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Localized acoustic waves in one-dimensional periodically modulated structures

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Abstract: **A number of one-dimensional phononic crystals, which are periodic thin-film structures of various geometries, consisting of sets of columns and metal inclusions located on a piezoelectric half-space, have been proposed and studied. The features of propagation in such structures of acoustic waves localized near the free surface and inhomogeneous inclusions have been studied. An unusual behavior of the dispersion curves for the studied localized modes was discovered. Particular attention is drawn to the so-called forbidden zones, i.e. frequency ranges in which there are no propagating localized modes. The influence of mechanical and electrical boundary conditions on the spectrum of the waves under study is discussed in detail.**

Keywords: **surface acoustic waves, one-dimensional phononic crystals, zinc oxide, zero group velocity, Love waves, Sezawa waves, leaky waves**

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CONTENTS

1. INTRODUCTION

Wave processes in periodic structures are currently one of the most popular objects for research in acoustics [1-6]. Unusual acoustic phenomena observed in such structures can be used to design sensors and signal processing devices, to control the acoustic wavefront, etc. These structures can be created in various ways. One of the most widespread approaches at the microscale is the use of photolithography technology, for example, the deposition of metal electrodes to the surface of a piezoelectric sample. However, for technological reasons, the thickness of such a metal layer usually does not exceed several hundred nanometers, therefore, its influence on acoustic waves in such structures is also small. In piezoelectric media, electrical boundary conditions can be easily changed using metal structures on the surface of acoustic waveguide. For example, from "floating," i.e. electrodes not connected to a voltage source, to electrically shorted, when a zero potential is applied to them. Another way to design periodic structures is to deposit various dielectric or piezoelectric films to the surface of a piezoelectric waveguide. ZnO films are considered in this work, which have good piezoelectric properties, and this allows them to be used as a top coating for the sensitive part of sensors [7]. In addition, deposition of a piezoelectric ZnO film with a system of electrodes on the surface of non-piezoelectric crystals allows for the efficient excitation of acoustic waves in such structures. It should be noted that within the state-of-the-art technology, the thickness of such a film can reach tens of microns, maintaining high crystallographic quality. This allows to significantly influence the spectrum of acoustic modes in similar structures [1-4,7,8]. The conductivity of ZnO was not taken into account in the current studies, but such consideration in the model is easy to implement, and it may have an additional impact on the dispersion curves.

2. GEOMETRIC PARAMETERS OF PERIODIC STRUCTURES AND INVESTIGATION METHODS

This work investigated theoretically the influence of geometric parameters on the spectrum of acoustic localized waves in periodic structures located on the half-space of *YZ* lithium niobate. The surface of the half-space is periodically modulated by various structures, electrodes at the interface between the ZnO film and the half-space, zinc oxide columns with aluminum inclusions, or by replacing the metal with a void in a homogeneous film (**Fig. 1**). The film and unit cell geometries are characterized by the values shown in Fig. 1. Height of film/column $h_{\mathrm{ZnO}} = 1$ μm, period of structure $d = 4$ μm, height of aluminum inclusion $v = 0.25$ μm, its width $w = d/2$. Further, the h_{ZnO} parameter is varied to evaluate the influence of geometric parameter variations on the spectrum of acoustic waves in the corresponding waveguides.

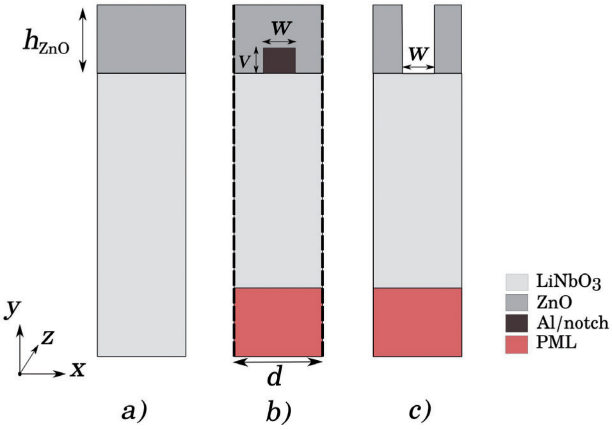

Fig. 1. *Schematic representation of single cells of periodic waveguides. a) homogenous ZnO film, b) ZnO film with aluminum inclusion, c) ZnO columns on the lithium niobate half-space. Film height* h_{ZnO}, *structure period d, basic inclusion size values with height v and width w.*

The problem of searching for acoustic modes was solved numerically using the finite element method. In this case, the sample in the *YX* plane was divided into two-dimensional quadrilateral elements. The one-dimensional wavevector was directed along the *X* axis. In the *Z* direction, the structure was considered infinite. This method and its implementation have been frequently tested in problems of propagation of acoustic waves in plates, of surface and edge waves, including periodic structures [5]. The Floquet-Bloch theorem was used to model dispersion relations. Within this approach, the solution was sought only in the area of a unit cell. At the ends of the unit cells, periodic boundary conditions were set (Fig. 1*b*, dashed lines). The unit cells had finite dimensions in the *Y* direction. This led to additional resonances of bulk acoustic waves that can be reflected from the lower boundary of the cell. These resonances are located at higher frequencies and do not overlap the region of existence of the studied localized modes. To study the conditions for the existence of pseudo-waves, or localized "leaky waves", the response of the system to a sinusoidal source acting on the upper surface of the structure was considered. In this case, the high-frequency region of the acoustic spectrum in the resonance region was analyzed. The modeling of a semi-infinite substrate using a perfectly matched layer (PML) placed at the bottom was used to prevent the reflection of acoustic waves generated by the source from the bottom boundary of the acoustic waveguide (Fig. 1*b*).

Material constants for lithium niobate were taken from the website of the manufacturer of crystals BostonPiezooptics [9], for zinc oxide from [3], the following parameters were used for aluminum: density 2700 kg/m^3, Young's modulus 70 GPa Poisson's ratio 0.33.

3. HOMOGENEOUS ZNO FILM

Consider the basic geometry in the absence of periodic structures, which is a homogeneous isotropic film (ZnO) on the half-space (*Y* cut lithium niobate) (Fig. 1*a*). The waves propagate in the *YZ* direction of lithium niobate. With the film thickness of ZnO $h_{\mathrm{ZnO}} = 1$ μm and the cell period of $d = 4$ μm, the calculated dispersion relations are as follows (**Fig. 2**).

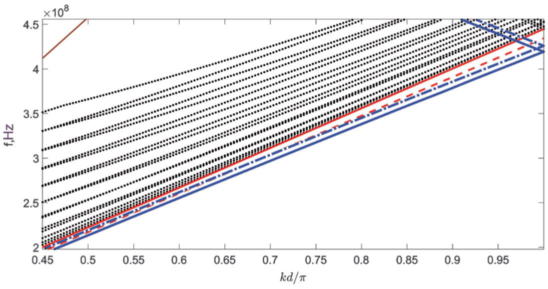

Fig. 2. *Dispersion relations for modes in the ZnO film system ($h_{ZnO} = 1$ μm) on a half-space of YZ lithium niobate. The red and brown solid lines correspond to the lowest transverse and longitudinal bulk waves in the Y section of lithium niobate, respectively. The dashed red line corresponds to the surface acoustic wave (SAW) in YZ lithium niobate. The black dashed lines correspond to the resonances of the bulk acoustic waves (BAW). The blue lines are solid and the dotted line corresponds to the 1st and 2nd localized surface waves. f – wave frequency, k – wavenumber.*

It can be seen that in this structure there are two localized modes (blue solid and blue dotted lines) in the range of the normalized value of the wave vector kd/π from 0.45 to 1. Separately, we note that since the depth of the modeled geometry is finite and in this case is 18 periods, then with small values of the wavenumbers, the lowest boundary of the structure affects the acoustic modes. Thus, the resulting dispersion relations at small *k* cease to plausibly describe the system.

As for the large values of the wavenumbers, due to the artificiality of choosing the period of the cell, dispersion dependencies exist beyond the Brillouin zone in the form of "reflected" or "folded" branches that go beyond the continuum of bulk and surface resonances. At the boundary of the Brillouin zone, the first localized mode (blue continuous) exists at frequency f_1 = 419.3 MHz and has sagittal polarization. This mode corresponds to the Rayleigh type of acoustic waves. At low

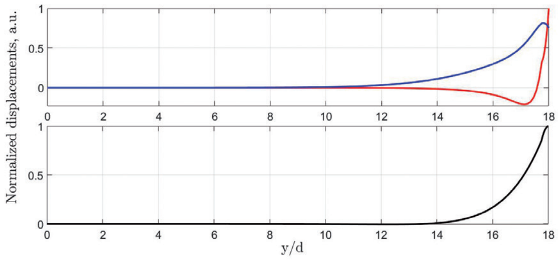

Fig. 3. *The distribution of the normalized displacement fields of the two lowest localized modes in the ZnO layer/YZ half-space structure LiNBO$_3$ at the boundary of the Brillouin zone in the Y direction. a) Rayleigh type mode with sagittal polarization (Fig. 2, blue solid), b) Love mode with shear horizontal polarization (Fig. 2, blue dotted line). u_x is the blue curve, u_y is the red curve, u_z is the black curve. Displacements for the Love mode and Rayleigh type mode are normalized on the surface to the u_z and u_y components, respectively.*

wavenumbers, this dispersion curve has the asymptotic of surface acoustic waves (SAW) in *YZ* lithium niobate in the absence of a film. A second localized mode (blue dotted line) at the boundary of the Brillouin zone exists at f_2 = 425.9 MHz and has shear horizontal (*SH*) polarization. Thus, it can be concluded that it is a Love wave. Near kd/π = 0.7, it crosses the asymptotic line for SAW in *YZ* lithium niobate (red dotted line). Branches above the asymptotic lines corresponding to BAW (black lines in Fig. 2), are bulk resonances. Fig. 2 shows only the first 20 eigenmodes. Dependencies of the distribution of normalized displacement fields of the two lower localized modes (Fig. 2, blue dotted line and blue solid) in depth in the *Y* direction at the boundary of the Brillouin zone are shown in **Fig. 3**.

4. ZNO FILM WITH ALUMINIUM INCLUSIONS.

To the structure described above (Fig. 1*a*) an aluminum electrode with a thickness of v = 0.25 µm and a width of w = 2 µm was added between the ZnO film and lithium niobate as a periodic inhomogeneity (Fig. 1*b*). The problem was solved by the method described above. As electrical boundary conditions, either the situation with electrically shorted electrodes or with electrodes not connected to a voltage source was used. **Fig. 4** shows the obtained theoretical dispersion relations.

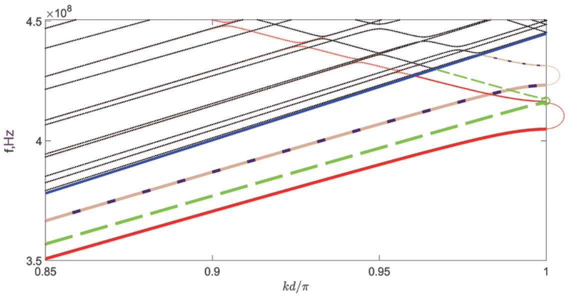

Fig. 4. *Dispersion relations for acoustic modes in the structure film ZnO (h_{ZnO} = 1 µm) – aluminum electrode (v = 0.25 µm, w = 2 µm) – Y LiNbO$_3$ half-space. Solid lines correspond to modes in the structure with short-circuited electrodes, dashed lines correspond to modes in the structure with electrodes not connected to voltage source. The blue straight line corresponds to the shear BAW in the substrate. Thin semicircular lines on the right show the corresponding band gaps.*

It can be seen that in this case band gaps appear (highlighted with a semi-oval). As shown in Fig. 4, the dispersion dependence of the lower Rayleigh mode (green bold dotted line) shifts to the low frequency region (red thick solid) when the electrodes are electrically shorted. In this case, the width of the forbidden zone for unconnected electrodes is 1.8 MHz, and when they are shorted, this value increases to 11.5 MHz. As for the Love waves, the corresponding dispersion relationship do not respond to changes in boundary conditions. This is due to the fact that the Love wave in this structure is nonpiezoactive and the width of its band gap for both boundary conditions is 8.1 MHz.

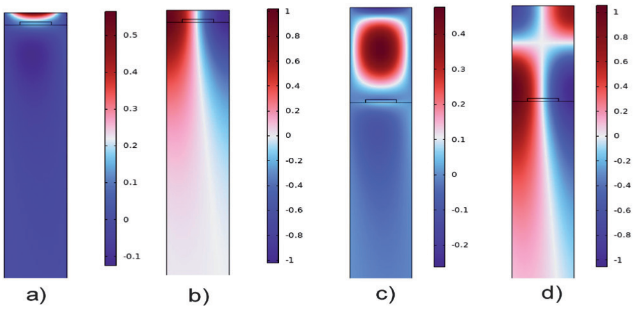

Fig. 5. *Displacement fields ux (a) and uy (b) for the Rayleigh mode at* h_{ZnO} *= 1 μm and for the Sezawa mode at* h_{ZnO} *= 8 μm ux (c) and uy (d) at the boundary of the Brillouin zone on the branches below the band gaps.*

To determine the polarization of the studied waves, the components of their mechanical displacements were calculated. **Figs. 5***a,b* show the displacement fields for the lower Rayleigh mode at 404.9 MHz at the boundary of the Brillouin zone.

Next, the influence of ZnO film thickness on the acoustic spectrum under study was analyzed. As a result, it was found that when the film thickness of ZnO is increased from 1 μm to 8 μm, higher localized modes appear (**Fig. 6**). It can be seen that in addition to Rayleigh type waves, Sezawa type modes appear that have sagittal polarization (black and orange lines). It should be noted that with the increase of thickness of the ZnO film, the piezoactivity of Rayleigh type waves is significantly reduced, while the emerging Sezawa type modes are more piezoactive. It was also found that when shorted, the band gap of this mode dramatically increases from 100 kHz (black semicircle) to 6.9 MHz (orange semicircle) (Fig. 6). Figs. 5*c,d* show the calculated mechanical displacement fields for the lower branch of Sesawa mode at the boundary of the Brillouin zone for h_{ZnO} = 8 μm. Unlike the Rayleigh mode, the components of the Sezawa mode field change sign inside the film, which corresponds to a phase change of $\pi/2$.

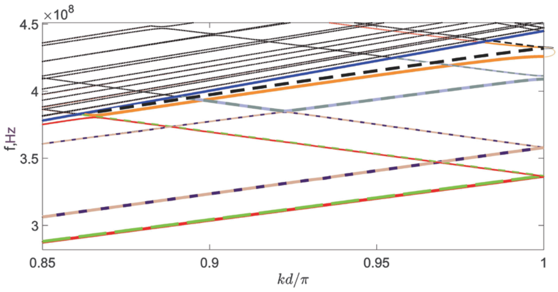

Fig. 6. *Dispersion relations for modes in the ZnO film system (*h_{ZnO} *= 8 μm) with a thin aluminum inclusion v = 0.25 μm and w = 2 μm (electrode) on a Y LiNbO*$_3$ *half-space. Solid lines correspond to modes in the system with shorted boundary conditions on electrodes, dashed lines correspond to modes in the system with "floating" boundary conditions on electrodes (not connected to a voltage source). The blue straight line describes the bulk shear wave in the substrate. Red and light green lines correspond to lower Rayleigh modes, orange and black lines correspond to Sezawa modes, dark blue and beige correspond to 1st order Love modes, dark green and purple correspond to 2nd order Love modes.*

5. RECTANGULAR NOTCH IN ZNO FILM OR ZNO COLUMN IN Y CUT LINBO$_3$ HALF-SPACE

It is of interest to evaluate the effect of other types of periodic inclusions on the spectrum of acoustic localized waves. It was found that when replacing the aluminum inclusion with a notch, a strong change in the behavior of dispersion dependencies occurs (**Fig. 7**).

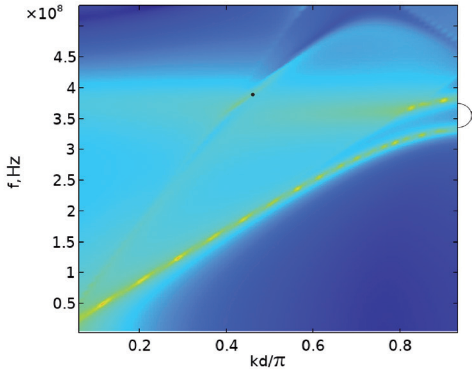

Fig. 7. *Dispersion dependencies in the form of a response to external mechanical action (force source) for modes in the ZnO film system (*h_{ZnO} *= 1 μm) with a notch v = 0.25 μm and w = 2 μm on a half-space of Y LiNbO*$_3$*. The semicirlce corresponds to band gap for guided modes.*

The study of the response of the system to an external force clearly demonstrates the existence of two localized lower modes emerging from the low-frequency continuum. Both observed branches have sagittal character of displacement fields. It should be noted that in such geometry there is a significant frequency range with a width of about 50 MHz, in which propagating guided modes are prohibited (Fig. 7, black semicircle).

In addition, the existence of pseudo-localized solutions with other asymptotics in the form of BAW with a higher velocity is observed. Distribution of displacement fields for leaky wave at frequency 386.25 MHz and at value of normalized wave number kd/π = 0.46346 (black dot in Fig. 7) is shown in **Fig. 8**.

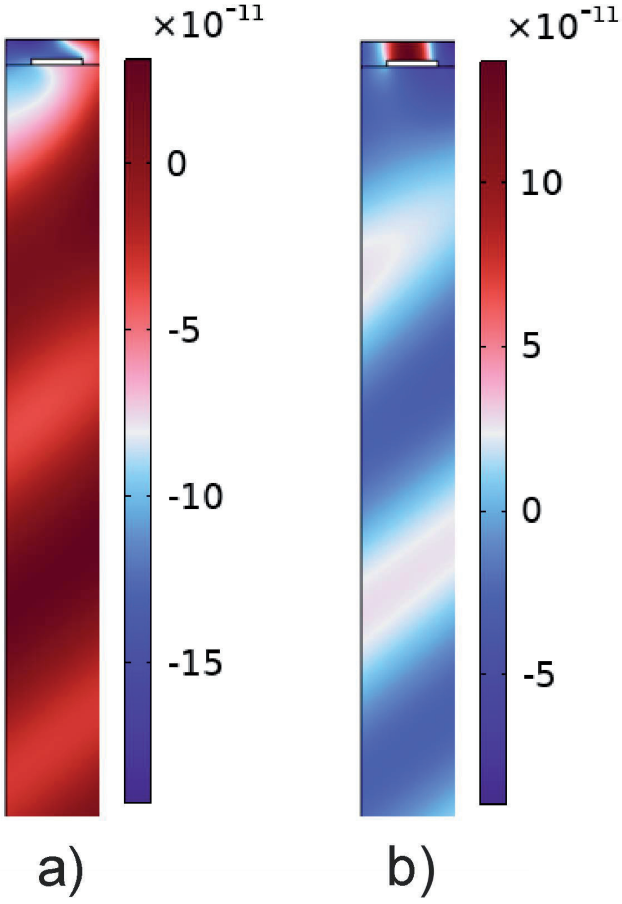

Fig. 8. *Displacement fields for a pseudo-localized leaky wave at a frequency of 386.25 MHz and at a normalized wave number kd/π = 0.46346 in a structure with a notch v = 0.25 μm and w = 2 μm in a ZnO film (h_{ZnO} = 1 μm) on Y LiNbO$_3$ half-space. a) ux component, b) uy component.*

The above structure has a geometry related to one-dimensional columns on the crystal surface [1, 2]. In this regard, to compare dispersion relations, the limiting case of an empty void $v \rightarrow h_{ZnO}$ in the form of columns with a height of h_{ZnO} = 1 μm and w = 2 μm was calculated (Fig. 1c). **Fig. 9** shows the dispersion curves for this structure. There are only two localized modes (blue lines are solid and dotted) lying below the BAW branch. Moreover, one of them exists in a wide wavevector and frequency range, the second in a small range – the from the border of the continuum to the boundary of the Brillouin zone. This mode branch is almost horizontal, that is, in this case, a wave with an almost zero group velocity is possible. There is also a very wide gap in the spectrum with a band of 62.5 MHz (Fig. 9, thin semicircle).

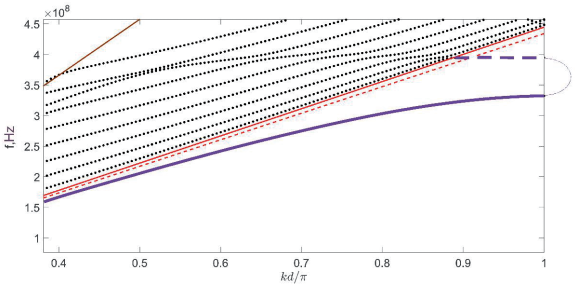

Fig. 9. *Dispersion relations for acoustic modes in the structure with columns ZnO (h_{ZnO} = 1 μm) and w = 2 μm on Y LiNbO$_3$ half-space. The red and brown solid lines correspond to the lowest transverse and longitudinal BAW in the Y cut of the LiNbO$_3$, respectively. The dashed red line corresponds to the SAW in YZ LiNbO$_3$. The blue lines correspond to the 1st and 2nd localized SAW, respectively. Thin semicircular lines on the right show band gap.*

6. CONCLUSION

Localized acoustic modes in one-dimensional periodic piezoelectric structures based on thin metal inclusions, notches, and grooves have been investigated. Based on the analysis of the fields of mechanical displacements, it was found that these modes in structures with periodic thin aluminum electrodes correspond to Love and Sezawa waves in homogeneous media. It has been shown that the change in mechanical and electrical boundary conditions has a strong effect on the behavior of dispersion curves near the boundary of the Brillouin zone. This allows to manipulate the existence of band gaps existence, as well as their width. On the other hand, it was found that these effects are negligibly small for non-piezoactive modes observed simultaneously in the same structure. More complex modifications of structures in the form of a combination of voids and grooves/columns also strongly affect the behavior of dispersion curves. In the structures appears wide band gaps, extensive ranges of modes with zero group velocity, and pseudo-waves branches. State-of-the-art technologies for deposition of films and objects of complex geometry make it possible to design acoustic waveguides with unique characteristics that are suitable for various applications, whether they are components of signal processing devices, sensors, or wavefront manipulation systems.

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