Analysis of Rayleigh Waves in Piezoelectric Solids with Metal Coatings by the Rayleigh-Ritz Method

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***Summary*—Analyzing Rayleigh waves in structures of a piezoelectric solid coated with a patterned metal film layer is of great importance in developing acoustic wave resonators. The Rayleigh-Ritz method is used to analyze the problem of surface acoustic wave (SAW) propagation in the two-dimensional resonator structure with simplification as an effort to validate novel techniques and methods. Following a standard formulation, relatively accurate results are obtained from the approximate eigenvalue problem with the consideration of the boundary conditions in the analytical procedure. The computational cost is relatively low in comparison with the finite element analysis, thus making it more practical and preferable as an innovative modeling tool for an efficient design procedure.**

Keywords—Rayleigh waves; piezoelectric; film; Rayleigh-Ritz method

I. INTRODUCTION

Since White and Voltmer discovered that the metal electrodes can enable the surface acoustic waves in piezoelectric materials [1], numerous studies on the analysis of Rayleigh waves have been published, mainly adopting analytical, semi-analytical, experimental, and the finite element method to help product design over the following few decades [2]–[9]. In this study, we undertook a thorough study of the Rayleigh waves in the structure of a piezoelectric substrate covered with a metal film by the Rayleigh-Ritz method for a better analysis of the displacement and electric fields with a novel approach.

As a popular numerical method, the Rayleigh-Ritz method (RRM) can find the approximate frequency of vibrations of elastic solids by generating an approximate eigenvalue equation with the assumed displacements meeting certain requirements such as satisfying the essential boundary conditions to obtain the frequency, mode shapes, and phase velocity as part of the procedure for device design.

II. BASIC EQUATIONS

A layered structure of Au/ZnO is used in this study for the dispersion curves with different boundary conditions. To analyze the propagation characteristics in the layered Au/ZnO structure, a 2D model is considered. To reduce the complexity of the numerical calculation, a unit cell of layered Au/ZnO structure with one wavelength (λ) wide (a) and nine wavelengths thickness (h) is shown in Fig. 1.

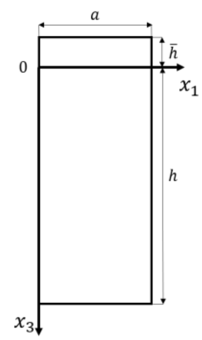

Fig. 1. A unit cell of layered Au/ZnO structure

The displacements of the Au film are assumed as

$$\bar{u}_i = \bar{f}(x_3)\left[\sum_{n=0}^{N} \bar{A}_{in} P_n\left(\frac{2x_3}{\bar{h}}+1\right)\sin(kx_1) + \sum_{n=0}^{N} \bar{B}_{in} P_n\left(\frac{2x_3}{\bar{h}}+1\right)\cos(kx_1)\right]e^{j\omega t} \quad (1)$$

The displacements of the substrate are

$$u_i = f(x_3)\left[\sum_{n=0}^{N} A_{in} P_n\left(\frac{2x_3}{h}-1\right)\sin(kx_1) + \sum_{n=0}^{N} B_{in} P_n\left(\frac{2x_3}{h}-1\right)\cos(kx_1)\right]e^{j\omega t} \quad (2)$$

The electrical potential of the Au film layer is

$$\varphi = \tilde{f}(x_3)\left[\sum_{n=0}^{N} \tilde{A}_{in} P_n\left(\frac{2x_3}{h}-1\right)\sin(kx_1) + \sum_{n=0}^{N} \tilde{B}_{in} P_n\left(\frac{2x_3}{h}-1\right)\cos(kx_1)\right]e^{j\omega t} \quad (3)$$

In the above equations, $i = 1,3$, k is the wavenumber, h is the thickness of the substrate, $\bar{h}$ is the thickness of the film, $P_n(x)$ are the Legendre polynomials, $f(x_3)$, $\bar{f}(x_3)$, and $\tilde{f}(x_3)$ are the boundary condition functions, respectively.

For the open circuit case the electrical boundary conditions are expressed as

$$D_3(x_3 = 0) = 0 \quad (4)$$

The traction-free boundary conditions are expressed as

$$\bar{\sigma}_{3i}(x_3 = -\bar{h}) = 0$$
$$\sigma_{3i}(x_3 = h) = 0 \tag{5}$$

For a shorted circuit case, the electrical boundary condition is expressed as

$$\varphi_3(x_3 = 0) = 0 \tag{6}$$

The continuity conditions of stresses and displacements are expressed as

$$u_i(x_3 = 0) = \bar{u}_i(x_3 = 0)$$
$$\sigma_{3i}(x_3 = 0) = \bar{\sigma}_{3i}(x_3 = 0) \tag{7}$$

The constitutive relation are

$$\sigma_{ij} = c_{ijkl}\gamma_{kl} - e_{kij}E_k$$
$$D_i = e_{ikl}\gamma_{kl} + \varepsilon_{ik}E_k \tag{8}$$

where σ_{ij} and D_i are the stresses and electric displacements, γ_{kl} and E_k are the strains and electric fields, c_{ijkl}, e_{kij} and ε_{ik} are elastic constants, piezoelectric coefficients and dielectric permittivity coefficients, respectively

Substituting (1)-(3) and (8) into the following variational equations

$$\iint \delta u_i\left(\sigma_{ij,j} - \rho\ddot{u}_i\right) \mathrm{d}x_1 \mathrm{d}x_3 = 0$$
$$\iint \delta\varphi\left(D_{i,i}\right) \mathrm{d}x_1 \mathrm{d}x_3 = 0 \tag{9}$$

and following a standard formulation by the RRM, the stiffness and mass matrices are

$$[K_{ik}] = \iint \left(\frac{1}{2}c_{ijkl}u_{i,j}u_{k,l} + \frac{1}{2}\bar{c}_{ijkl}\bar{u}_{i,j}\bar{u}_{k,l} - e_{kij}\varphi_{,k}u_{i,j} - \frac{1}{2}\varepsilon_{ik}\varphi_{,k}\varphi_{,i}\right) \mathrm{d}x_1 \mathrm{d}x_3 \tag{10}$$
$$[M_{ik}] = \iint \left(\frac{1}{2}\rho\dot{u}_i\dot{u}_k + \frac{1}{2}\bar{\rho}\dot{\bar{u}}_i\dot{\bar{u}}_k\right) \mathrm{d}x_1 \mathrm{d}x_3$$

The following eigenvalue equation is obtained

$$\begin{bmatrix} \mathbf{K}^{uu} & \mathbf{K}^{uw} & \mathbf{K}^{u\varphi} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}^{wu} & \mathbf{K}^{ww} & \mathbf{K}^{w\varphi} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}^{\varphi u} & \mathbf{K}^{\varphi w} & \mathbf{K}^{\varphi\varphi} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{K}^{\bar{u}\bar{u}} & \mathbf{K}^{\bar{u}\bar{w}} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{K}^{\bar{w}\bar{u}} & \mathbf{K}^{\bar{w}\bar{w}} \end{bmatrix}\boldsymbol{\alpha} - \omega^2 \begin{bmatrix} \mathbf{M}^{uu} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{M}^{ww} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{M}^{\bar{u}\bar{u}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{M}^{\bar{w}\bar{w}} \end{bmatrix}\boldsymbol{\alpha} = \begin{Bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{Bmatrix} \tag{11}$$

and the phase velocity of the SAW is $c_R = \frac{\omega}{k}$.

To obtain the relationship among the unknown amplitudes from the boundary conditions, there is a transformative matrix $\mathbf{S}_1$ such that

$$\boldsymbol{\alpha} = \mathbf{S_1}\bar{\boldsymbol{\alpha}} \tag{12}$$

where

$$\boldsymbol{\alpha} = \{\mathbf{A_1} \quad \mathbf{B_1} \quad \mathbf{A_3} \quad \mathbf{B_3} \quad \tilde{\mathbf{A}} \quad \tilde{\mathbf{B}} \quad \bar{\mathbf{A}}_\mathbf{1} \quad \bar{\mathbf{B}}_\mathbf{1} \quad \bar{\mathbf{A}}_\mathbf{3} \quad \bar{\mathbf{B}}_\mathbf{3}\}^{\mathrm{T}}$$
$$\bar{\boldsymbol{\alpha}} = \{\mathbf{AA_1} \quad \mathbf{BB_1} \quad \mathbf{AA_3} \quad \mathbf{BB_3} \quad \widetilde{\mathbf{AA}} \quad \widetilde{\mathbf{BB}} \quad \bar{\mathbf{A}}_\mathbf{1} \quad \bar{\mathbf{B}}_\mathbf{1} \quad \bar{\mathbf{A}}_\mathbf{3} \quad \bar{\mathbf{B}}_\mathbf{3}\} \tag{13}$$

and

$$\begin{aligned} \mathbf{A_1} &= [A_{11} \quad A_{12} \quad A_{13} \quad \dots \quad A_{1N}]^{\mathrm{T}} \\ &\vdots \\ \mathbf{B_3} &= [B_{31} \quad B_{32} \quad B_{33} \quad \dots \quad B_{3N}]^{\mathrm{T}} \\ \tilde{\mathbf{A}} &= [\tilde{A}_{11} \quad \tilde{A}_{12} \quad \tilde{A}_{13} \quad \dots \quad \tilde{A}_{1N}]^{\mathrm{T}} \\ \tilde{\mathbf{B}} &= [\tilde{B}_{11} \quad \tilde{B}_{12} \quad \tilde{B}_{13} \quad \dots \quad \tilde{B}_{1N}]^{\mathrm{T}} \\ \mathbf{AA_1} &= [A_{12} \quad A_{13} \quad A_{14} \quad \dots \quad A_{1N}]^{\mathrm{T}} \\ &\vdots \\ \mathbf{BB_3} &= [B_{32} \quad B_{33} \quad B_{34} \quad \dots \quad B_{3N}]^{\boldsymbol{T}} \\ \widetilde{\mathbf{AA}} &= [\tilde{A}_{14} \quad \tilde{A}_{15} \quad \tilde{A}_{16} \quad \dots \quad \tilde{A}_{1N}]^{\boldsymbol{T}} \\ \widetilde{\mathbf{BB}} &= [\tilde{B}_{14} \quad \tilde{B}_{15} \quad \tilde{B}_{16} \quad \dots \quad \tilde{B}_{1N}]^{\boldsymbol{T}} \\ \bar{\mathbf{A}}_\mathbf{1} &= [\bar{A}_{11} \quad \bar{A}_{12} \quad \bar{A}_{13} \quad \dots \quad \bar{A}_{1N}]^{\boldsymbol{T}} \\ &\vdots \\ \bar{\mathbf{B}}_\mathbf{3} &= [\bar{B}_{31} \quad \bar{B}_{32} \quad \bar{B}_{33} \quad \dots \quad \bar{B}_{3N}]^{\boldsymbol{T}} \end{aligned} \tag{14}$$

Then the modified stiffness and mass matrices can be expressed as

$$\widetilde{\mathbf{K}} = \mathbf{S_1^T K S_1}, \widetilde{\mathbf{M}} = \mathbf{S_1^T M S_1}, \widetilde{\boldsymbol{\alpha}} = \mathbf{S_1^T} \boldsymbol{\alpha} \mathbf{S_1} \tag{15}$$

So (11) can be rewritten in a modified and reduced form with independent amplitudes $\widetilde{\boldsymbol{\alpha}}$ as

$$\left(\widetilde{\mathbf{K}} - \omega^2\widetilde{\mathbf{M}}\right)\widetilde{\boldsymbol{\alpha}} = \mathbf{0} \tag{16}$$

III. Numerical Results

To calculate the SAWs in the finite layered Au/ZnO structure, the material parameters of Au and ZnO [10] are listed in Table 1.

TABLE I. MATERIAL PROPERTIES OF ZNO AND AU

Materials	Properties			
	Elastic constants (GPa)	Piezoelectric coefficients $(\mathrm{C/m^2})$	Dielectric permittivity coefficients $(10^{-11}\mathrm{C/Vm})$	Density $(\mathrm{kg/m^3})$
ZnO	$c_{11} = c_{22} = 210$, $c_{12} = 121$, $c_{13} = 105$, $c_{33} = 211$, $c_{44} = c_{55} = 43$, $c_{66} = 44.5$	$e_{15} = e_{24} = -0.48$, $e_{31} = e_{32} = -0.57$, $e_{33} = 1.32$	$\varepsilon_{11} = \varepsilon_{22} = 7.61$, $\varepsilon_{33} = 8.85$	5700
Au	$c_{11} = c_{22} = c_{33} = 193.3$, $c_{12} = c_{13} = c_{23} = 137.7$, $c_{44} = c_{55} = c_{66} = 27.8$	/	/	19300

To show the effect of the boundary conditions on the SAWs, we present the dispersion curves of the Rayleigh waves in a ZnO substrate covered by the Au thin film. The dispersion curves with the consideration of elastic properties and piezoelectric properties of ZnO on an open circuit are shown in Fig. 2. The dispersion curves from a shorted circuit boundary condition at the bottom of the substrate and an open circuit at the interface and different mechanical boundary conditions at the bottom of the substrate are shown in Fig. 3.

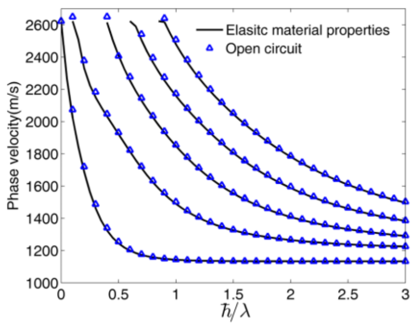

Fig. 2. Dispersion curves of SAW propagation in a layered Au/ZnO structure with free boundary condition

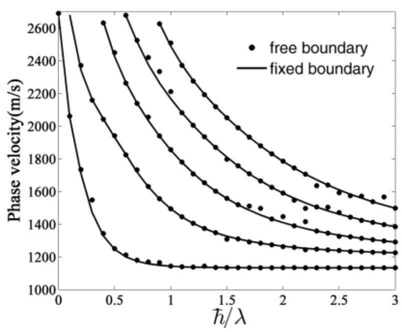

Fig. 3. Dispersion curves of SAW propagation in a layered Au/ZnO structure with different boundary conditions

The first wave mode always starts from the fundamental Rayleigh wave of the ZnO layer in both cases of open circuit and shorted circuit conditions.

IV. Conclusions

By utilizing the standard Rayleigh-Ritz method with the consideration of boundary conditions, the analysis of Rayleigh wave propagation in a layered finite structure of an Au film and a finite piezoelectric ZnO substrate with thickness h=9λ is performed. The results have been validated with other methods. The lowest branch of dispersion curves starts from the Rayleigh wave velocity of the substrate material. This demonstrates the Rayleigh-Ritz method is an effective approach for the relatively complicated structure of SAW resonators. This is part of the RRM procedure for the study of vibrations of SAW resonators with the consideration of piezoelectric effects.

References

[1] R. M. White and F. W. Voltmer, 'Direct Piezoelectric Coupling to Surface Elastic Waves', *Appl. Phys. Lett.*, vol. 7, no. 12, pp. 314–316, Dec. 1965, doi: 10.1063/1.1754276.

[2] D. Barnett and J. Lothe, 'Free surface (Rayleigh) waves in anisotropic elastic half-spaces: the surface impedance method', *Proc. R. Soc. Lond. A*, vol. 402, no. 1822, pp. 135–152, Dec. 1985, doi: 10.1098/rspa.1985.0111.

[3] I. Ben Salah and M. H. Ben Ghozlen, 'Rayleigh waves in piezoelectric material', *Physics Procedia*, vol. 2, no. 3, pp. 1377–1383, Nov. 2009, doi: 10.1016/j.phpro.2009.11.105.

[4] X. Cao, F. Jin, and Z. Wang, 'On dispersion relations of Rayleigh waves in a functionally graded piezoelectric material (FGPM) half-spaces, *Acta Mech*, vol. 200, no. 3–4, pp. 247–261, Oct. 2008, doi: 10.1007/s00707-008-0002-1.

[5] S. Chaudhary, S. A. Sahu, and A. Singhal, 'Analytic model for Rayleigh wave propagation in piezoelectric layer overlaid orthotropic substratum', *Acta Mech*, vol. 228, no. 2, pp. 495–529, Feb. 2017, doi: 10.1007/s00707-016-1708-0.

[6] V. T. N. Anh and P. C. Vinh, 'The incompressible limit method and Rayleigh waves in incompressible layered nonlocal orthotropic elastic media', *Acta Mech*, Sep. 2022, doi: 10.1007/s00707-022-03319-y.

[7] J. Wang and J. Lin, 'A Two-dimensional Theory for Surface Acoustic Wave Propagation in Finite Piezoelectric Solids', *Journal of Intelligent Material Systems and Structures*, vol. 16, no. 7–8, pp. 623–629, Jul. 2005, doi: 10.1177/1045389X05051628.

[8] N. Favretto-Cristini, D. Komatitsch, J. M. Carcione, and F. Cavallini, 'Elastic surface waves in crystals. Part 1: Review of the physics', *Ultrasonics*, vol. 51, no. 6, pp. 653–660, 2011, doi: https://doi.org/10.1016/j.ultras.2011.02.007.

[9] Z. Weijian and C. Weiqiu, 'Surface waves in a piezoelectric half-space with surface effect', *Chinese Journal of Theoretical and Applied Mechanics*, vol. 49, no. 3, pp. 597–604, 2017.

[10] R. Tian, G. Nie, J. Liu, E. Pan, and Y. Wang, 'On Rayleigh waves in a piezoelectric semiconductor thin film over an elastic half-space, *International Journal of Mechanical Sciences*, vol. 204, p. 106565, Aug. 2021, doi: 10.1016/j.ijmecsci.2021.106565.