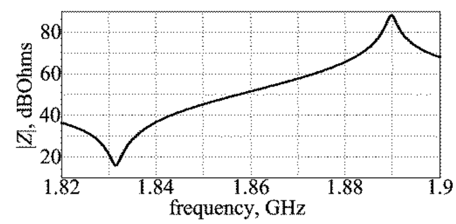

Fig. 6. The dependence $|Z(f)|$ using logarithmic scale for Z.

The received values of the resonance frequencies and Q-factors allow to calculate τ_p = 0.2435ps using formula (9).

B. Optimizing the mBVD Parameters

The best way for matching both frequency responses – the one obtained from COMSOL and the second calculated from mBVD model – is to minimize the relative difference between them. In fact the relative difference is the relative error of approximation of the real frequency response, received from COMSOL, with the mBVD model. The frequency response of the mBVD model can be calculated by replacing the determined above parameters in formula (5). Then, by varying these parameters a minimization of the relative error will be achieved.

Let us first consider the relative error between the imaginary parts of the frequency responses, calculated as (Im{Z_{mBVD}}–Im{Z_{COMSOL}})/Im{Z_{COMSOL}}. It is shown by dashed line in Fig. 7. It can be seen that the relative error is about 1% in the whole frequency range except around resonance frequencies. It can be reduced simply by increasing the capacitance C_0 by 1%, since C_0 divides the imaginary part of Z. Fig. 7 shows the result when C_0 is changed to 215.8fF – the error is very close to 0 for the curves with solid line.

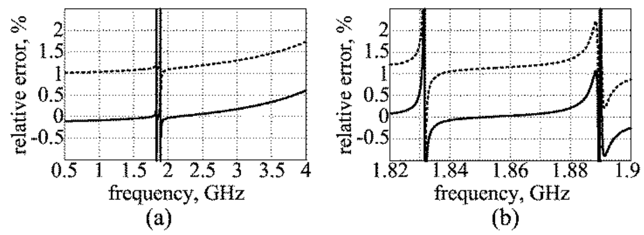

Fig. 7. Relative error of approximation of the imaginary part of the impedance. (a) In the frequency range 0.5-4GHz; (b) in the frequency range around resonance frequencies. The dashed lines are at C_0 = 213.4fF (the initial value), the solid lines are for C_0 = 215.8fF (improved value).

The large error around the resonances in Fig. 7 is due to determining of f_p and f_s with accuracy of 10 kHz. It could be reduced if increase the accuracy. Fig. 8 shows the effect of varying the kilohertz of their values – the error is decreased significantly. The more accurate values are f_s = 1.831602GHz and f_p = 1.889772GHz.

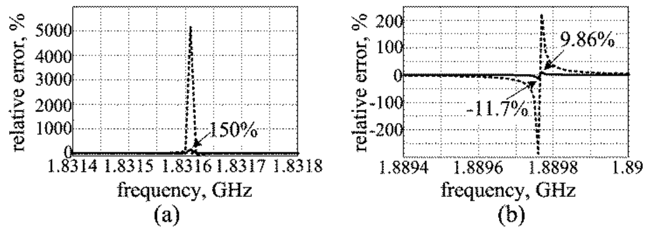

Fig. 8. Relative errors for imaginary parts of the impedance: (a) Around f_s; (b) around f_p. The dashed lines are for initial values f_s = 1.83161GHz and f_p = 1.88976GHz; solid lines are for more accurate f_s = 1.831602GHz and f_p = 1.889772GHz.

The real part of the impedance is influenced to great extent by the Q-factors and the resistance R_s. Thus the values of these parameters can be tuned by using the relative error for the real part of Z as criterion. Fig. 9 shows the effect of varying of R_s and Q_s on the error – the error reduction is significant in the area around resonances, when R_s is changed from 0.09Ω to 0.55Ω and Q_s – from 1300 to 1120. The other quality factor Q_p is also varied but without success and its value remains 1080. Regardless of the improvement, the relative error of the real part of the impedance is still large – several per cents in the area around the resonances and huge (thousands of percents) outside of this area. This means that mBVD model does not approximate the real part of FBAR impedance for frequencies far from resonances.

The elements of the mBVD model are calculated using the improved parameters. The corresponding formulas follow from (7) and (8):

$$C_m = C_0\left[\left(\frac{\omega_p}{\omega_s}\right)^2 - 1\right]; \qquad L_m = \frac{1}{\omega_s^2 C_m}; \tag{10}$$

$$R_m = \frac{\omega_s L_m}{Q_s}; \quad R_0 = R_m\left(\frac{Q_s}{Q_p}\frac{\omega_p}{\omega_s} - 1\right). \tag{11}$$

The values, calculated with these formulas, are: C_m = 13.927fF; L_m = 0.54213μH; R_m = 5.5706Ω; and R_0 = 0.39045 Ω.

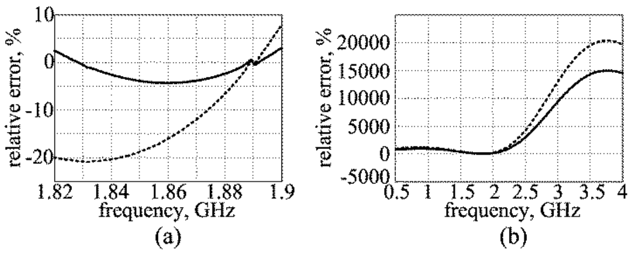

Fig. 9. Relative error in approximation of the real part of the impedance: (a) In the range around the resonances; (b) in wide frequency range. The dashed lines are for initial values R_s = 0.09Ω, Q_s = 1300; the solid lines are for improved values R_s = 0.55Ω, Q_s = 1120.

V. Conclusions

A methodology for deriving the parameters of the mBVD model of a FBAR from the results received by physical simulation based on FEM analysis is proposed. The extracted parameters give very good matching when compared to the FEM results especially for their imaginary parts, when the relative difference is less than 1%. It is also demonstrated that the resonance frequencies can be found with accuracy, better than the step between frequency points in the FEM analysis.

VI. Acknowledgments

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