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Features of the Metallization Influence on Phase Velocities of Acoustic Waves in Piezoelectric Plates

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The paper presents an analysis of the influence of the load represented by two metal layers on the change in the phase velocity of the dispersion modes of the elastic Lamb and SH-waves in "Me/ZnO/Me" and "Me/AlN/Me" structures depending on the elastic wave frequency and the ratio of the metal layer to the piezoelectric layer thickness. Aluminum (Al), molybdenum (Mo) and platinum (Pt) are considered as the metal layer materials (Me). Only the elastic Lamb wave modes have localized maxima of the sensitivity curve S for all types of structures. Systems with low values of acoustic impedances for layers and plates materials have maximum values of S for metallization with thin layers, and also have minimal differences in the profiles of the components of the displacement vectors of the elastic wave. Systems with the most different values of acoustic impedances of layers and plates materials have maximum values of S when metallized with thick layers, and also have maximum differences in the profiles of the components of the displacement vectors of the elastic wave.
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Introduction

Acoustic Lamb waves in piezoelectric plates are a promising object for the development of microwave resonators and sensors of the next generation. Due to the high interest in this issue, many experimental and theoretical studies of acoustoelectronic devices based on piezoelectric plates operating on various modes of elastic waves have appeared [1, 2].

In devices created on the basis of a single-layer or multilayer piezoelectric structure, the thickness of the electrodes can be comparable to the thickness of the piezoelectric plate. At the same time, precious metals such as gold or platinum, which are most often used in sensors for various biochemical applications, have significant values of acoustic impedance [3]. Thus, taking into account the influence of metal layers on the change in the dispersion characteristics of various

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modes of an elastic wave in a piezoelectric plate is important for improving the characteristics of devices on such structures [4].

In this paper, we performed a computer simulation of two thin metal layers influence on the dispersion characteristics of the elastic Lamb wave modes in zinc oxide ("Me/ZnO/Me" structures) and aluminum nitride ("Me/AlN/Me" structures) plates. These piezoelectrics have large values of the electromechanical coupling coefficient and significant values of the phase velocities of bulk and surface acoustic waves. Due to these properties, the materials in question are actively used in the development of various acoustoelectronic devices. As materials of metal layers (Me), aluminum (Al), molybdenum (Mo) and platinum (Pt) were used in the form of a sputtered thin film, that are metals often used as electrodes [5]. All materials used for layers and plates modeling have different values of acoustic impedance $Z = \rho v$, calculated for bulk longitudinal wave, which are related as $Z_{\mathrm{Al}} < Z_{\mathrm{AlN}} < Z_{\mathrm{ZnO}} < Z_{\mathrm{Mo}} < Z_{\mathrm{Pt}}$. The values of material constants for aluminum and molybdenum are taken in [5], ZnO — in [6], AlN — in [7], platinum — in [8].

1. Theoretical foundations for elastic waves propagation in a layered piezoelectric medium

The equation of motion, the equation of electrostatics, and the equations of state of the piezoelectric medium, describing the propagation of an elastic wave in a piezoelectric, have the form of [9]

$$\begin{aligned} \rho_0 \ddot{\mathbf{U}}_A = \tau_{AB,B}, &\qquad \mathbf{D}_{M,M} = 0, \\ \tau_{AB} = c^E_{ABCD}\eta_{CD} - e_{MAB}E_M, &\qquad \mathbf{D}_M = \varepsilon^{\eta}_{MN}E_N + e_{MAB}\eta_{AB}, \end{aligned} \tag{1}$$

where ρ_0 is the crystal density in undeformed state; $\mathbf{U}_A$ is the vector of dynamic elastic displacements; τ_{AB} is the thermodynamic stress tensor; $\mathbf{D}_M$ is the vector of electrical induction; η_{CD} is the small strain tensor; c^E_{ABCD}, e_{MAB}, ε^{η}_{MN} — elastic, piezoelectric and dielectric constants of the second order. The comma after the index denotes the spatial derivative, the Latin coordinate indices vary from 1 to 3. Hereinafter implies the summation of the twice-repeated index.

In a working orthogonal system of axis, the X_3 axis is directed along the outer normal to the layer surface and X_1 axis coincides with the direction of wave propagation (Fig. 1, *a*). The boundary conditions, in particular, for the "Me/Piezoelectric/Me" three-layer structure are: the equality to zero of normal components of the stress tensor at the "metal/vacuum" interface; the normal components equality of the stress tensor, the equality of the displacement vectors and the equality to zero of the electric potential wave at the "metal/piezoelectric" interface [10]:

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

Here d_1, d_2 and h are the thicknesses of the upper and lower metal layer and piezoelectric layer, respectively. In the present paper, the condition $d_1 = d_2$ is met, i.e. the thickness of the upper and lower metal layers are equal. The equality to zero of the boundary conditions determinant matrix (2), which size in this case is 20×20 elements, makes it possible to calculate the phase velocities of symmetric and antisymmetric modes of the Lamb and SH-wave. Boundary conditions variations (2) determine all types of elastic waves propagating in the three-layer plate.

2. Analysis of the loading on the wave velocities in three-layer plates

There are several determinations of the sensitivity parameter in the piezoelectric structure to a mass loading [11, 12]. In particular, the mass sensitivity S of a multilayer resonator can be defined as a relative frequency shift of the resonator, normalized to the surface mass density [12]. However, the disadvantage of this approach is that for large values of f frequencies, the changes of phase velocity are smoothed in case of increase in the metal layer thickness.

In the present work, the following formula to determine the mass sensitivity of an elastic wave is used:

$$S = \frac{1}{D\rho_0}\left(\frac{\Delta v}{v}\right), \tag{3}$$

where $\Delta v = v - v_{met}$ is the change in the phase velocity of the elastic wave during the deposition of a metal layer with bulk density ρ_0, D is the total thickness of the metal layers. The velocity shift is calculated relative to the velocity of the elastic wave when an infinitely thin layer is applied, which does not change the mechanical boundary conditions [13, 14]. Note that as shown by the computer experiment, this condition is fulfilled at a layer thickness of less than 1 nm. Also, condition (3), eliminates the effect of the piezoelectric effect and, therefore, S parameter doesn't depend on the type of the piezoelectric layer.

A schematic representation of the investigated layered structures is presented in Fig. 1, *a*. The dispersion dependences of phase velocities for the fundamental and first modes of Lamb and SH-waves on parameter $u = h \cdot f$ value (the product of the piezoelectric thickness and frequency) for the "Al/ZnO/Al" layered structure with the [100](001) layer orientation is presented in Fig. 1, *b*, similar dependences for the "Al/AlN/Al" layered structure with the [100] (001) layer orientation are shown in Fig. 1, *c*. In contrast to the "Me/ZnO/Me" structure with the maximum value of u = 10000 m/s, the range of variation of the parameter u to 20000 m/s was increased to calculate the second structure due to the fact that the values of the phase velocities of all elastic wave modes become much larger.

The phase velocities of zero modes of the elastic Lamb wave in the "Me/ZnO/Me" structure during metallization with infinitely thin layers tend to the phase velocity of the Rayleigh wave in ZnO with metallized surfaces (v = 2677.6 m/s). In the "Me/AlN/Me" structure the phase velocities of the traveling modes of an elastic wave change in the same way and tend to the Rayleigh wave phase velocity in AlN with metallized surfaces (v = 5485 m/s). The speeds of higher-order traveling modes of the Lamb wave with increasing u parameter decrease from several tens of km/s and tend to the speed of a slow shear bulk wave in a piezoelectric. The phase velocities of all the SH-wave modes tend to the speed of a fast shear bulk wave in a piezoelectric.

The use of metal in a multilayer plate can significantly affect the redistribution of the elastic wave energy due to the acoustic properties of the layers, as well as the interference between the incident and reflected elastic wave modes from the layer boundaries. For example, in the "Al/AlN/Al" structure the increasing u parameter and using of maximum thickness metal layers (d/h = 0.05), the phase velocities of the elastic wave fundamental modes decrease significantly and tend to the value of the phase velocity of the fast shear wave in aluminum (Fig. 1, *c*). A similar situation manifests itself when using other considered metals in the multilayer structure. It is noted that in the "Me/AlN/Me" structure the velocities of the elastic wave modes with the same metal type and u value decrease more significantly than in the "Me/ZnO/Me" structure.

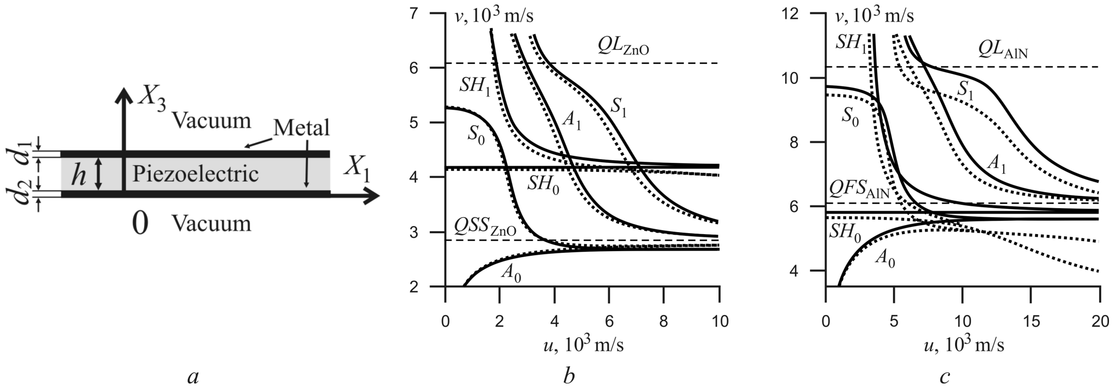

Fig. 1. Dispersion dependences of phase velocities on u parameter for the "Al/Piezoelectric/Al" layered structure: a — the layered structure scheme; b — fundamental and first Lamb and SH-wave modes in the "Al/ZnO/Al" structure; c — the fundamental and first Lamb and SH-wave modes in the "Al/AlN/Al" structure. Solid lines — the mode velocities for infinitely thin metal layers, dotted lines — the velocities for the metal and layer ratio $d/h = 0.05$

Fig. 2 represents the graphs of sensitivity S calculated by the formula (3) for the fundamental modes A_0, S_0, the first modes A_1, S_1 of the Lamb wave, and also the fundamental and two first modes of the SH-wave, depending on the parameter u in the "Al/ZnO/Al" (Fig. 2, a) and "Al/AlN/Al" (Fig. 2, b) structures with the d/h ratio = 0.001.

It can be noted that the all modes of the elastic Lamb wave (except A_0 mode) have sensitivity S maxima that appear at almost equal intervals of the parameter u values.

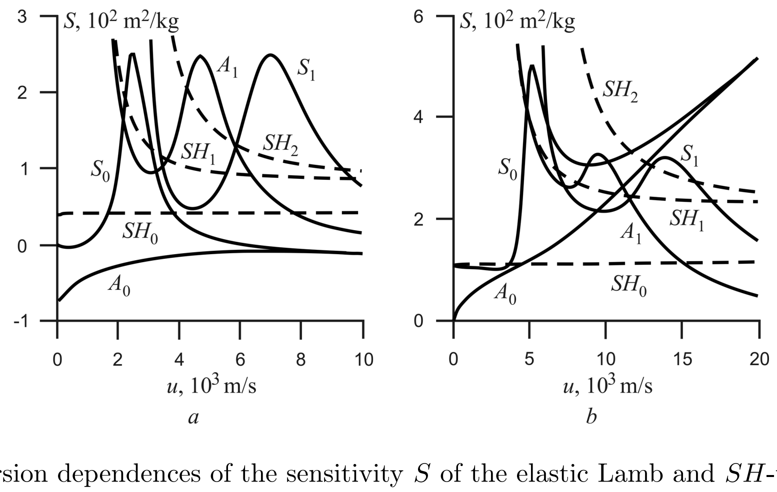

Fig. 2. Dispersion dependences of the sensitivity S of the elastic Lamb and SH-wave modes on the parameter u with the ratio of the thicknesses of the metal and piezoelectric $d/h = 0.001$: a — "Al/ZnO/Al" structure; b — "Al/AlN/Al" structure

It is noted that the maximum values of S in the "Al/AlN/Al" structure exceed the similar values for the same modes of the elastic Lamb wave by two times. At the same time, the acoustic impedances of the bulk longitudinal wave for the piezoelectric layer are not so different and equal for $Z_{\text{AlN}} = 3.35 \cdot 10^7$ kg·m/s^2 and $Z_{\text{ZnO}} = 3.45 \cdot 10^7$ kg·m/s^2.

The sensitivity graphs of S for the fundamental antisymmetric wave mode A_0 and SH-modes with transverse-horizontal polarization on the studied frequency range have no features. It can be noted that a decrease (in absolute value) of S in the "Al/ZnO/Al" structure is associated with a gradual increase of A_0 mode speed with an increase in the u parameter values (Fig. 2, a). On the contrary, the increase of S values in the "Al/AlN/Al" structure is associated with a significant drop in A_0 mode speed with an increase in the u parameter values (Fig. 2, b). The decrease in S values for modes with transverse-horizontal polarization is associated with a gradual decrease in the velocities of these modes when increasing the parameter u values. In the following, only features of the behavior of sensitivity curves S for the elastic Lamb wave modes are considered.

Next, we calculated the phase velocities change for the modes of the elastic wave with the ratio of one metal layer to the piezoelectric thickness $d/h = 0.005$; 0.01; 0.025; 0.05. The maximum sensitivity values for the S_0, A_1 and S_1 modes of Lamb wave depending on the type of metal layer, the d/h ratio and the u value in the "Me/ZnO/Me" structure are shown in Tab. 1.

A significant decrease in the maximum sensitivity S for the elastic wave modes considerated appears at a ratio $d/h > 0.025$. This decrease in S values with increasing d/h is especially evident when using Pt — a metal with a high acoustic impedance value. The numerical values of the S maxima for all types of metal differ only with significant layer thicknesses (Tab. 1).

Table 1. Maximum values of sensitivity S in the structure "Me/ZnO/Me"

d/h	Mode	S_0			A_1			S_1		
	Metall	**Al**	**Mo**	**Pt**	**Al**	**Mo**	**Pt**	**Al**	**Mo**	**Pt**
0.001	S, m^2/kg	251	246	275	248	247	248	249	248	246
	u, m/s	2500	2400	2500	4700	4700	4700	7000	7000	6900
0.005	S, m^2/kg	248	244	269	246	242	238	248	243	236
	u, m/s	2500	2400	2500	4700	4700	4700	7000	7000	6900
0.01	S, m^2/kg	246	240	258	244	237	225	245	237	221
	u, m/s	2400	2400	2500	4700	4600	4600	6900	6900	6700
0.025	S, m^2/kg	239	223	226	238	220	188	240	214	189
	u, m/s	2400	2400	2400	4600	4500	4300	6800	6800	6000
0.05	S, m^2/kg	225	199	180	228	190	142	233	177	152
	u, m/s	2400	2300	2200	4500	4400	3900	6700	6500	5300
Mean value of u in maximum S, m/s		2440± 136	2380± 284	2420± 393	4640± 305	4580± 786	4440± 2565	6880± 1010	6840± 1070	6360± 1120

The maximum sensitivity values for the S_0, A_1 and S_1 modes of Lamb wave depending on the type of metal layer, the d/h ratio and the u value in the "Me/AlN/Me" structure are shown in Tab. 2.

A significant decrease of sensitivity S for the elastic wave modes considerated is manifested when ratio $d/h > 0.025$, especially for using Mo and Pt. The numerical values of the S maxima for all types of metals differ only with significant thicknesses of the layers. The maximum values of S parameter for all modes are 1.5–2 times higher than the similar values for the "Me/ZnO/Me" structure.

At the same time in contrast to the "Me/ZnO/Me" structure, for the considered S_0, A_1, S_1 modes of the elastic Lamb wave, a significant increase in the S values was observed when using thick Al layers. In this case, the value of S for large values of u parameter can be comparable or even exceed the values at the local maximum. A similar effect was found for the S_0 mode only in the "Pt/ZnO/Pt" structure. At the same time, the situation is possible, for example, for mode A_1, when the maximum sensitivity is noted at the time of the wave, then a local minimum is observed and subsequently the S value becomes practically dispersionless or begins to increase, which corresponds to a decrease in the phase velocity of a particular mode with increasing thickness of the metal layer.

Table 2. Maximum values of sensitivity S in the structure "Me/AlN/Me"

d/h	Mode	S_0			A_1			S_1		
	Metall	**Al**	**Mo**	**Pt**	**Al**	**Mo**	**Pt**	**Al**	**Mo**	**Pt**
0.001	S, m^2/kg	502	493	532	329	327	326	323	321	319
	u, m/s	5200	5200	5200	9600	9600	9600	14000	13800	13800
0.005	S, m^2/kg	500	489	525	327	318	303	321	312	336
	u, m/s	5200	5000	5000	9600	9400	9200	13800	13600	11800
0.01	S, m^2/kg	497	479	497	324	306	—	319	302	387
	u, m/s	5200	5000	4800	9400	9200	—	13800	13400	11600
0.025	S, m^2/kg	494	433	390	318	270	—	319	285	425
	u, m/s	5000	4800	4600	9400	8800	—	13400	12400	12400
0.05	S, m^2/kg	476	349	263	313	229	258	364	264	298
	u, m/s	5000	4600	4400	9000	8000	7800	12000	11800	11800
Mean value of u in maximum S, m/s		5120± 136	4920± 284	4800± 393	9400± 305	9000± 786	8867± 2565	13400± 1010	13000± 1070	12280± 1120

In general, the character of S parameter changes in the "Me/AlN/Me" structures is similar to the changes in S in a three-layer "Me/ZnO/Me" plate.

3. Features of the S sensitivity curves of Lamb and SH-waves in the "Me/ZnO/Me" and "Me/AlN/Me" structures

For both structures the characteristic feature is that only the S_0, A_1 and S_1 modes of the elastic Lamb wave have localized maxima of S curves. Other modes haven't pronounced features of sensitivity curves on the studied frequency range.

When comparing the same structures with different thickness of metal layers, it have found that increasing the thickness of the metal layer, as a rule, reduces the propagation velocity of the acoustic waves of first and higher orders. An increase in the thickness of the metal layers leads to a shift of the maxima of S values to the low-frequency region. In this case the amplitude and width of the peaks of S with metal thickness increasing for the "Me/ZnO/Me" plate are less dependent on the type of metal and the u parameter than for "Me/AlN/Me" structure.

When comparing various "Me/Piezoelectric/Me" structures, it is noted that the sensitivity values of the Lamb elastic wave modes at d/h ratio = 0.001; 0,005; 0.01 differ slightly. A significant decrease in the sensitivity S for these modes at the ratio $d/h > 0.025$, especially when using Mo and Pt, may limit the use of metals with high acoustic impedance values and considerable thickness of layers in sensor devices.

A specific feature of the S_0 elastic wave mode propagation in the "Me/ZnO/Me" layered structure is the occurrence of negative values of the S parameter then using Al and Mo, i.e., the value of the elastic wave phase velocity when metal layers are applied can increase compared to the wave velocity in the unloaded piezoelectric plate (Fig. 2, *a*). Moreover, in the "Mo/ZnO/Mo" structure, a negative values of the S parameter are present only for metallization by layers of minimum thickness ($d/h = 0.001$), and in the "Al/ZnO/Al" structure, on the contrary, the values of S become negative and further decrease with increasing d/h ratio. This effect is not observed in the "Me/AlN/Me" layered structure for any of the elastic Lamb wave modes.

Fig. 3 shows the components of the elastic displacement vectors U_1 and U_3 of modes S_0, A_1 and S_1 distributed over the depth of a three-layer plate in local maxima of S sensitivity curves.

The profiles of components of the displacement vectors for S_0 mode are constructed for local maxima of the S curves in the "Me/ZnO/Me" structures at u = 2200–2400 m/s (Fig. 3, *a*) and in the "Me/AlN/Me" structures at u = 4400–5000 m/s (Fig. 3, *b*). It was noted that in general, the nature of the profiles in both structures is the same, and the differences lie in the initial phases of oscillations. The elastic oscillations of S_0 mode occur in the piezoelectric thickness, and the deformation in metal layers is insignificant. The components U_1 and U_3 have a maximum amplitude in both structures when using Al layers. In this case, the components of the displacements using Mo and Pt are of the same order of magnitude, and their amplitude is approximately 5 times smaller than when using Al.

The profiles of components of the displacement vectors for A_1 mode are constructed for the local maxima of the S curves in the "Me/ZnO/Me" structures at u = 3900–4500 m/s (Fig. 3, *c*) and in the "Me/AlN/Me" structures at u = 7800–9000 m/s (Fig. 3, *d*). It was also noted that the profiles of the elastic displacement vectors in both structures are similar and the elastic vibrations occur mainly in the thickness of the piezoelectric. But differences were found from the previous mode in the various metals influence on the amplitude of oscillations. The components U_1 and U_3 have the maximum amplitude in the "Me/ZnO/Me" structures using Al and Pt layers (Fig. 3, *c*). In contrast, in the "Me/AlN/Me" structures, the components U_1 and U_3 have the maximum amplitude when using Mo layers, and then, in descending order, Al and Pt (Fig. 3, *d*). In addition, when using Pt, both components of the oscillations rapidly decay by as much as a quarter of the piezoelectric layer thickness.

The profiles of components of the displacement vectors for S_1 mode are constructed for local maxima of S curves in the "Me/ZnO/Me" structures at u = 5300–6700 m/s (Fig. 3, *e*) and in the "Me/AlN/Me" structures at u = 11800–12000 m/s (Fig. 3, *f*). The profiles of the vectors of elastic displacements in both structures already differ significantly. The components U_1 and U_3 have the maximum amplitude in the "Me/ZnO/Me" structures when using Pt layers, while the minimum displacements are observed with Al and Mo, i.e. the picture of displacements is opposite to the observed picture for the S_0 mode (Fig. 3, *a*). On the contrary, in the "Me/AlN/Me" structures, the U_1 and U_3 components have the maximum amplitude when using Al and Mo layers, and when using Pt, the oscillation amplitude decreases by 3 orders of magnitude, and both components quickly decay by a quarter of the thickness of the piezoelectric layer (U_1 and U_3 for Pt are not shown in Fig. 3, *f*). In addition, in these structures elastic oscillations occur both in the metal layers and in the thickness of the plate with a sharp change of amplitude and phase at the metal-piezoelectric boundary, especially for the U_1 component for all types of metals.

It is also noted that the minimal differences in the profiles of the elastic wave displacement vectors are achieved for the S_0 mode and for "Al/Piezoelectric/Al" configuration of layered system, i.e. in the systems with low acoustic impedances of the layers and piezoelectric materials. The maximum differences in these profiles are achieved for the S_1 mode and for "Pt/Piezoelectric/Pt" configuration of layered system, i.e. in systems with the most different values of materials acoustic impedances.

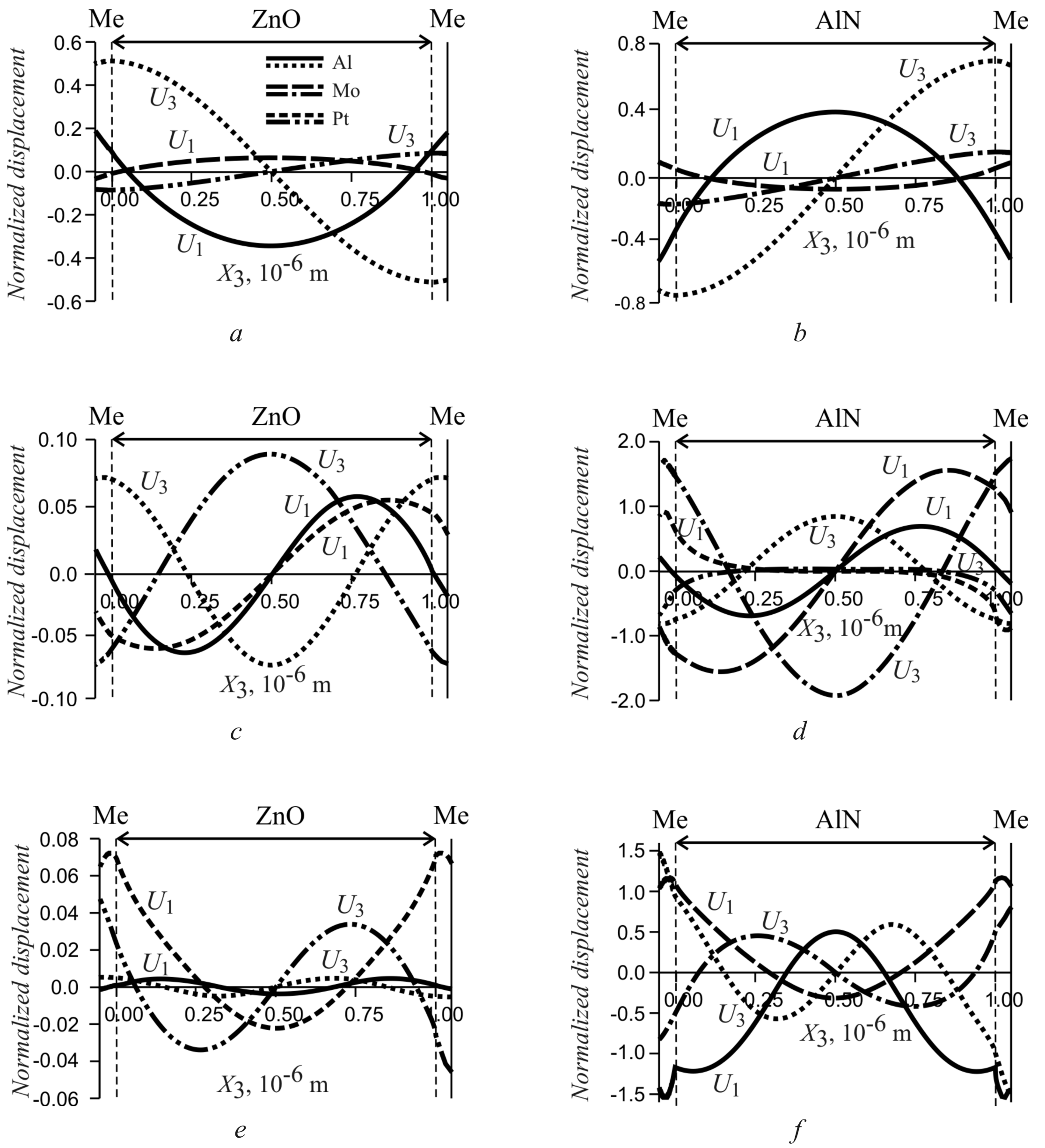

Fig. 3. The profiles of components of elastic displacements vectors U_1 and U_3 for Lamb wave modes in the maxima of S curves for "Me/ZnO/Me" and "Me/AlN/Me" layered structures: a–b — S_0 mode; c–d — A_1 mode, e–f — S_1 mode. The thickness of metal and piezoelectric ratio $d/h = 0.05$

Conclusion

The sensitivity S of the elastic wave dispersive modes in the piezoelectric layered structures "Me/ZnO/Me" and "Me/AlN/Me" depends on the ratio of metal layer and piezoelectric material acoustic impedance, as well as the d/h ratio and the u parameter.

Note that the maximum values of sensitivity S for elastic wave modes with large thicknesses of both metal layers (5 % and 10 % thickness of the piezoelectric plate) are reached with

"Al/AlN/Al" layered system configuration, i.e. in the system with low acoustic impedances for bulk longitudinal wave for materials of the metal and piezoelectric layers, which was shown earlier in [14]. However, when plating with thin layers, the maximum sensitivity S values, in particular, for S_0 modes of the elastic Lamb wave, are reached both "Pt/ZnO/Pt" and "Pt/AlN/Pt" configuration of layered system , i.e. in systems with the most different acoustic impedances of layers and piezoelectric materials.

The study of component profiles of the elastic displacement vector of the elastic Lamb wave modes in local maxima of sensitivity curves S in "Me/ZnO/Me" and "Me/AlN/Me" structures confirmed the above results about the metals with different acoustic impedances influence on amplitude and attenuation of elastic vibrations in layered structures. It is noted that minimal differences in the profiles of the displacement vectors are reached for systems with low values of acoustic impedances the materials of all layers. The maximum differences in these profiles are reached for systems with the most different acoustic impedance values.

It is noted that with an increase in the mode number of the elastic wave, the maximum and minimum of the sensitivity curve S shift to the region of large values of the parameter u, which explains the increase of the recorded differences in the profiles of elastic waves.

The results obtained by computer simulation can be useful in the development of the acoustoelectronic devices based on Lamb and SH-waves.

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Особенности влияния металлизации на фазовые скорости акустических волн в пьезоэлектрических пластинах

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В работе выполнен анализ влияния нагрузки в виде двух металлических слоев на изменение фазовой скорости дисперсионных мод упругой волны Лэмба и SH–волны в структурах вида "Me/ZnO/Me"и "Me/AlN/Me"в зависимости от частоты упругой волны и отношения толщин слоев металла и пьезоэлектрика. В качестве материалов металлического слоя (Me) использовали алюминий (Al), молибден (Mo) и платину (Pt). Только моды упругой волны Лэмба обладают локализованными максимумами чувствительности S для всех типов структур. Системы с низкими значениями акустических импедансов материалов слоев и пластин обладают максимальными значениями S при металлизации тонкими слоями, а также имеют минимальные отличия профилей компонент векторов смещений упругой волны. Системы с максимально различными значениями акустических импедансов материалов слоев и пластин обладают максимальными значениями S при металлизации толстыми слоями, а также имеют максимальные отличия профилей компонент векторов смещений упругой волны.

Ключевые слова: пьезоэлектрическая пластина, волна Лэмба, SH–волна, массовая нагрузка, компьютерное моделирование