Extension of the Legendre polynomial approach for analyzing composite BAW resonators

A. Raherison and F. E. Ratolojanahary
Laboratoire de Physique Appliquée (LAPAUF)
Université de Fianarantsoa
301 Fianarantsoa, Madagascar
faniry@univ-fianar.mg

J. E. Lefebvre, T. Gryba and E. Ntagwirumugara
IEMN, UMR CNRS 8520, Département OAE
Université de Valenciennes,
59313-Valenciennes Cedex 9, France
jean-etienne.lefebvre@univ-valenciennes.fr

Abstract— **We present a new 1D resonator modeling through a polynomial approach. We have determined, for different values of the metallization thickness, the series and parallel resonance frequencies, the field profiles within the structure, and the effective electromechanical coupling coefficient and the Q-factor as well. To assess and validate the approach, the results are compared against other calculations from the literature.**

I. INTRODUCTION

The tremendous growth in wireless and mobile communication systems leads to a great demand for radiofrequency filters in the 1 to 10GHz range. Conventional surface acoustic wave technology comes up against its limits and cannot meet the required specifications in this new frequency range [1]-[3]. Bulk acoustic wave technology is extensively investigated to develop the required high-performance components. There is a need for models, which enable design and optimization of these components.

Till now the Legendre polynomial approach has been used for studying devices with guided waves. The method's convergence depends on the constituent materials parameters of the multilayered structure i.e. good convergence for those with constituent materials parameters close to each other and poor convergence for those with very dissimilar materials in nature [4]-[6].

In this paper, we extend the Legendre polynomial formulation to study BAW resonators i.e. devices with standing rather than travelling waves and with very dissimilar materials. The aim is to have an access to modal and harmonic analysis of composite BAW resonators.

In Sec. II, the Legendre polynomial method formulation is described. We take into account two models of excitation (voltage and current sources). In Sec. III, this method is implemented for numerical simulation. On the one hand, through a modal analysis, we calculate for different values of the metallization thickness, the series and the antiresonance frequencies for the first six modes and the field profiles within this structure. We then calculate two key parameters for the BAW resonator: the effective electromechanical coupling coefficient K^2 and the Q-factor. On the other hand, we calculate through a harmonic analysis the input electrical impedance under two types of excitation: voltage and current excitation.

To validate the approach, it is applied to the study of a three-layer structure (Al/ZnO/Al); the results are compared against the results obtained from a numerical approach using a matrix algorithm [7]. A conclusion is given in Sec. IV.

II. LEGENDRE POLYNOMIAL METHOD FORMULATION

A. Structure

The structure is shown in Fig. 1. The x_3 axis is in the direction of propagation. Throughout this paper, a harmonic time dependence exp(jωt) is implied.

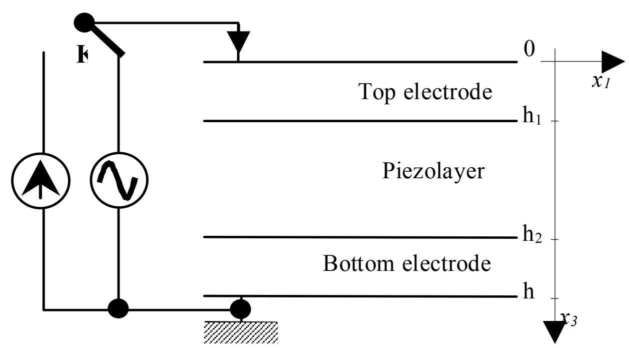

Figure 1. Schematic view of a composite bulk acoustic wave resonator (BAW) with one piezolayer. Definition of the two resonator excitation methods.

B. Mathematical formulation

The field equations governing wave propagation into the structure are given by:

$$\frac{\partial T_{ac}}{\partial x_c} = \rho^s \frac{\partial^2 u_a}{\partial t^2} , \tag{1}$$

$$\frac{\partial D_c}{\partial x_c} = 0, \tag{2}$$

$$J(s,t) = \frac{\partial D_3}{\partial t}. \tag{3}$$

where u_a stands for the components of particle displacement, T_{ac} and D_c are the stress and the electrical displacement. The subscript S represents the effective quantity of the structure [5]. Summation over repeated indices is implied throughout this article.

The boundary conditions for this structure are:

- Continuity of stress, particle displacement components and electric potential across interfaces,
- Vanishing of stress at upmost and lowest surfaces,

Piezoelectric materials are anisotropic: they imply a coupling between electrical and mechanical properties. By introducing the rectangular window function $\pi_{0,h}$ the boundary conditions are automatically incorporated in the constitutive equations for piezoelectric materials [5]:

$$T_{ac} = \left(c^{s}_{abcd} \cdot \frac{\partial u_b}{\partial x_d} + e^{s}_{dac} \cdot \frac{\partial \phi}{\partial x_d} \right) . \pi_{0,h}(x_3) \ , \tag{4}$$

$$D_c = e^{s}_{cbd} \cdot \frac{\partial u_b}{\partial x_d} - \varepsilon^{s}_{cd} \cdot \frac{\partial \phi}{\partial x_d} \ . \tag{5}$$

where ϕ stands for the electric potential.

Till now, the polynomial approach was thought to be efficient for multilayered structures with very similar neighboring materials. Indeed, for dissimilar neighboring materials, the convergence is poor due to the discontinuities in slope exhibited at interfaces by field quantities such as particle displacement components and electric potential.

In this paper, we propose an alternative approach allowing to overcome this difficulty: in each layer, we choose a specific polynomial expansion in order to fit, by anticipation, the slope discontinuities at the interfaces.

1) Polynomial resolution:

The spatial coordinates have been transformed to be dimensionless:

$q = x_3/\text{h}$, h is resonator thickness.

- In piezolayer numbered (2)

The expression of particle displacement is [5]:

$$u^{(2)}_{a}(q) = \sum_{m=0}^{+\infty} p_m \, Q_m(q) \ , \tag{6}$$

The expression of electric potential depends on the used excitation method:

- For the case of the voltage excitation method:

$$\phi^{(2)}(q) = \sum_{m=0}^{+\infty} r_m (q_1 - q).(q_2 - q) Q_m(q) + \left(\frac{q_2 - q}{q_2 - q_1} \right)^2 . V_0 \ , \tag{7}$$

- and for the case of the current excitation method:

$$\phi^{(2)}(q) = \sum_{m=0}^{+\infty} r_m (q_2 - q).Q_m(q) \ , \tag{8}$$

- In the metal electrodes

By fulfilling the stress continuity across the interfaces, we can determine the particle displacement in metal electrodes that anticipate the slope's discontinuities.

Expressions of the electric potential:

- Top electrode numbered (1)

$$\phi^{(1)}(q) = \phi^{(2)}(q_1), \tag{9}$$

- Bottom electrode numbered (3)

$$\phi^{(3)}(q) = 0 \, . \tag{10}$$

2) Analytic solution:

Combining the equations above and exploiting the orthonormality of the Legendre polynomial, we obtain:

- Voltage excitation:

$$(\omega \text{h})^2 . \delta_{jm} . p^{b}_{m} = \text{A}_{jm} . p^{b}_{m} + \text{B}^{b}_{j} . V_0 \, , \tag{11}$$

$$\delta_{jm} . r_m = \text{C}^{b}_{jm} . p^{b}_{m} + \text{D}_j . V_0 \, . \tag{12}$$

where: $\delta_{jm} = \begin{cases} 1 \text{ if } j = m, \\ 0 \text{ if } j \neq m. \end{cases}$

- Current excitation :

$$(\omega \text{h})^2 . \delta_{jm} . p^{b}_{m} = \text{AA}_{jm} . p^{b}_{m} + \text{BB}^{b}_{j} . I_0 \, , \tag{13}$$

$$\delta_{jm} . r_m = \text{CC}^{b}_{jm} . p^{b}_{m} + \text{DD}_j . I_0 \, . \tag{14}$$

The modal analysis can be treated as a specific case of the here-above harmonic analysis by setting the electrical excitations to zero.

III. Applications - Numerical simulation

Table I indicates the parameters of the materials and the truncature order which have been used in calculations.

TABLE I. MATERIAL PARAMETERS USED IN SIMULATIONS

Parameters	Symbol	ZnO	Al
Mass density($kg.m^{-3}$)	ρ	5.676	2 .7
Elastic stiffness ($10^{10} N.m^2$)	c_{33}	21.09	10.7
Elastic viscosity (10^{-3} $Pa.s$)	η	11.96	—
Piezoelectric constant ($c.m^{-2}$)	e_{33}	1.14	—
Permittivity ($10^{-10} F.m^{-1}$)	ε_{33}	0.783	—
Layer thickness (μm)	h	2	modifiable
Legendre Polynomials truncature order: M = 11			

A. Modal analysis

1) Series and parallel resonance frequencies

As mentioned above, modal analysis is obtained by vanishing the electrical excitations. Under these conditions, both the voltage excitation equation (11) and the current excitation equation (13) are reduced to eigenvalue equations. For the first case $V_0 = 0$ (short-circuited electrodes), eigenvalues yield the series resonance frequencies; for the second case $I_0 = 0$ (open-circuit), eigenvalues yield the antiresonance frequencies. In both cases, the corresponding eigenvectors p_m and r_m yield the field profiles.

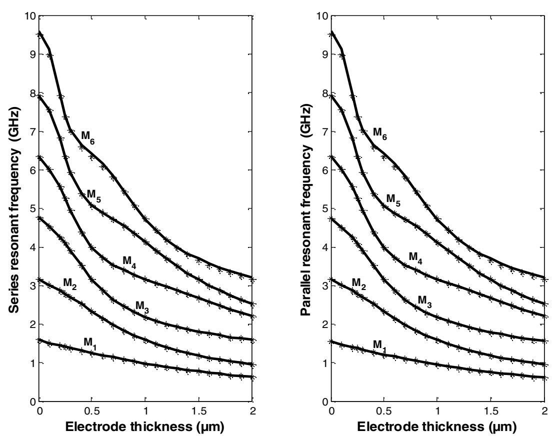

Figure 2. Effect of electrodes thickness on series and parallel resonance frequencies for the first six modes for a 2 µm thick ZnO layer and Al metal electrode (+: analytic; —: polynomial method with anticipation). M = 11.

Fig. 2 illustrates the effect of electrodes thickness on resonance frequencies. This figure reveals a good agreement between the analytic method and the polynomial approach with anticipation.

2) Effective coupling electromechanical coefficient

The effective coupling electromechanical coefficient and the Q-factor are calculated from the series and parallel resonance frequencies f_S and f_P as follows [8]:

$$K^2 = \frac{f_p^2 - f_s^2}{f_p^2}, \tag{15}$$

$$Q = \frac{2\pi}{f_s \eta}. \tag{16}$$

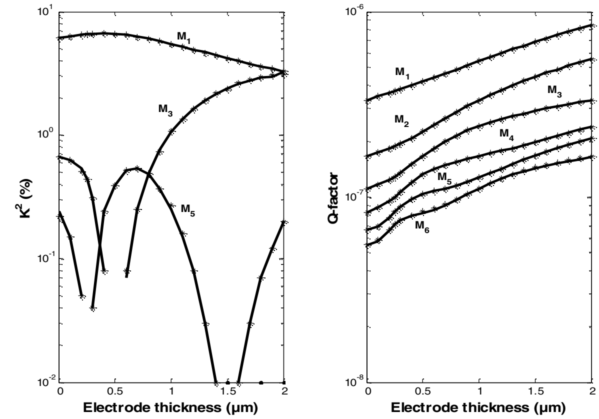

Figure 3. Effect of electrodes thickness on effective coupling electromechanical coefficient and Q-factor for the first six modes for a 2 µm thick ZnO layer and Al metal electrode. (+: analytic; —: polynomial method with anticipation). M = 11.

Fig. 3 also shows a good agreement between the analytic method and the polynomial approach with anticipation for the calculation of the effective coupling electromechanical coefficient and the Q-factor. These curves reveal an optimum electrode thickness for which the effective coupling electromechanical coefficient is maximum: ≈ 0.5 µm for the first mode and ≈ 0.7 µm for the fifth mode.

3) Fields profiles

Fig.4 and Fig.5 show respectively the calculated profiles, of the particle displacement and the electric potential within the studied three-layer structure, obtained by using the analytic method and the polynomial approaches with and without anticipation for each method of excitation.

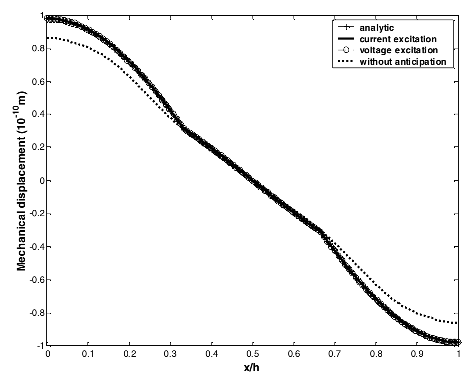

Figure 4. Particle displacement within 2 µm Al/ZnO/Al structure without anticipation for two methods of excitation (V_0 = 1 V, I_0 = 400 nA) at the resonance frequency (0.625 GHz). M = 11.

For both figures 4 and 5, the analytic curve and those calculated by the polynomial approach with anticipation show a good agreement. The discontinuities in slope at the interfaces are correctly restituted.

However, the obtained profiles with the polynomial approach without anticipation and the analytic method exhibit a discrepancy especially in the metal electrodes. In addition, the discontinuities in slope at the interfaces are not restituted by the polynomial approach without anticipation.

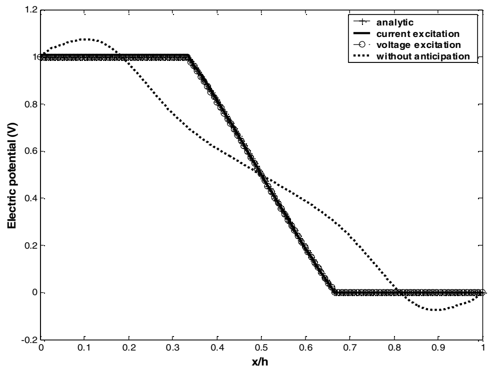

Figure 5. Electric potential within 2 µm Al/ZnO/Al structure without anticipation for two methods of excitation (V_0 = 1 V, I_0 = 400 nA) at the resonance frequency (0.625 GHz). M = 11.

B. Harmonic analysis

The input impedance of a composite BAW resonator with two electrodes can be written [7]:

$$Z_{in} = \frac{1}{j\omega C_0}\left[1 + \frac{k^2}{\varphi}\frac{j(z_t + z_b)z_p \sin\varphi - 2z_p^2(1-\cos\varphi)}{(z_p^2 + z_t z_b)\sin\varphi - j(z_t + z_b)z_p\cos\varphi}\right], \quad (17)$$

where z_t, z_b and z_p are respectively the acoustic impedances of the top and the bottom electrodes and the piezolayer.

$\varphi=\omega h/V_p$, V_p is the thickness mode velocity on the piezolayer, k^2 is the coupling electromechanical coefficient.

For the Legendre polynomial method, this input electric impedance is given by:

$$Z_{in} = V/I = \phi(0)/I, \quad (18)$$

and the electric admittance can be written:

$$Y_{in} = 1/\, Z_{in}. \quad (19)$$

Fig. 6 permits to compare the curves of electric admittance computed with the analytic and polynomial methods. A good agreement is obtained between the results from the polynomial approach with anticipation and the analytic method for both current and voltage excitations. For the polynomial method without anticipation, the result is incorrect due to the slope's problems of the particle displacement and the electric potential at the interfaces.

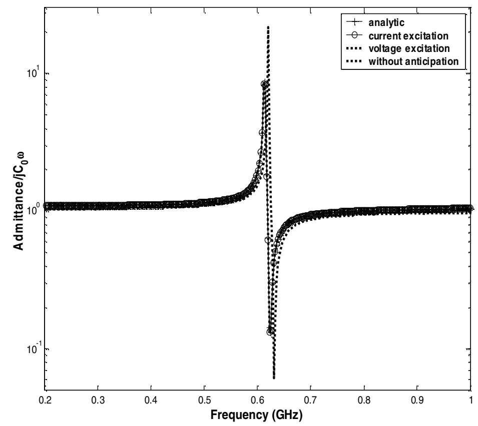

Figure 6. Comparison of the input admittances calculated for the 2µm Al/ZnO/Al structure with and without anticipation for two methods of excitation (V_0 = 1 V, I_0 = 400 nA). M = 11.

IV. CONCLUSION

The advantages of the polynomial approach with anticipation are (i) an efficient computation of the series and parallel resonance frequencies (eigenvalues), the effective coupling electromechanical coefficient and the Q-factor as well as the mode shapes (eigenvectors) (ii) the efficiency of the method for the calculation of the input electric impedance (iii) a good accuracy (better than 2%). The obtained results are satisfying and the resonance frequencies can be retrieved easily. Therefore, this method is a powerful tool for calculation of the composite BAW resonator performances. This approach is thought to have potentialities for a bidimensional modeling of BAW composite resonators. This study will be considered in a subsequent paper.

V. REFERENCES

[1] G. V. Tsarenkov, "10 GHz Piezoelectric BAW Resonators Based on Semiconductor Multilayer Heterostructures," *IEEE Ultrasonics Symposium*, pp. 939–942, 1999.

[2] J. Kim, S. Lee, J. Ahn and J. Lee, "AlN piezoelectric materials for wireless communication thin film components*", Journal of ceramic Processing Research*, vol. 3, No. 1, pp. 25–28, 2002.

[3] M. Dubois, "Thin film bulk acoustic wave resonators: a technology overview", *MEMSWAVE 03*, Toulouse, France, July 2–4, 2003.

[4] S. Datta and B. J. Hunsiger, "Surface acoustic waves in periodic structures", *J. Appl. Phys*, vol. 50, No. 5, pp. 3370–3375, May 1979.

[5] J. E. Lefebvre, V. Zhang, J. Gazalet and T. Gryba, "Legendre polynomial approach for modeling free ultrasonic waves in multilayered plates", *J. Appl. Phys*, vol. 85, pp. 3419–3427, 1999.

[6] L. Elmaimouni, J. E. Lefebvre, V. Zhang, J. Gazalet and T. Gryba, "Guided waves in inhomogeneous cylinders of Functionally Graded Materials (FGM)", *NDT&E International*, vol. 38, pp. 344–353, 2005.

[7] M. Dubois, P. Murelt and V. Plessky, "BAW resonators based on Aluminium nitride thin filter*", IEEE Ultrasonics Symposium*, pp. 907–910, 1999.

[8] ANSI/IEEE Std 176-1987, IEEE Standard on Piezoelectricity (The Institute of Electrical and Electronics Engineers), New York, 1989.