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Analysis of the metal layer thickness influence on the dispersion characteristics of acoustic waves propagating in the layered piezoelectric structure "Me/AlN/Me/diamond"

S.I. Burkov [a,*], O.P. Zolotova [b], B.P. Sorokin [c,d]

[a] Siberian Federal University, 79 Svobodny Ave., 660041 Krasnoyarsk, Russian Federation
[b] Siberian State Aerospace University, 31 Krasnoyarsky Rabochy Ave., 660014 Krasnoyarsk, Russian Federation
[c] Technological Institute for Superhard and Novel Carbon Materials, 7a Central'naya Str., 142190 Moscow, Troitsk, Russian Federation
[d] Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Russian Federation

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ABSTRACT

The paper presents the results of computer simulation of the acoustic waves propagation in piezoelectric layered structures based on diamond substrate under the influence of various metal film deposition. It has been observed that the maximum phase velocity change $\Delta v/v$ is achieved with an "Au/(001) AlN/Au/(100) diamond" PLS configuration. However, if the acoustic impedance of the metal layer is greater than the acoustic impedance of the substrate, an elastic wave reflection can be observed, reducing the $\Delta v/v$ quantities. Obtained results may be useful in the development of resonant and sensor acousto-electronic devices based on the Rayleigh and Love waves.

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1. Introduction

Multilayer piezoelectric structures with layer thickness comparable to the acoustic wavelength are widely used for the development of microwave acoustoelectronic (AE) devices. Recently, one of the most heavily used acoustoelectronic devices have been thin-film resonators on acoustic waves with high quality factors and low form factors, operating in the 2–12 GHz frequency range [1,2]. Resonators of this type provide the basis for the development of sensors of physical and mechanical quantities, as well as biosensors [3]. Depending on the number of layers in the structure and the presence (or absence) of the substrate, different types of acoustic waves as bulk acoustic waves (BAW), Rayleigh, Lamb, Love, and SH-waves, can propagate in the such structures. Earlier the boundary conditions and computer calculations of the phase velocity variations in the piezoelectric layered structures (PLS) have been obtained under the influence of a bias electric field [4] and uniaxial pressure application [5].

Thin-film AE-resonators offer a sensor active area which is highly sensitive to the external parameters, and this peculiarity is indispensable for applications, for example, in medical, biological, and chemical sensors [6–9].

The simplest design is a thin-film microwave acoustoelectronic resonator consisting of two electrodes separated by a thin piezoelectric layer. The center frequency of the resonator is determined by the piezoelectric layer thickness and BAW velocity, and by the thickness and type of the electrode material [10–13]. In AE-devices, the different metals can be used as electrodes: aluminum (Al), molybdenum (Mo), silver (Ag), gold (Au), platinum (Pt), and their alloys in various combinations. The total thickness of the electrodes can build up to 30% of the thickness of all the structure [14].

In this paper, we consider the mass loading of the two thin metal layers as an influence on the dispersion characteristics of the Rayleigh and Love wave modes in the "Me/AlN/Me/diamond" PLS. These materials have a lot of important properties, such as high electromechanical coupling of AlN and higher BAW and SAW velocities of diamond, and are widely used in the development of various AE-devices. A true layer material choice influence on the successful practical application of AE-devices in particular by the difference in the acoustical impedance of the metals.

* Corresponding author.
E-mail addresses: sburkov@sfu-kras.ru (S.I. Burkov), zolotova@sibsau.ru (O.P. Zolotova), bpsorokin2@rambler.ru (B.P. Sorokin).

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The main objective of this paper is the computer simulation of the influence of Al, Mo, and Au deposited films on the acoustic wave propagation in the "Me/AlN/Me/diamond" piezoelectric layered structure.

2. Theory of elastic wave propagation in a layered piezoelectric medium

Let us consider the small amplitude elastic wave propagation in the undisturbed piezoelectric crystal. The equation of motion, and equations of electrostatics and state of the piezoelectric media, are the following [15]:

$$\rho_0 \ddot{U}_i = \tau_{ij,j}; \quad D_{m,m} = 0; \\ \tau_{ab} = c^E_{abcd}\eta_{cd} - e_{mab}E_m; \quad D_m = \varepsilon^{\eta}_{mn}E_n + e_{mab}\eta_{ab}, \tag{1}$$

where ρ_0 is the density of the crystal in undeformed state; U_i is a dynamic elastic displacement vector; τ_{ab} is a thermodynamic stress tensor; D_m is an electric induction vector; η_{cd} is a tensor of small deformations; c^E_{abcd}, e_{mab}, and ε^{η}_{mn} are second-order elastic, piezoelectric and clamped dielectric constants, respectively. Note, that the elastic, piezoelectric, and dielectric constants are forth-order, third-order and second-order tensors, respectively. For elastic displacements and electrical potentials taken in the form of plane monochromatic waves of small amplitude, the system of equations can be written as the well-known Green-Christoffel's equations, and its solutions should be necessary to obtain for each PLS layer [15,16].

In order to examine the conditions of elastic wave propagation in a PLS let's introduce a working orthogonal coordinate system where the X_3 axis is directed along the outer normal to the layer surface, and the X_1 axis coincides with the direction of wave propagation. So, only the Rayleigh and Love type modes will be taken into account. Note, that some relevant boundary conditions should be complied with. Boundary conditions, particularly for a four-layer structure "metal/piezoelectric film/metal/dielectric substrate" (Fig. 1a) can be put down as: an equality to zero a normal component of the stress tensor at the top metal/vacuum interface; an equality of the normal components of the stress tensor and displacement vectors at top and bottom metal/piezoelectric interfaces; an equality to zero an electrical potential at the top and bottom piezoelectric film surfaces [16]:

$$\begin{aligned} &\tau^{(1)}_{3j}\big|_{x_3=d_1} = 0; \\ &\tau^{(1)}_{3j} = \tau^{(2)}_{3j}\Big|_{x_3=h}; \varphi^{(2)} = 0\big|_{x_3=h}; U^{\to(1)} = U^{\to(2)}\big|_{x_3=h}; \\ &\tau^{(2)}_{3j} = \tau^{(3)}_{3j}\Big|_{x_3=d_2}; \varphi^{(2)} = 0\big|_{x_3=d_2}; U^{\to(1)} = U^{\to(3)}\big|_{x_3=d_2}; \\ &\tau^{(3)}_{3j} = \tau^{(4)}_{3j}\Big|_{x_3=0}; U^{\to(3)} = U^{\to(4)}\big|_{x_3=0}. \end{aligned} \tag{2}$$

Here d_1, d_2 and h values are associated with the top and bottom layers of metals, and piezoelectric film, respectively. First the condition $d_1 = d_2$ has been applied as a special case. When the boundary condition matrix determinant (2), the size of which in this case is 24×24, is equal to zero, we can obtain a characteristic equation determining all the parameters of elastic waves propagation.

Let us to substitute the elastic wave solutions in the form of linear combinations of partial waves into the boundary conditions (2) as:

$$\begin{aligned} U_i &= \sum_n C^{(m)}_n \alpha^{(n)}_i \exp[i(k_1x_1 + k^{(n)}_3 x_3 - \omega t)], \\ \varphi &= \sum_n C^{(m)}_4 \alpha^{(n)}_4 \exp[i(k_1x_1 + k^{(n)}_3 x_3 - \omega t)], \end{aligned} \tag{3}$$

where the superscript n corresponds to the number of partial waves in the corresponding crystalline layer. Variations of the boundary conditions (2) determine all the types of elastic waves propagating in a layered structure. For example, the first equation in (2) determines the propagation of the surface Rayleigh wave; also the first and last equations describe the propagation of an elastic wave in a piezoelectric plate. For the PLS "Me/AlN/Me/diamond" taken into consideration, the system of boundary condition equations (2) is divided into two independent systems. The system of equations 8×8 for the SH-modes (Love waves) and the system of equations 16×16 for the Rayleigh mode will be written as:

$$\begin{aligned} &C^{(1)}_n\left(C_{11}k_1\alpha^{(n)}_1 + C_{12}k^{(n)}_3\alpha^{(n)}_3\right)\exp\left(ik^{(n)}_3 d_1\right) = 0, \\ &C^{(1)}_n\left(k_1\alpha^{(n)}_3 + k^{(n)}_3\alpha^{(n)}_1\right)\exp\left(ik^{(n)}_3 d_1\right) = 0, \\ &C^{(1)}_n\left(k_1\alpha^{(n)}_3 + k^{(n)}_3\alpha^{(n)}_1\right)\exp\left(ik^{(n)}_3 h\right) - \\ &C^{(2)}_n\left[C^{(2)}_{44}\left(k^{(n)}_3\alpha^{(n)}_1 + k_1\alpha^{(n)}_3\right) + e_{15}k_1\alpha^{(n)}_4\right]\exp\left(ik^{(n)}_3 h\right) = 0, \\ &C^{(1)}_n\left(C_{11}k_1\alpha^{(n)}_1 + C_{12}k^{(n)}_3\alpha^{(n)}_3\right)\exp\left(ik^{(n)}_3 h\right) - \\ &C^{(2)}_n\left(C^{(2)}_{33}k^{(n)}_3\alpha^{(n)}_3 + C^{(2)}_{13}k_1\alpha^{(n)}_3 + e_{33}k^{(n)}_3\alpha^{(n)}_4\right)\exp\left(ik^{(n)}_3 h\right) = 0, \\ &C^{(2)}_n\left[C^{(2)}_{44}\left(k^{(n)}_3\alpha^{(n)}_1 + k_1\alpha^{(n)}_3\right) + e_{15}k_1\alpha^{(n)}_4\right]\exp(ik^{(n)}_3 d_2) - \\ &C^{(3)}_n\left(k_1\alpha^{(n)}_3 + k^{(n)}_3\alpha^{(n)}_1\right)\exp\left(ik^{(n)}_3 d_2\right) = 0, \\ &C^{(2)}_n\left[C^{(2)}_{33}k^{(n)}_3\alpha^{(n)}_3 + C^{(2)}_{13}k_1\alpha^{(n)}_3 + e_{33}k^{(n)}_3\alpha^{(n)}_4\right]\exp\left(ik^{(n)}_3 d_2\right) - \\ &C^{(3)}_n\left(C_{11}k_1\alpha^{(n)}_1 + C_{12}k^{(n)}_3\alpha^{(n)}_3\right)\exp\left(ik^{(n)}_3 d_2\right) = 0, \\ &C^{(1)}_m\alpha^{(m)}_i\exp\left(ik^{(m)}_3 h\right) - C^{(2)}_n\alpha^{(n)}_i\exp\left(ik^{(n)}_3 h\right) = 0, \\ &C^{(3)}_m\alpha^{(m)}_i\exp\left(ik^{(m)}_3 d_2\right) - C^{(2)}_n\alpha^{(n)}_i\exp\left(ik^{(n)}_3 d_2\right) = 0, \\ &C^{(3)}_n\left(k_1\alpha^{(n)}_3 + k^{(n)}_3\alpha^{(n)}_1\right) - C^{(4)}_n\left(k^{(n)}_3\alpha^{(n)}_1 + k_1\alpha^{(n)}_3\right) = 0, \\ &C^{(3)}_n\left(C_{11}k_1\alpha^{(n)}_1 + C_{12}k^{(n)}_3\alpha^{(n)}_3\right) - C^{(4)}_n\left(C^{(4)}_{11}k^{(n)}_3\alpha^{(n)}_3 + C^{(4)}_{12}k_1\alpha^{(n)}_3\right) = 0, \\ &C^{(3)}_m\alpha^{(m)}_i - C^{(4)}_n\alpha^{(n)}_i = 0. \end{aligned} \tag{4}$$

Here the superscripts 1–4 denote the layers and the substrate, respectively, similarly to Eq. (2), and k_n is the wave vector.

In a layered structure describing by Eq. (4), the films of the isotropic metals, a piezoelectric film belonging to the 6mm point symmetry group, and a dielectric substrate of a cubic crystal were used. Only computer simulation gives us an instrument of the solution of the basic system (4).

3. Analysis of the mass loading influence on the acoustic wave propagation in a layered piezoelectric structure

Determination of a normalized mass sensitivity S of a multilayer resonator has done primarily in terms of the energy balance variation under a frequency changing, i.e. it was convenient to introduce a shift of the relative frequency of the resonator normalized to the surface mass density ρ_s [17,18] as

$$S = \frac{1}{f\rho_s}\left(\frac{\Delta f}{f_0}\right) = \frac{1}{f\rho_s}\left(\frac{\Delta v}{v}\right), \tag{5}$$

where v is the phase velocity of the elastic wave, f and f_0 are the operating and resonant frequency, respectively. But Eq. (5) has a one disadvantage, namely, at large frequency values, the phase velocity change will be smoothed with the metal thickness increasing. Therefore, in this paper, we will use the following formula to determine the sensitivity:

$$S_v = \frac{\Delta v}{v_{ml}} = \frac{v - v_{mt}}{v_{ml}}, \tag{6}$$

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