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ACCURATE EXPLICIT FORMULAE OF THE FUNDAMENTAL MODE RESONANT FREQUENCIES FOR FBAR WITH THICK ELECTRODES

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Abstract - **Parallel and series resonant frequencies are the most important parameters for designing and analyzing the acoustic resonators. Explicit formulae that link the two resonant frequencies to the physical parameters of the piezo-layer and electrodes were given, when the electrode is thin enough to be ignored or taken as a mass loading only. For FBAR, however, the electrode is "thick", and the resonant frequencies have to be calculated by using the multi-layered acoustic transmission line. The transmission line model is accurate, but it is an inversion procedure for design. Accurate explicit formulae available for thick electrode are necessary in practice.**

This paper presents the explicit formulae of the parallel and series resonant frequencies of the fundamental thickness mode for the FBAR structures with improved accuracy. A hypothesis is proposed that the input acoustic impedance becomes continuous under resonance, at the two opposite faces of a virtual cut plane at any position along with the acoustic transmission line, no matter at interfaces or not. On the other words, only correct resonant frequency can meet the input acoustic impedance continuity condition. When the frequency deviation is small, the input acoustic impedance can be approximated as a linear function of frequency around the resonant frequency. We deduce the frequency correction formulae to eliminate the input impedance difference. The proposed parallel/series resonant frequency formulae are composed of two parts. The first part is the resonant frequency with mass loading effect, and the second part is the correction item for the input acoustic impedance difference correction mentioned above.

To check the accuracy of the proposed formulae, the simulations with different thickness and material combinations of the piezo-layer (ZnO and AlN) and the electrodes (Al, Au, Ag, Cu, Mo, W) are conducted. We calculate the electrical impedance of the multi-layered transmission line and get the maximum resistance/conductance frequencies as the parallel/series resonant frequencies for comparison. The results show, the errors of the explicit formulae we proposed can be lower than 0.3% under the conditions that the unit area mass ratio of electrodes to piezo-layer is less than 0.5 for heavy metal (Au, Ag, Cu, Mo, W), and thickness ratio is less than 0.25 for light metal (Al). These conditions are suitable for usual FBAR. Under the same conditions, the error of our formulae can be decreased to less than 5% of the formulae with mass loading effect only.

Keywords - **FBAR, series resonant frequency, parallel resonant frequency, explicit formulae**

I. INTRODUCTION

Duplexers for 1900 MHz PCS handsets based on film-bulk-acoustic-resonator (FBAR) had been realized by micro-machined thin film AlN devices [1-5]. Samples of 3.5 GHz, even 6.0 to 8.0 GHz were reported [6-9]. A miniature FBAR filter for 5GHz WLAN applications was announced last year [10]. FBAR will be a strong candidate in the high frequency RF filter technologies.

The series and parallel resonant frequencies are important and fundamental parameters of resonators and also affect the bandwidth of impedance element filter built by the mentioned resonators. These two frequencies can deduce other important parameters of resonators, including effective electromechanical coupling factor and the motional conductance and inductance (with given static capacitance) of BVD equivalent circuit. The relationship between these two resonant frequencies (series and parallel) and the physical parameters of FBAR is important to design and analysis. Accurate explicit formulae available for thick electrode are necessary in practice.

There are two types of FBAR, which use different means to prevent acoustic emission into the substrates. The first is a membrane configuration with air interfaces on both sides. The other is Solidly Mounted Resonator (SMR) with one side free and acoustic reflector on the other side to make mechanical supported but acoustically free. In this paper, we only discuss the FBAR with membrane configuration type.

For single piezoelectric plate resonator, neglect the electrodes, the formula for fundamental mode parallel resonant frequency is well known and simply as half of the ratio of acoustic velocity to plate thickness. An accurate approximated series resonant frequency can be also deduced from parallel resonant frequency and electromechanical coupling factor without difficult.

For the piezo-plate with thin enough electrodes, which can be modeled as mass-loading on piezo-plate, we had deduced a formula for the parallel resonant frequency with mass-loading effect [11].

However, FBAR is multi-layer structure, and the electrodes are not thin. Many requirements and restrictions [6] posed on the thickness of electrodes: (1) low acoustic attenuation, (2) high electric conductivity, (3) coupling coefficient enhancement [12], (4) process compatibility and (5) temperature compensation [4]. To those demands, thickness of the electrodes is not thin usually. That means, the electrodes cannot be treated as mass-loading only and should be modeled as acoustic layers.

This paper proposes a hypothesis that the input acoustic impedance becomes continuous under resonance, at the two opposite faces of a virtual cut plane at any position along with the acoustic transmission line, no matter at interfaces or not. On the other words, only correct resonant frequency can meet the input acoustic impedance continuity condition. When the frequency deviation is small, the input acoustic impedance can be approximated as a linear function of frequency around the resonant frequency. The method to improve the accuracy of the explicit formulae for series and parallel resonant frequencies of FBAR in single or multi layer electrodes with or without symmetry (the same material and thickness to up and bottom electrodes) will be introduced in section II. However, for simplicity, only the example of explicit formulae for single layer and symmetrical electrode will be shown in section III.

To check the accuracy of the proposed formulae, the simulations with different thickness and material combinations of the piezo-layer (ZnO and AlN) and the electrodes (Al, Au, Ag, Cu, Mo, W) are conducted. We calculate the electrical impedance of the multi-layered transmission line and get the maximum resistance/conductance frequencies as the parallel/series resonant frequencies for comparison.

II. Approximation Methodology

When the relative thickness of electrode to piezoelectric layer is very small and can be neglected, the bulk acoustic wave (BAW) resonator can be modeled as only one piezoelectric layer, and the fundamental mode parallel resonant frequency is well known as

$$f_{p0} = \frac{V_0}{2l_0} \tag{1}$$

where f_{p0}, V_0 and l_0 are the parallel resonant frequency, acoustic velocity and thickness of the piezoelectric layer. The series resonant frequency can be deduced from the electromechanical coupling factor equation which as following

$$k_t^2 = \frac{\pi^2}{4}\cdot\frac{f_{s0}}{f_{p0}}\cdot\left(1-\frac{f_{s0}}{f_{p0}}\right) \tag{2}$$

where k_t^2 and f_{s0} are electromechanical coupling factor and series resonant frequency.

After some operations, we can get the series resonant frequency as

$$f_{s0} = f_{p0}\left(\frac{1}{2}+\sqrt{\frac{1}{4}-\frac{4}{\pi^2}k_t^2}\right). \tag{3}$$

When the electrode is thin enough, it can be modeled as mass loading[11], and the parallel resonant frequency is as

$$f_p = \frac{V_0}{2l_0}\cdot\frac{1}{1+2\rho_E l_E/\rho_0 l_0} = f_{p0}\cdot\left(1+2\rho_E l_E/\rho_0 l_0\right)^{-1} \tag{4}$$

where ρ_E, ρ_0, l_E, and l_0 are density and thickness of electrode and piezoelectric film. Comparing with the resonator where the electrodes are ignored, the parallel resonance frequency decreases by a factor of $1+2\rho_E l_E/\rho_0 l_0$, which is just the unit area mass ratio of the film coated by two electrodes to the bare film. The effective coupling factor is approximated as [11]

$$k_{eff}^2 = \frac{\pi^2}{4}\cdot\frac{f_s}{f_p}\cdot\left(1-\frac{f_s}{f_p}\right) = k_t^2\cdot\left(1+\frac{2\rho_E\cdot l_E}{\rho_0\cdot l_0}\right) \tag{5}$$

However, the electrode thickness used in practice [1-6] is not “thin” and cannot be treated as mass loading only, where the formulae were deduced from electrical impedance equations [11]. In this paper, we will derive a set of explicit formulae suitable for all the electrodes used in [1-6] based on a hypothesis.

HYPOTHESIS: Usually, at the interfaces, the acoustic impedance is not continuous when the two media have different values. However, if a vibration system consisting of multi-layer, as shown in figure 1, is in resonance, the impedance at the interfaces seems (becomes) continuous. In other words, at the two opposite faces of a virtual cut plane at any position along with the acoustic transmission line, no matter at interfaces or not (Fig. 1), the input acoustic impedance Z_1 is equal to minus Z_2.

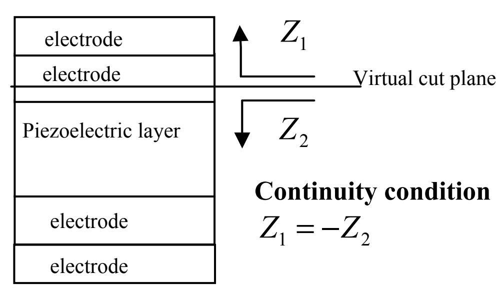

Fig. 1 Acoustic continuity condition

METHOD: Based on above hypothesis, only correct resonant frequency can meet the acoustic continuity condition, i.e., if an approximated resonant frequency is not accurate enough, the impedance Z_1 will have a deviation from minus Z_2. When the frequency deviation is small, we assume that the impedance function Z_1 and Z_2 can be given approximately by a linear function in a small frequency range near the resonant frequency. Then we can calculate the frequency correction by using Z_1, Z_2 and their slope functions at the approximated resonant frequency, as illustrated in Fig.2 .

PEOCEDURE: The frequency correction can be expressed as

$$\varepsilon = (Z_1 - Z_2) \Big/ (Z_2' - Z_1') \tag{6}$$

, where Z_1' and Z_2' are the slope of Z_1 and Z_2 at first approximated resonant frequency (with mass-loading consideration). The general formulae form for parallel and series resonant frequencies can be expressed as $f_p = mf_{p0} + \varepsilon_p$ and $f_s = mf_{s0} + \varepsilon_s$, where m is mass loading correction coefficient, ε_p and ε_s are the acoustic impedance continuity correction terms, f_{p0} and f_{s0} are the parallel and series resonant frequencies of bare piezoelectric film.

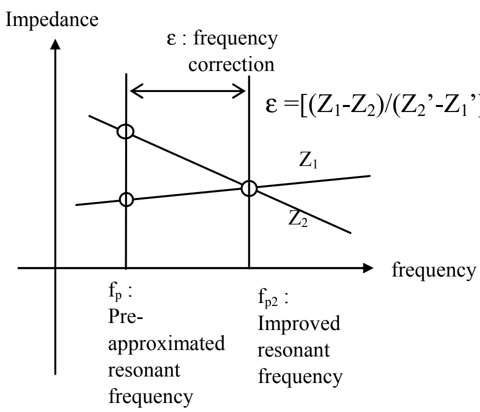

Fig.2 Accuracy improvement idea : move the approximated resonant frequency to eliminate the acoustic impedance discontinuity at specified interface inside FBAR.

III. FORMULAE EXAMPLE FOR SINGLE LAYER SYMMETRICAL ELECTRODE FBAR

For simplicity, this paper will show a formulae example of the single electrode and symmetric FBAR. That means, the upper and lower electrodes are the same. The single electrode and symmetric FBAR is shown as Fig. 3. The virtual cut plane is the interface between piezoelectric film and electrode.

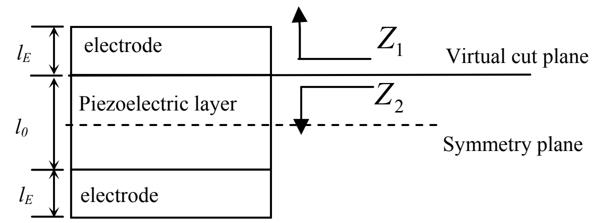

Fig. 3 Single electrode and symmetric FBAR

The input impedance of an one dimensional acoustic transmission line can be expressed as

$$Z_{in} = Z_T \frac{Z_L \cos\gamma + jZ_T \sin\gamma}{Z_T \cos\gamma + jZ_L \sin\gamma}, \tag{7}$$

where $Z_T = \rho_T V_T A$, ρ_T , V_T and A are density, acoustic velocity and section area of transmission line, $\gamma = \frac{2\pi f l_T}{V_T}$, f is frequency, l_T is transmission line length, and Z_L is acoustic load impedance on the other end.

For the input impedance of electrode side, $Z_L = 0$ and can be expressed as $Z_1 = jZ_E \tan\gamma_E$, where $Z_E = \rho_E V_E A$, ρ_E , V_E are density and acoustic velocity of electrode, $\gamma_E = \frac{2\pi f l_E}{V_E}$, l_E is electrode thickness.

For the acoustic impedance of piezoelectric film side under electrical open condition, $Z_L = \infty$ at the symmetry plane, and can be expressed as

$$Z_{2p} = -jZ_0 \Big/ \tan\frac{\gamma}{2} \tag{8}$$

, where $Z_0 = \rho_0 V_0 A$, ρ_0 , V_0 is density and acoustic velocity of piezoelectric film, A is section area of it, $\gamma = \frac{2\pi f l_0}{V_0}$, f is frequency, l_0 is piezoelectric film thickness. On the other hand, under the same acoustic boundary condition and electrical short condition, the acoustic input impedance can be expressed as

$$Z_{2s} = -jZ_0 \left(\frac{1}{\tan\frac{\gamma}{2}} - \frac{k_t^2}{\frac{\gamma}{2}} \right) \qquad (9)$$

, where k_t^2 is the electromechanical coupling factor. By satisfying the acoustic impedance continuity condition, we can get the equations for parallel and series resonant frequencies.

For parallel resonant frequency, $Z_{2p} = -Z_1$,

$$\frac{1}{\tan\frac{\gamma}{2}} = z_E \tan\gamma_E \qquad (10)$$

where $z_E = Z_E / Z_0$

For series resonant frequency, $Z_{2s} = -Z_1$,

$$\left(\frac{1}{\tan\frac{\gamma}{2}} - \frac{k_t^2}{\frac{\gamma}{2}}\right) = z_E \tan\gamma_E \qquad (11)$$

Before we find out the frequency correction, we should list out the derivatives of the input impedance functions.

The derivative for left-hand side of (10) is $-\frac{1}{2}\csc^2\frac{\gamma}{2}$, for the right hand side of (10) is $z_E \frac{V_0}{V_E}\frac{l_E}{l_0}\sec^2\gamma_E$, for the left hand side of (11) is $-\frac{1}{2}\csc^2\frac{\gamma}{2} + \frac{2k_t^2}{\gamma^2}$.

Based on (6), we can find out the frequency correction item for parallel resonant frequency is

$$\varepsilon_p = \frac{V_0}{2\pi l_0} \frac{\frac{1}{\tan\frac{\gamma_p}{2}} - z_E \tan\gamma_{Ep}}{z_E \frac{V_0}{V_E}\frac{l_E}{l_0}\sec^2\gamma_{Ep} + \frac{1}{2}\csc^2\frac{\gamma_p}{2}} \qquad (12)$$

where $\gamma_p = \frac{2\pi f_{pm} l_0}{V_0}$, $\gamma_{Ep} = \frac{2\pi f_{pm} l_E}{V_E}$, and

$$f_{pm} = f_{p0} \cdot (1 + 2 \cdot \rho_E l_E / \rho_0 l_0)^{-1} \qquad (13)$$

which is the approximated parallel resonant frequency with mass loading only, and $f_{p0} = V_0 / 2l_0$.

For series resonant frequency, the frequency correction item can be written as

$$\varepsilon_s = \frac{V_0}{2\pi l_0} \frac{\frac{1}{\tan\frac{\gamma_s}{2}} - \frac{k_t^2}{\gamma_s/2} - z_E \tan\gamma_{Es}}{z_E \frac{V_0}{V_E}\frac{l_E}{l_0}\sec^2\gamma_{Es} + \frac{1}{2}\csc^2\frac{\gamma_s}{2} - \frac{2k_t^2}{\gamma_s^2}} \qquad (14)$$

where $\gamma_s = \frac{2\pi f_{sm} l_0}{V_0}$, $\gamma_{Es} = \frac{2\pi f_{sm} l_E}{V_E}$,

$$f_{sm} = f_{s0} \cdot (1 + 2 \cdot \rho_E l_E / \rho_0 l_0)^{-1} \qquad (15)$$

which is approximated series resonant frequency with mass loading only, and $f_{s0} = f_{p0}\left(\frac{1}{2} + \sqrt{\frac{1}{4} - \frac{4}{\pi^2}k_t^2}\right)$.

The parallel and series resonant frequencies can be written as (16) and (17)

$$f_p = f_{p0} \cdot (1 + 2 \cdot \rho_E l_E / \rho_0 l_0)^{-1} + \varepsilon_p \qquad (16)$$

$$f_s = f_{s0} \cdot (1 + 2 \cdot \rho_E l_E / \rho_0 l_0)^{-1} + \varepsilon_s \qquad (17)$$

where ε_p and ε_s are expressed as (12) and (14).

Once we have the resonant frequencies, we can calculate the effective electromechanical coupling factor as (18) and also the motional conductance and inductance.

$$k_{eff}^2 = \frac{\pi^2}{4} \cdot \frac{f_s}{f_p} \cdot \left(1 - \frac{f_s}{f_p}\right) \qquad (18)$$

IV. Accuracy Verification by Numerical Simulation

To check the accuracy of the proposed formulae, the simulations with different thickness and material combinations of the piezo-layer (ZnO and AlN) and the electrodes (Al, Au, Ag, Cu, Mo, W) are conducted. We calculate the electrical impedance of the multi-layered transmission line and get the maximum resistance/conductance frequencies as the reference parallel/series resonant frequencies for comparison.

For simplicity, this paper neglects the acoustic attenuation in material. On the other hand, for numerical stability, we assume Q of all material is 100,000 to simulate no loss condition in the program of the maximum resistance/conductance frequencies calculation to get the reference parallel/series resonant frequencies. The piezoelectric film thickness is 1.5μm. The material constant adopted in simulation is shown as Table I.

TABLE I
MATERIAL CONSTANT IN SIMULATION

Material	Density (kg/m3)	Acoustic wave velocity (m/s)	Electro-mechanical coupling factor
AlN	3270	11350	5%
ZnO	5680	6070	7.80%
Al	2700	6420	NA
Ag	10600	3600	NA
Cu	8930	5010	NA
Mo	10000	6300	NA
Au	19490	3361	NA
W	19400	5200	NA

There are two kinds of electrode thickness variation. For most heavy metal, Au, Ag, Cu, Mo, W, the unit area mass ratio, $\rho_E l_E / \rho_0 l_0$, vary from 0 to 0.5. However, for light metal, Al, the thickness ratio to piezoelectric film is from 0 to 0.25. These conditions are suitable for usual FBAR.

Three kinds of parallel resonant frequencies were calculated for comparison, they are mass loading only approximation (13), proposed formula of this paper (16), and from transmission line model as reference frequency. The frequency deviation between approximation equation and reference frequency is the error of approximation and is shown as Table II. The effective coupling factor of (18) and (5) are calculated and compared to the result from transmission line model and also shown in Table II.

TABLE II
APPROXIMATION ERROR FOR f_p and k_{eff}^2

Piezo-electric layer	Electrode layer (*)	f_p error (%)	k_{eff}^2 error (%)	f_p error (%)	k_{eff}^2 error (%)
		Mass loading only		Proposed formulae	
AlN	Al	7.978	48.733	0.229	2.069
AlN	Ag	0.49019	97.94017	0.00011	0.00245
AlN	Cu	2.80382	88.23539	0.01626	0.01607
AlN	Mo	5.78897	76.64595	0.12893	0.41229
AlN	Au	6.01245	75.82835	0.14342	0.46479
AlN	W	7.58645	70.20277	0.27234	0.94247
ZnO	Al	1.813	14.555	0.007	0.086
ZnO	Ag	1.65922	93.28907	0.00356	0.00602
ZnO	Cu	3.63895	85.4881	0.0346	0.07138
ZnO	Mo	6.19695	76.06491	0.15587	0.48799
ZnO	Au	6.38884	75.39072	0.16964	0.53587
ZnO	W	7.74173	70.7509	0.28764	0.94859

(*)Note: The thickness ratio for electrode Al is 0.25. For other electrode material, the unit area mass ratio is 0.5.

The errors for parallel resonant frequency of the explicit formulae we proposed can be lower than 0.3% under the conditions that the unit area mass ratio of electrodes to piezoelectric layer is less than 0.5 for heavy metal (Au, Ag, Cu, Mo, W), and thickness ratio is less than 0.25 for light metal (Al). Under the same conditions, the error of our formulae can be decreased to less than 5% of the formulae with mass loading effect only.

The error for effective coupling factor of the proposed formulae can be lower then 1% for heavy electrode materials, and it is much lower than the formulae with mass loading effect only which have greater than 50% error.

For limited space, the distribution of parallel resonant frequency and the effective coupling factor along electrode thickness ratio or mass ratio are shown for two electrode materials, one light electrode Al with lowest acoustic impedance and one heavy electrode W with highest acoustic impedance. The relationship between the distribution results and the material combination are AlN + Al (Fig. 4,5), AlN +W (Fig. 6,7), ZnO + Al (Fig. 8,9), and ZnO + W(Fig. 10,11). In each figure, there are three types of lines: thick dashed line, thin dashed line, and solid line. Thick dashed line is calculated from transmission line model. Thin dashed line is from formulae with mass loading correction only. Solid line is from the proposed formulae.

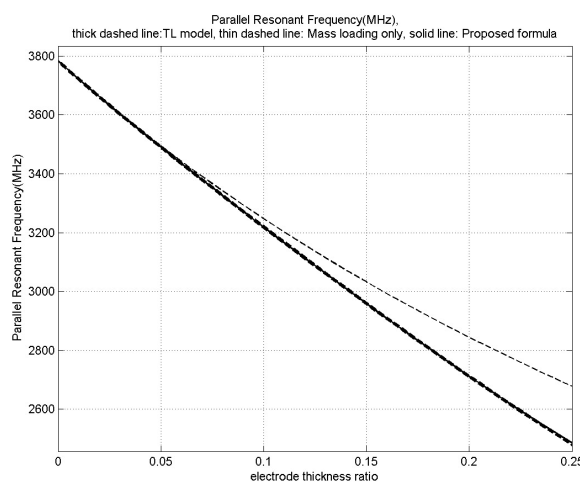

Fig. 4 The parallel resonant frequency distribution along electrode thickness ratio for AlN+Al

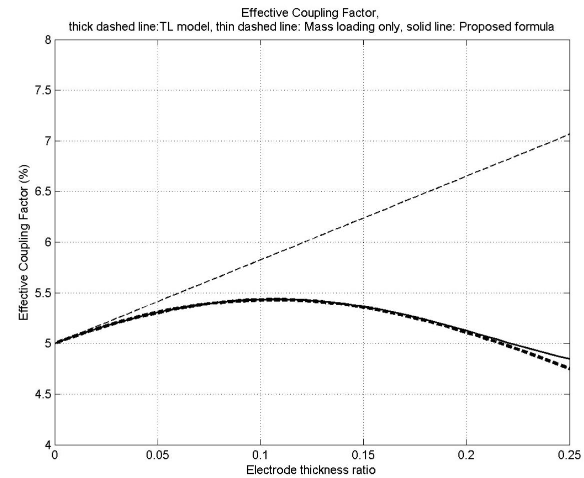

Fig. 5 The effective coupling factor distribution along electrode thickness ratio for AlN+Al

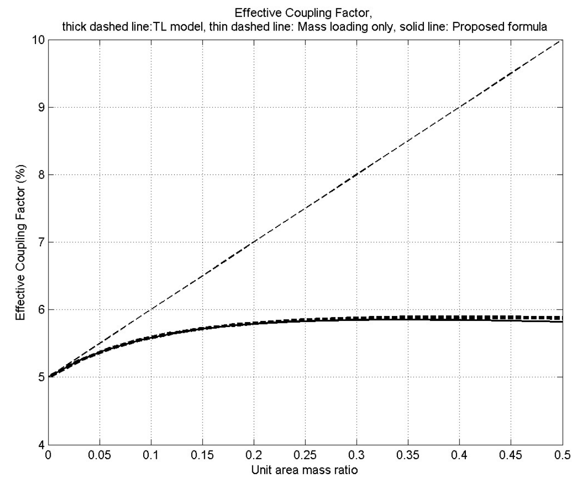

Fig. 7 The effective coupling factor distribution along mass ratio for AlN+W

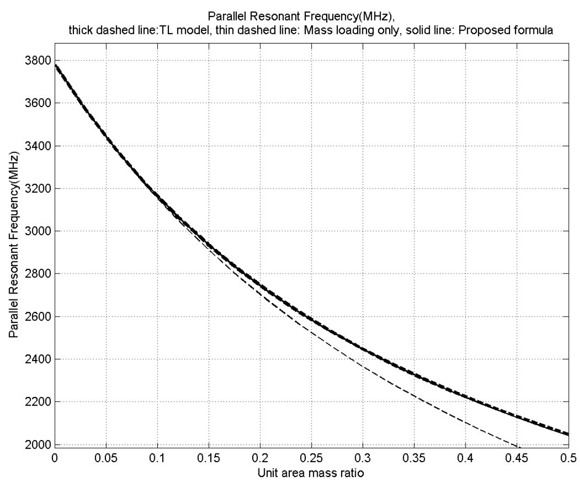

Fig. 6 The parallel resonant frequency distribution along mass ratio for AlN+W

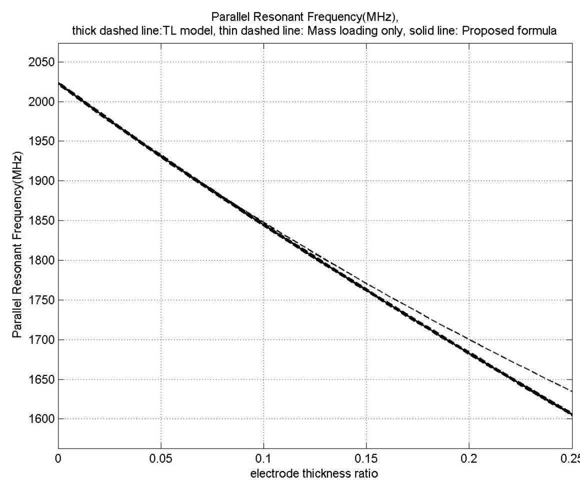

Fig. 8 The parallel resonant frequency distribution along electrode thickness ratio for ZnO+Al

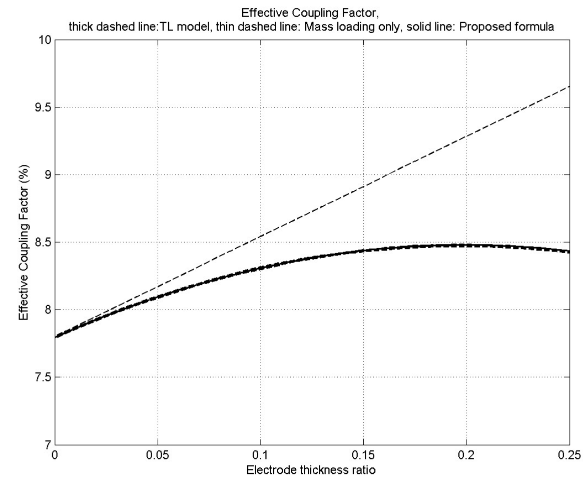

Fig. 9 The effective coupling factor distribution along electrode thickness ratio for ZnO+Al

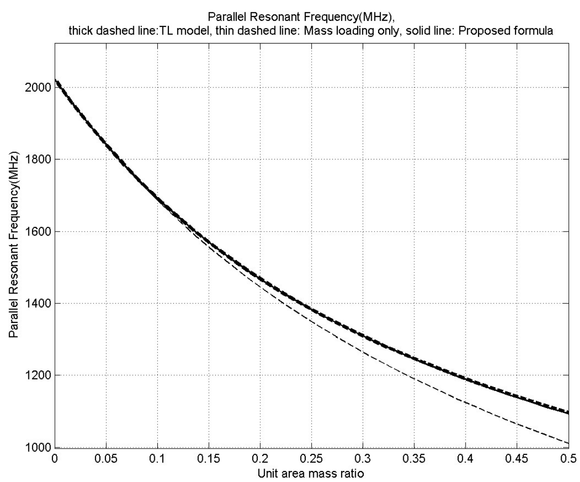

Fig. 10 The parallel resonant frequency distribution along mass ratio for ZnO+W

The simulation results show for both parallel resonant frequency and effective electromechanical coupling factor, the proposed formulae can approximate transmission line model very closely. The formulae with mass loading effect only can approximate well in very thin electrode region, but the error grows rapidly as the electrode get thicker.

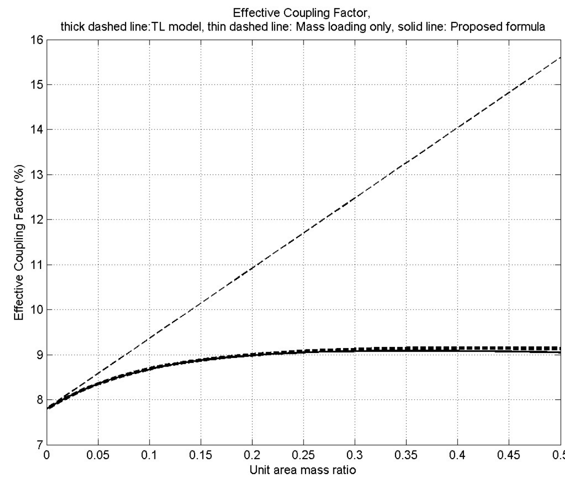

Fig. 11 The effective coupling factor distribution along mass ratio for ZnO+W

V. Conclusion

Accurate explicit formulae for the fundamental mode parallel/series resonant frequencies of FBAR with thick electrode were proposed. A hypothesis was described that the input acoustic impedance becomes continuous under resonance, at the two opposite faces of a virtual cut plane at any position along with the acoustic transmission line, no matter at interfaces or not. On the other words, only correct resonant frequency can meet the input acoustic impedance continuity condition. When the frequency deviation is small, the input acoustic impedance can be approximated as a linear function of frequency around the resonant frequency. We deduce the frequency correction formulae to eliminate the input impedance difference. The proposed parallel/series resonant frequency formulae are composed of two parts. The first part is the resonant frequency with mass loading effect, and the second part is the correction item for the input acoustic impedance difference correction mentioned above. Numerical simulations were conducted to check the accuracy of the proposed formulae.

The results show, for parallel resonant frequency, the errors of the proposed explicit formulae can be lower than 0.3% under the conditions that the unit area mass ratio of electrodes to piezo-layer is less than 0.5 for heavy metal (Au, Ag, Cu, Mo, W), and thickness ratio is less than 0.25 for light metal (Al). These conditions are suitable for usual FBAR. Under the same conditions, the error of our formulae can be decreased to less than 5% of the formulae with mass loading effect only. For effective coupling factor calculated from resonant frequencies, the error can be lower then 1% for heavy electrode materials, and it is much lower than the formulae with mass loading effect only which have greater than 50% error.

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