

This work studies propagation of different SH-SAWs treating various configurations using the cubic crystals  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{GeO}_{20}$ , which possess strong piezoelectric effect. Possible cuts for the wave propagation are treated when an even-order symmetry axis of a crystal is perpendicular to the sagittal plane, and when some analytical solutions can be obtained studying propagation direction [101] in the crystals. Calculations of the phase velocity and the CEMC versus the layer thickness were carried out. Numerical results on propagation of the seven-partial Love type waves were also introduced for different electrical boundary conditions: metallized and non-metallized surfaces. Also, new dispersive SAW possessing single mode was discovered concerning direction [101] in various layered systems consisting of the cubic crystals. It is thought that the obtained results can be also useful in the application of inter-digital transducers for excitation of different SAWs in structural health monitoring. In addition, a theoretical study of three-layer structures consisting of widely-used weak piezoelectrics ( $\text{GaAs}/\text{GaP}/\text{GaAs}$  and  $\text{GaAs}/\text{GaP}/\text{ZnTe}$ ) was also carried out.



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## Dispersive SAWs in Layered Systems Consisting of Cubic Piezoelectrics

New Dispersive Shear-Horizontal Waves and Love Type Waves in Layered Systems Consisting of Cubic Piezoelectrics



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## PREFACE

This book theoretically studies propagation of different shear-horizontal acoustic waves in two-layer systems. Various configurations are treated using the cubic crystals  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{GeO}_{20}$  which possess strong piezoelectric effect. Possible cuts for the wave propagation are treated when an even-order symmetry axis is perpendicular to the sagittal plane, and when some analytical solutions can be obtained studying propagation direction  $[101]$  in the crystals. Calculations of the phase velocity  $V_{ph}$  and the static coefficient of electromechanical coupling  $K^2$  versus the layer thickness were carried out. The calculation of the phase velocity  $V_{ph}$  can be useful for finding new shear-horizontal surface acoustic waves (SH-SAWs). Numerical results on propagation of the seven-partial Love type waves were also introduced for different electrical boundary conditions: metallized and non-metallized surfaces. Also, new dispersive SAW possessing single mode confined in suitable  $V_{ph}$ -range was discovered concerning direction  $[101]$  in various layered systems consisting of the cubic crystals. It was also found that speeds of non-dispersive surface and interfacial waves are possible limit speeds for the new dispersive SH-SAWs in the cases of the wavenumber  $k \rightarrow 0$  and  $k \rightarrow \infty$ . However, the  $V_{ph}$  for some modes of the new dispersive waves can approach other limit speeds for a large value of the wavenumber  $k$ . The new SH-SAW existence broadens choice of piezoelectric materials which can be used in SH-SAW technical devices. It is thought that the obtained results can be also useful in the application of inter-digital transducers for excitation of different SAWs in structural health monitoring. In addition, theoretical study of three-layer structures consisting of widely-used weak piezoelectrics ( $\text{GaAs}/\text{GaP}/\text{GaAs}$  and  $\text{GaAs}/\text{GaP}/\text{ZnTe}$ ) was carried out concerning any possibility to numerically find the new dispersive SH-SAWs.

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**Keywords:** piezoelectric cubic crystals, strong piezoelectric coupling, new SH-SAWs, Love type waves.

## COMMENTS BY THE AUTHOR

This book describes the theoretical work carried out for the International Institute of Zakharenko Waves (IIZWs) as an additional work to the PhD-thesis by the author: Aleksey Anatolievich Zakharenko, corresponding address is 660037, Krasnoyarsk-37, 17701, Krasnoyarsk, Russia (E-mail: [aazaaz@inbox.ru](mailto:aazaaz@inbox.ru)). It is thought that this book can be interesting for researchers and students who deal with piezoelectrics, piezomagnetism, and layered systems consisting of them. It is also thought that it can represent an interest for those who cope with piezoelectromagnetics. Indeed, knowledge of properties of cubic piezoelectrics is beneficial to design of smart devices, sensors, actuators, as well as applications in non-destructive testing. Also, the obtained results in this book can allow one to choose apt materials to constitute piezomagnetic/piezoelectric laminate composites in the microwave technology. It is well-known that innovative smart materials are also created for the aerospace industry.

The International Institute of Zakharenko Waves (IIZWs) was recently created for support of different Zakharenko waves, as well as for monitoring the non-dispersive Zakharenko type waves in complex systems such as layered and quantum systems. Indeed, any complex system in which dispersive waves can propagate is of a great interest for the IIZWs. The well-known examples of dispersive waves are dispersive Rayleigh and Bleustein-Gulyaev type waves as well as Love and Lamb type waves. There are currently more than twenty papers relevant to the IIZWs. The International Institute of Zakharenko Waves also studies different dispersive and non-dispersive waves both theoretically and experimentally, including different applications of the waves for signal processing (filters, sensors, etc.) and the structural health monitoring. Note that one can financially support the research of the International Institute of Zakharenko Waves, using the following bank account: Beneficiary's Bank is Krasnoyarsk Branch of National Bank TRUST, c/a № 30301978300450000038 with Moscow Branch of National Bank TRUST, Moscow,

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It is worth noting that the International Institute of Zakharenko waves possessively takes all the planets and smaller natural space bodies in the space outside the Solar System to develop both the IIZWs and the planets concerning economics, ecology, and population. Also, it is thought that this is necessary in order to exclude any sale of the planets and their surfaces by any human or other. This activity of the IIZWs was also created due to a problem to find a spot for the IIZWs on Earth. Note that the single person, namely Mr. Dennis Hope from the United States possesses the planets in the Solar System (but Earth) who sells surfaces of the planets to individuals. It is also noted that only about 500 planets orbiting stars can be currently observed in Star Systems which are situated relatively near the Solar System. This does not mean that only 500 planets exist outside the Solar System we can observe. It is expected that in average ten planets can orbit each star of enormous number of Star System in our Universe. It is thought that our Universe can accumulate more than  $10^{999}$  stars.

Aleksey A. Zakharenko  
Krasnoyarsk, Russia, 2010

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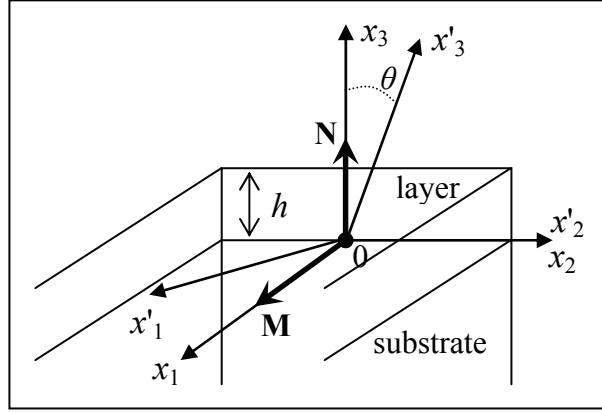
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## INTRODUCTION

It is well-known that there are two basic polarization types for surface acoustic waves (SAWs) in acoustics of solids such as the wave polarization in the sagittal plane and the polarization perpendicular to the sagittal plane. The sagittal plane is formed by the directional vector  $\mathbf{M}$  and the vector  $\mathbf{N}$  being the normal to both the free surface and interface shown in figure 1 along with the coordinate system for the layered system, consisting of a thin film (layer) on a substrate (half-space). The surface Rayleigh waves possessing hybridization of the displacement components  $U_1$  and  $U_3$  along the  $x_1$ - and  $x_3$ -axes are polarized in the sagittal plane. These waves were originally discovered in 1885 by Lord Rayleigh [1]. Note that Lord Rayleigh has studied isotropic mono-materials, namely the case of the layer thickness  $h = 0$  in figure 1. It is thought that the SAW simplest example concerning the polarization perpendicular to the sagittal plane is the Love wave [2] propagating in layered systems, consisting of two isotropic materials. Note that there is the following existence condition for Love waves: the speed  $V_{SH} = (C_{44}/\rho)^{1/2}$  of the bulk shear-horizontal (SH) wave for a substrate should be higher than that for a layer, where  $C_{44}$  and  $\rho$  are the shear elastic constant and material density, respectively. For the Love (type) waves, the displacement component  $U_2$  along the  $x_2$ -axis for a substrate is coupled with the component  $U_2$  for a layer at the layer-substrate interface. Therefore, they are hybridized due to their co-influence. The Love type wave (LTW) becomes the bulk SH-wave for zero layer thickness and cannot exist in homogeneous monocrystals.

SAWs with the Love-wave polarization can also exist in inhomogeneous media such as piezoelectric monocrystals. They were first discovered by Bleustein and Gulyaev simultaneously in the late 1960s [3, 4] studying transversely-isotropic piezoelectrics of class 6 mm. The surface Bleustein-Gulyaev type waves (BGTWs) are treated as the weakly-nonhomogeneous SAWs. They can exist only on certain cuts and propagate in certain directions of piezoelectric monocrystals characterized

by coupling between the elastic displacement component  $U_2$  and electrical potential  $U_4 = \varphi$ , where  $\varphi$  is electrostatically defined from the electrical field  $E_j = \partial\varphi/\partial x_j$  with the index  $j = 1, 2, 3$ . Hence, it is thought that there must be a coupling of at least two displacement components in the SAW simplest cases.



**Figure 1.** The right coordinate system with the directional vector  $\mathbf{M}||[100]$  and the vector-normal  $\mathbf{N}$  for the layered structure consisting of a layer on a substrate, where  $h$  is the layer thickness

Dispersive Rayleigh type waves (RTWs) can propagate in the layered systems shown in figure 1 in which the LTWs can also co-exist. In layered systems consisting of two piezoelectric materials, the “pure” RTWs are coupled with the electrical potential when LTWs represent pure mechanical waves and vice versa, according to Refs. [5, 6, 7]. See also the famous book [8] describing applications of the RTW, LTW, and BGTW. Recently, interest is growing in the study of propagation of dispersive BGTWs in various layered structures (for example see Ref. [9]) because the application of layered piezoelectric structures can significantly reduce the penetration depth, which is 10 – 100 times larger than the wavelength  $\lambda$  for the surface BG-waves in monocrystals. It is thought that the single mode of dispersive BGTWs can be treated as the LTW lowest-order mode, which represents the LTW first type. It is also thought that the LTW higher-order modes represent the LTW

second type in order to have an analogy with the dispersive RTWs, of which the first (lowest-order mode) and second types are separately studied.

In general, propagation of the dispersive and non-dispersive BGTWs is studied in the transversely-isotropic materials. Moreover, one of the BG-wave discoverers stated in Ref. [10] published in 2005 that the SAWs cannot exist in piezoelectric cubic monocrystals. Indeed, such surface waves were not found in Ref. [11] studying cubic piezocrystals of class 23 in propagation direction (001) [100]. It is noted that in 1966, Kaganov and Sklovskaya [12] reported a possible existence of new surface waves coupled with the electrical potential in piezoelectric cubic monocrystals in addition to the purely mechanical surface Rayleigh waves. Treating the case of elastically-isotropic medium with the non-zero piezoelectric constants  $e_{14} = e_{25} = e_{36}$ , they in Ref. [12] have found that the phase velocity  $V_{ph}$  of the new (additional) surface wave is higher than  $3^{1/2}c_t/2$  and lower than  $c_t$ , according to the paper text (the abstract in Ref. [12] was incorrectly written) where  $c_t$  represents the bulk shear wave velocity uncoupled with the electrical potential. In addition, they did not state that such new SAWs can propagate when the wave propagation direction is perpendicular to an even-order symmetry axis of a piezoelectric crystal. Indeed, utilization of cubic piezoelectrics in addition to the transversely-isotropic materials can broaden a list of suitable materials and represents an interest in engineering and design of SAW devices (filters, dispersive delay lines, etc.).

According to Ref. [13] by Al'shits and Lyubimov, the BG-wave existence in cubic piezocrystals of classes  $\bar{4}3m$  and 23 strongly depends on the piezoelectric constants and dielectric constant  $\varepsilon$ . Ref. [13] has discussed that existence sectors of the BG-waves being about  $\pi/4$ , when there is rotation around the axis directed along an even-order symmetry axis, can be significantly broadened using crystals with small dielectric constants. For the limit case of  $\varepsilon \rightarrow 0$  requiring small piezoelectric constants, the BG-waves can exist in any such propagation direction, except the exceptional angles  $0, \pi/2, \pi, \dots$ , where the single-partial exceptional bulk waves of first type can exist representing the boundaries of such SAW existence sectors. Also, only the exceptional bulk waves can exist in piezoelectric cubic monocrystals

possessing a very large dielectric constant  $\varepsilon \rightarrow \infty$  [13] for the second limit case. They also noted that there is an analogy of existence of exceptional bulk waves in optics, where surface optic waves can be converted to bulk waves for some frequencies and propagation directions. Indeed, different electrical boundary conditions (for example, the surface metallization) can also alter the existence sectors of the BG-waves. It is thought that the interesting case of  $\varepsilon \rightarrow \infty$  can be realized due to recent discovery of the giant dielectric effect found in the cubic perovskite-related materials  $\text{CdCu}_3\text{Ti}_4\text{O}_{12}$  and  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$  [14]. The latter has a tremendously high dielectric constant  $\varepsilon_s \sim 10^4$  at room temperatures. One of the most commonly used dielectric materials is silicon nitride with  $\varepsilon_s \sim 7$ . Materials with large static dielectric constants  $\varepsilon_s > 7$  are generally referred to as high-dielectric constant materials and are used in memory devices being highly called for the microelectronics industry. That is due to the fact that acting as a scaling factor, the static dielectric constant  $\varepsilon_s$  ultimately determines the miniaturization level.

The recent review paper [15] by Yamaguchi focused on early days of research about SH type acoustic waves. For instance, it was discussed in Ref. [15] that the surface skimming bulk waves (SSBWs) are closely related to the other SAWs known as the Bleustein-Gulyaev-Shimizu waves (BGSWs) on rotated  $Y$ -cuts of quartz, namely the SSBW velocities substantially coincide with those of BGSW. Also, some types of SH-SAWs in solids can be found in the famous review paper [16] by Gulyaev, see also the famous book [17] on wave phenomena in inhomogeneous media. A possible existence of two new types of SH-SAWs propagating in layered systems, consisting of a layer on a substrate, was recently introduced in Ref. [18], of which one can be used in addition to the Love type waves. Ref. [18] also shows the existence possibility of the supersonic three-partial Love type waves (LTW3) where the velocity equivalents for both layer and substrate, instead of the bulk SH-waves, should be analyzed for the wave existence condition. It is noted that the velocity equivalent is always lower than the bulk SH-wave speed for anisotropic materials. It is thought that these velocity equivalents can be also called the exceptional bulk waves. This paper studies different dispersive and non-dispersive waves with the

Love-wave polarization. The following section contains thermodynamic description of the material constants in the linear case. Also, the following section provides evolution of the piezoelectric constants caused by changes in the wave propagation directions when the elastic and dielectric constants are not changed.



## CHAPTER I. Material Properties

Piezoelectric ceramics are used in a variety of commercial applications due to their electromechanical nature displaying both a direct effect (generating effect) in which an electrical charge is generated by a mechanical stress, and the converse effect (motor effect) in which an electrical field produces a mechanical displacement. Note that piezoelectricity from the Greek word “piezo” means pressure electricity. Various solid-state or polymeric materials with piezoelectric characteristics are being applied to a variety of transducers and sensors, which include hydrophones, sonar, accelerometers, power supplies, ultrasonic motors, transformers, micropositioners, filters, robotic muscles, medical ultrasound, etc. Currently, piezoelectric ceramics are the most widely used materials, because they comparatively show the highest generative forces, accurate displacements, and best high frequency capabilities. When an AC voltage is applied to a sample piezoelectric material, it will cause vibrations and thus generate mechanical waves at the same frequency of the input AC field. Similarly, it would sense the input mechanical vibrations and produce the proportional charge at the matching frequency of the mechanical input. Quartz is a well-known single-crystal material, depicting such piezoelectric effects. The pioneer work by W.G. Cady [19] concerning applications of Quartz piezoelectric crystals attracted attention to the utilization of piezoelectric crystals in various technical devices. The famous review papers [20, 21] by W.P. Mason describe many applications of piezoelectrics over the last century, including different SAW technical devices.

According to the classical works [22, 23], the thermodynamic potentials derive the equations of piezoelectric medium. In order to describe thermoelectroelastic interactions in piezoelectric crystals, eight thermodynamic potentials are currently used, in which energetic terms are included and are coupled with elastic (stress  $\tau_{ij}$  or strain  $\eta_{ij}$ ), electric (electrical field  $E_i$  or electrical induction  $D_i$ ) and thermal (temperature  $T$  or disorder value called entropy  $S$ ) sub-systems [23]. General



equations for adiabatic rather than isothermal conditions may be obtained using the thermodynamic potential (electrical enthalpy  $H_{el}^a$ ) given by the following expression:

$$H_{el}^a = \tau_{ij}\eta_{ij} - D_m E_m - T_k S_k \quad (1)$$

It is thought that it is convenient to naturally take the mechanical strain tensor  $\eta_{ij}$  as an independent thermodynamic mechanical variable, because the wavelength of propagating acoustic waves is significantly smaller than line sizes of a sample crystal, and crystal vibrations as a whole can be neglected (mechanically-shortening condition). Also, the electrical field  $E_m$  is taken as a thermodynamic electrical variable, because the piezoactive propagation directions can exist in piezoelectric materials where the electrical potential is coupled with propagating elastic waves. The perfect differential of equation (1) is then written in the following way:

$$dH_{el}^a = \tau_{ij} d\eta_{ij} - D_m dE_m - T_k dS_k \quad (2)$$

Treating adiabatic processes with the constant entropy ( $S = \text{const}$  giving  $dS = 0$ ) and leaving only linear terms, it is possible to write a Taylor series for the electrical enthalpy  $H_{el}^a(\eta_{ij}, E_m, S)$  relative to an equilibrium condition  $H_{el}^a(0, 0, S_0)$ :

$$H_{el}^a(\eta_{ij}, E_m, S) - H_{el}^a(0, 0, S_0) = \frac{1}{2} C_{ijkl}^E \eta_{ij} \eta_{kl} - e_{mij} \eta_{ij} E_m - \frac{1}{2} \varepsilon_{mn}^\eta E_m E_n \quad (3)$$

With vibrating piezoelectric elements there is usually negligible heat interchange, and the adiabatic equations hold. Using equation (3), it is possible to write “mechanical” and “electrical” equations for the treated linear case. With the stress and electrical field as the independent variables, the equations are written as follows:

$$\tau_{ij} = \left( \frac{\partial H_{el}^a}{\partial \eta_{ij}} \right)_{E,S} = C_{ijkl}^E \eta_{kl} - e_{ijm} E_m \quad (4)$$

$$D_m = -\left(\frac{\partial H_{el}^a}{\partial E_m}\right)_{\eta,S} = \varepsilon_{mn}^{\eta} E_n + e_{mij} \eta_{ij} \quad (5)$$

The elastic constants  $C_{ijkl}$ , being components of the elastic stiffness tensor, relate two second-order symmetric tensors representing fourth-order tensors from equation (4) for linear elasticity with piezoelectric term:

$$C_{ijkl}^{E,S} = \left(\frac{\partial^2 H_{el}^a}{\partial \eta_{ij} \partial \eta_{kl}}\right)_{E,S} = \left(\frac{\partial \tau_{ij}}{\partial \eta_{kl}}\right)_{E,S} \quad (6)$$

The piezoelectric constants  $e_{mij}$  relate second-order symmetric tensors to vectors, and therefore they are third-order tensors, using equations (4) and (5):

$$e_{mij}^S = e_{ijm}^S = -\left(\frac{\partial^2 H_{el}^a}{\partial \eta_{ij} \partial E_m}\right)_S = -\left(\frac{\partial \tau_{ij}}{\partial E_m}\right)_{\eta,S} = \left(\frac{\partial D_m}{\partial \eta_{ij}}\right)_{E,S} \quad (7)$$

The dielectric constants  $\varepsilon_{mn}$ , also called dielectric permittivity, relate two vectors, and therefore represent second-order tensors. Using equation (5), they are defined as follows:

$$\varepsilon_{mn}^{\eta,S} = -\left(\frac{\partial^2 H_{el}^a}{\partial E_m \partial E_n}\right)_{\eta,S} = \left(\frac{\partial D_m}{\partial E_n}\right)_{\eta,S} \quad (8)$$

Accounting the fact, such as the sound velocity  $V$  in a crystal is very small compared with the light velocity  $c$ , allows usage of the quasi-electrostatic approximation

$$\text{rot}\mathbf{E} = 0 \quad \text{or} \quad E_m = -\frac{\partial \varphi}{\partial x_m} \quad (9)$$

with  $\varphi$  and  $x_m$  being the electrical potential and current rectangular coordinates of a material point, respectively. On the other hand, the electrical induction  $D_m$  must satisfy the Maxwell equation for a non-conducting medium

$$\operatorname{div}\mathbf{D} = \frac{\partial D_m}{\partial x_m} = 0 \quad (10)$$

Note that equation (8) gives the well-known relationship  $D_m = \varepsilon_{mn}E_n$  between the electrical induction  $D_m$  and the electrical field  $E_n$ .

The corresponding material tensors in equations from (6) to (8), being invariant relative to the crystallographic group of symmetry, are described in the famous book [24] by J.F. Nye. Note that crystal symmetry is coupled with symmetry of physical properties of a crystal. The fundamental postulate of crystallophysics known as the Neumann principle (for example see Ref. [24]) states the following: ‘‘Symmetry elements of any crystal physical property should include symmetry elements of crystal point group’’. Each crystal point group has its own set of independent components of material tensors. For instance, piezoelectric cubic crystal  $\text{Bi}_{12}\text{SiO}_{20}$  (class 23) has the following independent material constants (in the Voigt notation):  $C_{11} = C_{22} = C_{33}$ ,  $C_{12} = C_{13} = C_{23}$ ,  $C_{44} = C_{55} = C_{66}$ ;  $e_{14} = e_{25} = e_{36}$  and  $\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{33}$  in addition to the material density  $\rho$ . Material constants for cubic crystals  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{GeO}_{20}$  can be written following Ref. [25]. For  $\text{Bi}_{12}\text{SiO}_{20}$  there are the following material constants:  $\rho = 9070$  [ $\text{kg}/\text{m}^3$ ];  $C_{11} = 12.962 \times 10^{10}$  [ $\text{N}/\text{m}^2$ ],  $C_{44} = 2.451 \times 10^{10}$  [ $\text{N}/\text{m}^2$ ], and  $C_{12} = 2.985 \times 10^{10}$  [ $\text{N}/\text{m}^2$ ];  $e_{14} = 1.122$  [ $\text{C}/\text{m}^2$ ];  $\varepsilon_{11}/\varepsilon_0 = 41.1$  where  $\varepsilon_0$  is the free space dielectric permittivity ( $\varepsilon_0 = 8.854 \times 10^{-12}$  [ $\text{F}/\text{m}$ ]). For  $\text{Bi}_{12}\text{GeO}_{20}$  there are:  $\rho = 9200$  [ $\text{kg}/\text{m}^3$ ];  $C_{11} = 12.852 \times 10^{10}$  [ $\text{N}/\text{m}^2$ ],  $C_{44} = 2.562 \times 10^{10}$  [ $\text{N}/\text{m}^2$ ], and  $C_{12} = 2.934 \times 10^{10}$  [ $\text{N}/\text{m}^2$ ];  $e_{14} = 0.983$  [ $\text{C}/\text{m}^2$ ];  $\varepsilon_{11} = 3.336 \times 10^{10}$  [ $\text{F}/\text{m}$ ]. Transformations of any tensor component from the original coordinate system ( $x_1x_2x_3$  in figure 1) to the ‘‘work’’ coordinate system ( $x'_1x'_2x'_3$  in figure 1) are perfectly described in the excellent books [8, 24]. Transformed components  $\varepsilon_{ij}$  of the dielectric permittivity tensor can be

calculated using given original components  $\varepsilon_{mn}$  and corresponding components  $a_{im}$  and  $a_{jn}$  of the transformation matrix:

$$\varepsilon_{ij} = a_{im} a_{jn} \varepsilon_{mn} \quad (11)$$

Analogically, components of the piezoelectric and elastic tensors after transformations are obtained with the following formulae:

$$e_{ijk} = a_{im} a_{jn} a_{kp} e_{mnp} \quad (12)$$

$$C_{ijkl} = a_{im} a_{jn} a_{kp} a_{lq} C_{mnpq} \quad (13)$$

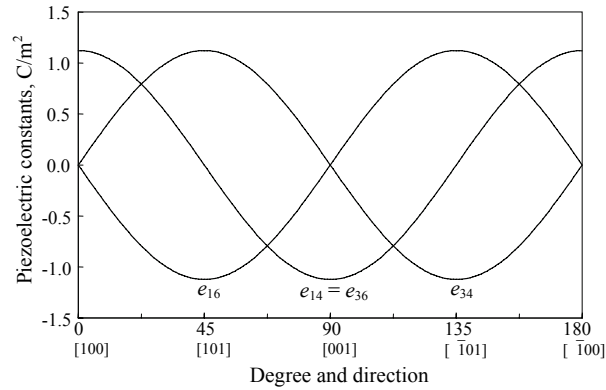
The crystallographic coordinates  $(X, Y, Z)$  coincide with the original coordinates  $(x_1, x_2, x_3)$  in figure 1. Acoustic waves propagate along the  $x'_1$ -axis in the work coordinate system  $(x'_1, x'_2, x'_3)$  obtained by rotation around the  $x'_2$ -axis, which must be directed along an even-order symmetry axis of a studied crystal. The direction of the cut normal is also changed with the Euler angles  $(0^\circ; \theta; 0^\circ)$ . Therefore, the coordinate transformations read:

$$a_{\mu\nu}^{(\theta)} = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix} \quad (14)$$

For instance, the components of the transformation matrix (14) for the angle  $\theta = \pi/4$  are as follows:

$$a_{\mu\nu}^{(\pi/4)} = \begin{pmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \end{pmatrix} \quad (15)$$

For piezoelectric cubic crystals, the transformations keep the material constants  $C_{44}(\theta)$  and  $\varepsilon_{11}(\theta)$ , but the piezoelectric constants  $e_{ij}(\theta)$  are changed as shown in figure 2 for the cubic crystal  $\text{Bi}_{12}\text{SiO}_{20}$ . That conveniently allows study of piezoelectric properties of crystals.



**Figure 2.** The dependence of the piezoelectric constants  $e_{14} = e_{36}$ ,  $e_{16}$ , and  $e_{34}$  on the propagation directions with the Euler angles  $\{0^\circ, \theta, 0^\circ\}$  for the cubic crystal  $\text{Bi}_{12}\text{SiO}_{20}$

This book describes wave propagation with the Love-wave polarization in various layered systems consisting of cubic crystals  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{GeO}_{20}$  with strong piezoelectric effect, when the propagation directions are perpendicular to the crystal second-order symmetry axis. Particularly, it will be shown below that the surface Bleustein-Gulyaev waves cannot exist in piezoelectric cubic crystals, supplementing Gulyaev's opinion written in Ref. [10] concerning the surface waves in the crystals mentioned in the previous section. The following section describes theory of wave propagation in different cuts and propagation directions, and the fourth and fifth sections provide boundary-condition determinants for finding the phase velocity  $V_{ph}$  of SH-waves in piezoelectric monocrystals and layered systems. The sixth section adds some obtained results of numerical investigations concerning the  $V_{ph}$  behavior in a set of configurations for complete understanding of the problem.

## CHAPTER II. Theory of Propagating Waves

The equation of motion of an elastic medium is written as follows [6, 7]:

$$\rho \frac{\partial^2 U_i}{\partial t^2} = \frac{\partial \tau_{ik}}{\partial x_k} \quad (16)$$

which represents the governing equation of stress equilibrium, where  $\rho$  denotes the material density.  $U_i$  and  $\tau_{ij}$  are the mechanical displacement components and components of the stress tensor thermodynamically defined in equation (4), respectively. In equation (14),  $t$  and  $x_k$  are time and the real space vector components  $\mathbf{r} \rightarrow \{x_1, x_2, x_3\}$  using the rectangular co-ordinate system. Substituting equations (4) and (5) into (16) and (10), respectively, and accounting expression (9) for the electrical field, one can write the coupled equations of motion for a piezoelectric medium in the common form:

$$\begin{aligned} \rho \frac{\partial^2 U_i}{\partial t^2} &= C_{ijkl} \frac{\partial^2 U_l}{\partial x_j \partial x_k} + e_{kij} \frac{\partial^2 U_4}{\partial x_j \partial x_k} \\ 0 &= e_{ijk} \frac{\partial^2 U_k}{\partial x_i \partial x_j} - \epsilon_{ij} \frac{\partial^2 U_4}{\partial x_i \partial x_j} \end{aligned} \quad (17)$$

where the component  $U_4$  represents the electrical potential  $\varphi$ . Solutions of homogeneous partial differential equations (17) of the second order can be found in the following form of plane wave:

$$U_i = U_i^0 \exp[j(\mathbf{kr} - \omega t)] \quad (18)$$

where the index  $i$  runs from 1 to 4, and  $U_i^0$  is an initial amplitude.  $j = (-1)^{1/2}$  and  $\mathbf{kr}$  denote the imaginary unity and scalar multiplication of two vectors, respectively. In

equation (18),  $\omega$  and  $\mathbf{k}$  are the angular frequency and wavevector with the following components:  $\{k_1, k_2, k_3\} = k\{n_1, n_2, n_3\}$  where  $k$  and  $\{n_1, n_2, n_3\}$  are the wavenumber in the wave propagation direction and the directional cosines.

In the treated case of wave propagation, the sagittal plane is always perpendicular to an even-order symmetry axis of a crystal. Coupled equations (17) of motion describe propagation of “pure” waves, according to Ref. [6, 7]. Hence, the coupled equations of motion can be readily written in the following simplified form, leaving only equations for waves with polarization perpendicular to the sagittal plane and non-zero components of the material tensors:

$$\begin{aligned} \rho \frac{\partial^2 U_2}{\partial t^2} &= C_{44} \left( \frac{\partial^2 U_2}{\partial x_1^2} + \frac{\partial^2 U_2}{\partial x_3^2} \right) + e_{16} \frac{\partial^2 \varphi}{\partial x_1^2} + e_{14} \frac{\partial^2 \varphi}{\partial x_1 \partial x_3} + e_{36} \frac{\partial^2 \varphi}{\partial x_3 \partial x_1} + e_{34} \frac{\partial^2 \varphi}{\partial x_3^2} \\ 0 &= e_{16} \frac{\partial^2 U_2}{\partial x_1^2} + e_{14} \frac{\partial^2 U_2}{\partial x_1 \partial x_3} + e_{36} \frac{\partial^2 U_2}{\partial x_3 \partial x_1} + e_{34} \frac{\partial^2 U_2}{\partial x_3^2} - \varepsilon_{11} \left( \frac{\partial^2 \varphi}{\partial x_1^2} + \frac{\partial^2 \varphi}{\partial x_3^2} \right) \end{aligned} \quad (19)$$

where the single mechanical displacement component  $U_2$  is directed along the  $x_2$ -axis in figure 1:

$$\begin{aligned} U_2 &= U_2^0 \exp[jk(n_1 x_1 + n_3 x_3 - V_{ph} t)] \\ \varphi &= \varphi^0 \exp[jk(n_1 x_1 + n_3 x_3 - V_{ph} t)] \end{aligned} \quad (20)$$

In equation (20), the phase velocity  $V_{ph}$  is defined as follows:  $V_{ph} = \omega/k$ .

Substituting the mechanical displacement  $U_2$  and electrical potential  $\varphi$  of equation (20) into equations (19) of motion, the equations of motion can be readily written in the well-known tensor form, using corresponding components of the well-known Green-Christoffel equation [6, 7]:  $GL_{22}$ ,  $GL_{42} = GL_{24}$  and  $GL_{44}$ . That gives the following system of two homogeneous equations, using  $n_3 = k_3/k$ :

$$\begin{pmatrix} GL_{22} - C_{44}(V_{ph}/V_{t4})^2 & GL_{24} \\ GL_{42} & GL_{44} \end{pmatrix} \begin{pmatrix} U_2^0 \\ \varphi^0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (21)$$

where

$$\begin{aligned}
GL_{22} &= C_{44}(1+n_3^2) \\
GL_{24} = GL_{42} &= e_{16} + (e_{14} + e_{36})n_3 + e_{34}n_3^2 \\
GL_{44} &= -\varepsilon_{11}(1+n_3^2)
\end{aligned} \tag{22}$$

In equations (21) and (22), the directional cosines are defined as follows:  $n_1 \equiv 1$ ,  $n_2 \equiv 0$  and  $n_3 = n_3$ . The parameter  $V_{t4} = (C_{44}/\rho)^{1/2}$  represents the speed of the bulk SH-wave in some particular cases. Setting the determinant of the coefficient matrix in equations (21) equal to zero, a suitable  $V_{ph}$  satisfying boundary conditions written in the following sections and four polynomial roots  $n_3^{(p)}(V_{ph})$  can be determined, with which the unknown  $U_2^0$  and  $\varphi^0$  can be also determined as functions of the  $V_{ph}$ . For example, they can be written in the following form, using equations (21) and (22):

$$\varphi^0 = GL_{42} \text{ and } U_2^0 = -GL_{44} \tag{23}$$

Expanding the determinant of matrix in equation (22), the secular equation is written as follows:

$$(1 + K_1^2)n_3^4 + K_2^2n_3^3 + (1 + A_t^2 + K_3^2)n_3^2 + K_4^2n_3 + (K^2 + A_t^2) = 0 \tag{24}$$

where there are the following non-dimensional values:

$$\begin{aligned}
A_t^2 &= 1 - (V_{ph}/V_{t4})^2 \\
K^2 &= e_{16}^2 / (C_{44}\varepsilon_{11}) \\
K_1^2 &= e_{34}^2 / (C_{44}\varepsilon_{11}) \\
K_2^2 &= 2e_{34}(e_{14} + e_{36}) / (C_{44}\varepsilon_{11}) \\
K_3^2 &= [(e_{14} + e_{36})^2 + 2e_{16}e_{34}] / (C_{44}\varepsilon_{11}) \\
K_4^2 &= 2e_{16}(e_{14} + e_{36}) / (C_{44}\varepsilon_{11})
\end{aligned}$$



Note that  $K^2$  is called the static coefficient of electromechanical coupling (CEMC). Equation (24) represents the fourth order polynomial for which there is a very complicated procedure to determine its roots  $n_3$ . Therefore, the polynomial roots are usually determined numerically. Notwithstanding, it is possible to treat some particular cases listed in table 1 in order to significantly simplify the problem for analytical investigations. Note that the following equalities  $e_{16} = -e_{34}$  and  $e_{14} = e_{36}$  always occur as shown in figure 2.

The first case in table 1 concerning propagation direction [100] was treated in Ref. [11], where the following equality  $e_{16} = e_{34} = 0$  (hence  $K^2 = K_1^2 = K_2^2 = K_4^2 = 0$ ) gives  $GL_{24} = GL_{42} = 2en_3$  with  $e = e_{14} = e_{36}$  and all completely imaginary roots of equation (24) for  $V_{ph} < V_t$ . This is true for case 5 in propagation direction [001] and the last case in the table. However, case 5 for negative piezoelectric constants  $e = e_{14} = e_{36}$  gives the same  $n_3$  and negative  $GL_{24} = GL_{42} = -2en_3$  resulting in negative  $\varphi^0$  in equation (23). Hence, the electrical field  $E$  in equation (9) will change its sign. In these cases, the speed  $V_t$  of the bulk SH-wave is equal to the  $V_{t4}$ . This indicates that these waves in propagation direction [100] are not coupled with the electrical potential. It is clearly seen from the last term of equation (24) that in any other treated case the bulk velocity  $V_t$  is equal to the following:

$$V_t = V_{t4}(1 + K^2)^{1/2} \quad (25)$$

The second particular case listed in table 1 is more complicated than the first and can be studied numerically for comparison with the other cases. That is very interesting, because here there is an equality of absolute values of all piezoelectric constants giving  $GL_{24} = GL_{42} = e(-1 + 2n_3 + n_3^2)$ . Therefore, other analogical cases 4, 6, and 8 in table 1 can be also studied numerically.

Some evaluations for the third case in table 1 concerning propagation direction [101] can be readily done analytically making substitution in equation (24) such as  $m_3 = 1 + n_3^2$  and using the piezoelectric constants  $e_{16} = -e_{34}$  and  $e_{14} = e_{36} = 0$ , which give  $GL_{24} = GL_{42} = e(-1 + n_3^2)$  for the case. For case 7 in the table there is  $GL_{24} = GL_{42} =$

$e(1 - n_3^2)$  that changes the electrical-field sign similarly to cases 1 and 5 discussed above. As the result of such transformations, the equation (24) is written in the following simplified form:

$$(1 + K^2)m_3^2 - Bm_3 + 4K^2 = 0 \text{ with } B = \left(\frac{V_{ph}}{V_{t4}}\right)^2 + 4K^2 \quad (26)$$

of which two roots are as follows:

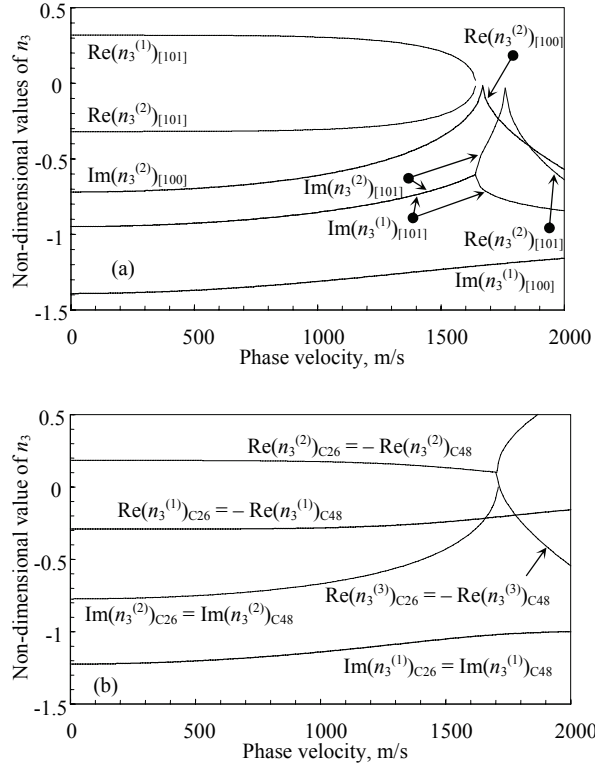
$$m_3^{(1,2)} = \frac{B \pm \sqrt{B^2 - 16K^2(1 + K^2)}}{2(1 + K^2)} \quad (27)$$

giving the following four polynomial roots of equation (24)

$$n_3^{(1,2,3,4)} = \pm \sqrt{-1 + m_3^{(1,2)}} \quad (28)$$

**Table 1.** The piezoelectric constants  $e_{14} = e_{36}$ ,  $e_{16}$ , and  $e_{34}$  [C/m<sup>2</sup>] in some highly-symmetric propagation directions for the cubic crystal Bi<sub>12</sub>SiO<sub>20</sub>

Case	Direction	Degree	$e_{14} = e_{36}$	$e_{16}$	$e_{34}$
1.	[100]	0°	1.122	0.0	0.0
2.	–	~ 22.5°	0.793	– 0.793	0.793
3.	[101]	45°	0.0	– 1.122	1.122
4.	–	~ 67.5°	– 0.793	– 0.793	0.793
5.	[001]	90°	– 1.122	0.0	0.0
6.	–	~ 112.5°	– 0.793	0.793	– 0.793
7.	[ $\bar{1}01$ ]	135°	0.0	1.122	– 1.122
8.	–	~ 157.5°	0.793	0.793	– 0.793
9.	[ $\bar{1}00$ ]	180°	1.122	0.0	0.0



**Figure 3.** The  $n_3$  real and imaginary parts along the  $x_3$ -axis for the propagation directions listed in table 1: (a) cases 1, 3, 5, 7, and 9 for Bi<sub>12</sub>GeO<sub>20</sub>; (b) cases 2, 4, 6, and 8 with the corresponding subscripts “C26” and “C48” for Bi<sub>12</sub>GeO<sub>20</sub>

The polynomial roots  $n_3^{(1,2,3,4)}$ , representing eigenvalues, are shown in figure 3 for the cases listed in table 1. Each eigenvalue  $n_3$  has its own eigenvector  $\{U_2^0, \varphi^0\}$  in equation (23) shown in figure 4. Figure 3a compares eigenvalues for cases 1 and 3 listed in table 1. It is clearly seen that the eigenvalues for direction [100] are completely imaginary or real, while they can be complex for direction [101]. As the result, the eigenvectors corresponding to direction [100] are completely imaginary or real, but they can be complex for direction [101] as shown in figure 4a.

Also, it is clearly seen in figure 3 that absolute values of all  $n_3$  imaginary parts begin to decrease with increase in  $V_{ph}$  starting at  $V_{ph} = 0$ . It is well-known that the SAW penetration depth depends on values of  $\text{Im}(n_3)$ . For comparison, purely imaginary roots for cases 2, 4, 6, and 8 listed in table 1 cannot exist that is clearly seen in figure 3b. That statement can be significant in order to choose crystal cuts for

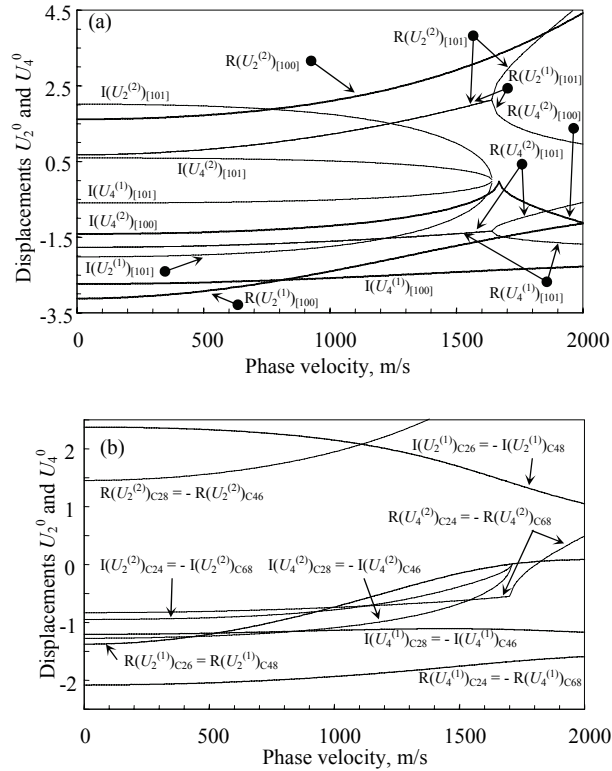
finding SAWs. Each eigenvalue  $n_3$  shown in figure 3b possesses its own eigenvector, of which the real and imaginary parts are drawn in figure 4b.

Further analyzing the roots for propagation direction [101] in equations (27) and (28), it can be found that all complex roots can be calculated, when sign of the expression under square root in equation (27) is negative. This fulfills for velocities  $V_{ph}$  being lower some velocity  $V_{ph0}$  obtained solving the following equation:

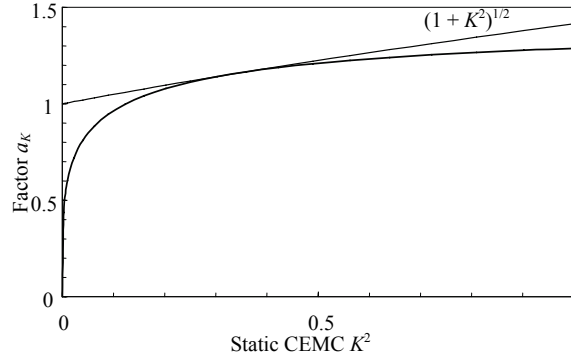
$$B^2 - 16K^2(1 + K^2) = 0 \quad (29)$$

The velocity  $V_{ph0}$  is defined by the following formula:

$$V_{ph0} = a_K V_{t4} \quad \text{with} \quad a_K = 2\sqrt{K\sqrt{1+K^2} - K^2} \quad (30)$$



**Figure 4.** The behavior of the eigenvector  $\{U_2^0, U_4^0 = \varphi^0\}$ : (a) propagation directions [100] (bold lines) and [101] (thin lines) for  $\text{Bi}_{12}\text{GeO}_{20}$ ; (b) cases 2, 4, 6, and 8 with the corresponding subscripts such as “C26”, etc., for  $\text{Bi}_{12}\text{GeO}_{20}$



**Figure 5.** The dependence of the non-dimensional factor  $a_K$  on the non-dimensional value of static CEMC  $K^2$ . The function  $(1 + K^2)^{1/2}$  is shown for comparison

It is clearly seen in equation (30) that the factor  $a_K$  is a function of the CEMC  $K^2$  shown in figure 5 together with the other function  $f(K^2) = (1 + K^2)^{1/2}$  from equation (25). It is clearly seen in figure 5 that about  $K_0^2 = 1/3$  the function  $a_K(K^2)$  approaches the function  $f(K^2) = (1 + K^2)^{1/2}$  giving the following equality:  $V_{ph0} = V_t$ . Hence, only complex polynomial roots can exist for  $V_{ph} < V_{ph0}$ . The CEMC  $K_0^2 = 1/3$  is readily calculated by substituting the velocity  $V_t$  from equation (25) instead of the  $V_{ph}$  in equation (29). However, the form of polynomial roots depends on the  $K^2$ : for  $K^2 < K_0^2$  there are all imaginary roots for  $V_{ph} > V_{ph0}$ , but a large  $K^2 > K_0^2$  gives real roots for  $V_{ph} > V_{ph0}$ . Note that formula (30) represents the velocity  $V_{ph0}$ , at which the complex roots become completely imaginary for  $K^2 < K_0^2$ . Moreover, the absolute values of all four imaginary roots are equal to each other giving the solution  $V_{ph0}$ . Indeed, two equal negative imaginary roots give the same set of eigenvector components. As a consequence, the boundary-condition determinant written in the following section will become equal to zero. Note that only complex/imaginary roots with negative imaginary parts are chosen in order to have wave damping towards depth of a crystal corresponding to negative values of the  $x_3$ -axis shown in figure 1. For comparison, table 2 lists characteristics for some weak piezoelectrics with the cubic symmetry.

**Table 2.** The characteristics of piezoelectric cubic crystals of class  $\bar{4}3m$ . The material constants  $C_{44}$ ,  $e_{14}$ ,  $\epsilon_{11}$ , and  $\rho$  are written here following those in Ref. [25]. The velocity  $V_{ph0} = a_K V_{t4}$  was calculated using equation (30) for propagation direction [101]. The used ZnTe dielectric constant  $\epsilon_{11}$  was announced in Ref. [26]. Noted that the SAW velocity  $V_{SAW}$  listed in this table for the weak piezoelectrics differs from the Bleustein-Gulyaev wave velocity calculated with the following well-known formula:  $V_{BG} = V_t \{1 - (K^2 / [(1 + K^2) \times (1 + \epsilon_{11} / \epsilon_0)])^2\}^{1/2}$  where  $\epsilon_0 = 0.08854 \times 10^{-10}$  [F/m]. Some of the weak piezoelectrics were also studied in Refs. [39-42]

Crystal	$C_{44}, 10^{10}$ N/m <sup>2</sup>	$e_{14}, C/m^2$	$\epsilon_{11}, 10^{-10}$ F/m	$\rho, kg/m^3$	$K^2, \%$
GaAs	5.940	-0.160	1.107	5316	0.389319
GaP	6.260	-0.100	0.983	4301	0.162507
$\beta$ -ZnS	4.613	0.147	0.735	4091	0.637329
ZnSe	3.920	0.049	0.779	5264	0.078626
InSb	3.040	0.080	1.549	5790	0.135911
ZnTe	3.120	0.0284	0.894	5636	0.028916
Bi <sub>4</sub> (GeO <sub>4</sub> ) <sub>3</sub>	4.360	0.0376	1.417	7120	0.022883
Bi <sub>4</sub> (SiO <sub>4</sub> ) <sub>3</sub>	5.180	0.0830	1.434	6800	0.092742

Crystal	$a_K$	$V_{t4}, m/s$	$V_b, m/s$	$V_{SAW}, m/s$	$V_{ph0}, m/s$
GaAs	0.484246	3342.725669	3349.226288	3349.226145	1618.702294
GaP	0.393547	3815.069424	3818.168042	3818.168010	1501.409546
$\beta$ -ZnS	0.543005	3357.971359	3368.655030	3368.654232	1823.395247
ZnSe	0.330243	2728.884115	2729.956717	2729.956707	901.195778
InSb	0.376999	2291.382067	2292.938660	2292.938653	863.848699
ZnTe	0.258597	2352.836803	2353.176957	2353.176955	608.436933
Bi <sub>4</sub> (GeO <sub>4</sub> ) <sub>3</sub>	0.244132	2474.589967	2474.873085181	2474.873085	604.127170
Bi <sub>4</sub> (SiO <sub>4</sub> ) <sub>3</sub>	0.343746	2760.008525	2761.288076	2761.288069	948.741383

However, it is commonly thought that it is necessary to account the piezoelectric effect only for strong piezoelectric crystals with  $K^2 > 1\%$ . The interesting feature of cubic crystals with a weak piezoelectric effect is a slow velocity  $V_{ph0}$  in equation (30), depending on both  $V_{t4}$  and  $a_K$ . In general, values of the factor  $a_K$  are confined between 0.2 and 0.5 for piezoelectrics of class  $\bar{4}3m$ , and a small value of  $V_{t4}$  (for example,  $V_{t4}(\text{Ti}_3\text{TaS}_4) \sim 687$  m/s and  $V_{t4}(\text{Ti}_3\text{TaSe}_4) \sim 751$  m/s [25]) can give a slow  $V_{ph0}$ . Hence, using the factor  $a_K$  of formula (30) and figure 3, one can examine that the penetration depth in weak piezoelectrics with the cubic symmetry can be comparable with that in stronger ones. Note that the  $V_{ph0}$  for cubic piezoelectrics with  $K^2 < 1/3$  must be experimentally verified, because it has “latent” characteristics. In addition to table 2, the strong piezoelectrics of class 23 have the following CEMCs:  $K^2(\text{Bi}_{12}\text{SiO}_{20}) \sim 0.141$  and  $K^2(\text{Bi}_{12}\text{GeO}_{20}) \sim 0.113$ .

Note that the SAWs cannot be found in cubic crystals with a large  $K^2 > 1/3$  in the  $V_{ph}$ -range:  $V_{ph0} < V_{ph} < V_t$ . That can manifest a strong instability of such piezoelectric crystals concerning SH-SAW propagation. Here, there are all complex roots for  $V_{ph} < V_{ph0}$ , all real roots for  $V_{ph0} < V_{ph} < V_t$ , and one pair of complex conjugated roots with two real roots for  $V_{ph} > V_t$ . It is thought that a large  $K^2$  can be observed in complex compounds, as well as in simple ones including cubic piezoelectrics. For instance, the classic ferroelectric  $\text{PbTiO}_3$  has been known to have a single ferroelectric tetragonal (T) to paraelectric cubic phase transition with increased temperature or pressure. Results of Ref. [27] studying  $\text{PbTiO}_3$  discuss an unexpected tetragonal-to-monoclinic-to-rhombohedral-to-cubic phase transition sequence induced by hydrostatic pressure and a morphotropic phase boundary in a pure compound. In the transition regions,  $\text{PbTiO}_3$  can possess huge dielectric and piezoelectric coupling constants similar to those observed in the new complex single-crystal solid-solution piezoelectrics  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - $\text{PbTiO}_3$  (PMN-PT) and  $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - $\text{PbTiO}_3$  (PZN-PT) which are expected to revolutionize electromechanical applications. The complex piezoelectrics, for instance, the most widely used piezoelectric material  $\text{PbZrO}_3$ - $\text{PbTiO}_3$  (PZT), being ubiquitous in modern technology, have piezoelectric coefficients an order of magnitude larger than

those of conventional ferroelectric simple compounds [28]. In addition, Ref. [27] suggests that the giant piezoelectric effect can be studied in simple systems, because this effect as well as the morphotropic phase boundary effect does not require intrinsic disorder.





### CHAPTER III. Boundary Conditions for SH-waves in Monocrystals

Boundary conditions studying SH-waves in monocrystals ( $h = 0$  in figure 1) are based on several requirements which must be satisfied. There is the single mechanical boundary condition on the normal component of the stress tensor  $\tau_{32}$  at  $x_3 = 0$  ( $\tau_{32} = 0$ ) where

$$\tau_{32} = \sum_{p=1,2} F^{(p)} [C_{44}k_3^{(p)}U_2^{(p)} + (e_{14}k_1 + e_{34}k_3^{(p)})\phi^{(p)}] \quad (31)$$

There are two electrical boundary conditions: continuity of the normal component  $D_3$  of the electrical displacements at  $x_3 = 0$ , namely at the interface between a vacuum ( $D_3^f$ ) and the crystal surface, where

$$D_3 = \sum_{p=1,2} F^{(p)} [(e_{36}k_1 + e_{34}k_3^{(p)})U_2^{(p)} - \varepsilon_{33}k_3^{(p)}\phi^{(p)}] \\ D_3^f = -F^{(0)}\phi_0^f jk_1\varepsilon_0 \quad (32)$$

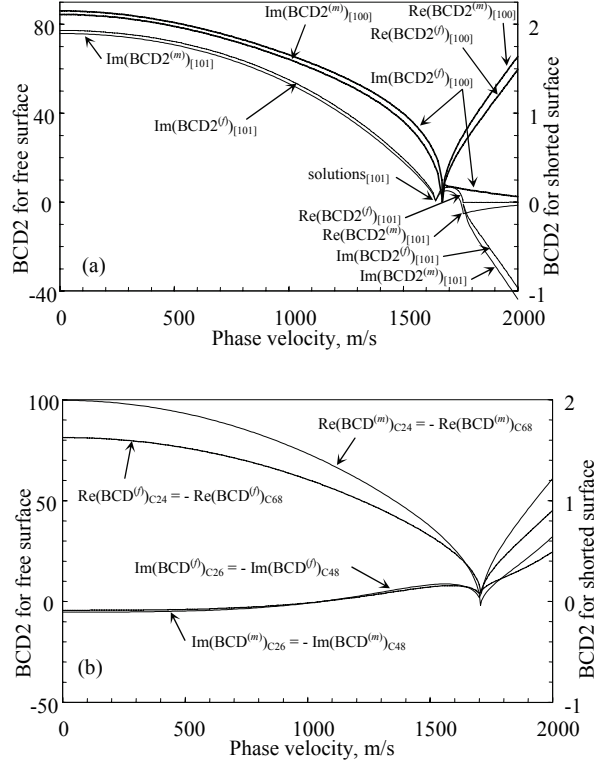
and continuity of the electrical potential  $\phi$  at  $x_3 = 0$  ( $\phi = \phi^f$ ) where

$$\phi = \sum_{p=1,2} F^{(p)}\phi^{(p)} \quad \text{and} \quad \phi^f = F^{(0)}\phi_0^f \quad (33)$$

Therefore, the third-order boundary-condition determinant (BCD3) of a matrix can be readily formed from equations (31) – (33), using the weight functions  $F^{(0)}$ ,  $F^{(1)}$ , and  $F^{(2)}$  as unknown factors. It is noted that BCD3 can be readily reduced to BCD2 for finding the  $V_{ph}$ , because values of the electrical potential  $\phi$  and the electrical displacement component  $D_3$  can be taken to be not independent, for example, see Refs. [6, 7, 29]. Once  $\phi$  is given, a fixed value of  $D_3$  is also given. Therefore, two

electrical boundary conditions (32) and (33) at the free surface can be written as follows:

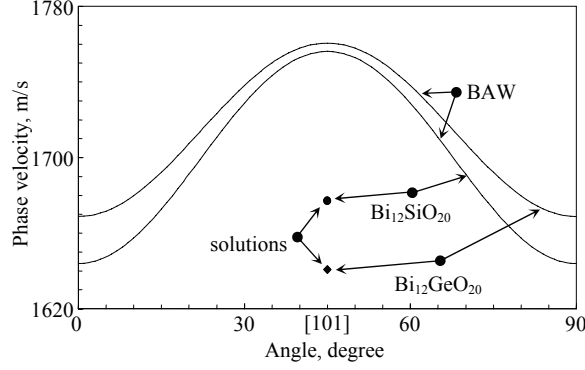
$$D_3 = \sum_{p=1,2} F^{(p)} [(e_{36}k_1 + e_{34}k_3^{(p)})U_2^{(p)} - (\varepsilon_{33}k_3^{(p)} - jk_1\varepsilon_0)\phi^{(p)}] \quad (34)$$



**Figure 6.** The behavior of the non-dimensional value of determinant BCD2 using the material constants of  $\text{Bi}_{12}\text{GeO}_{20}$ : (a) propagation directions [100] and [101] of cases 1 and 3 listed in table 1; (b) cases 2, 4, 6, and 8 of table 1. Different electrical boundary conditions of free surface (see “ $f$ ”) and surface metallization (“ $m$ ”) are shown

Figure 6 shows behavior of the determinants corresponding to the cases listed in table 1 for different electrical boundary conditions of free surface and surface metallization. Figure 6a compares the BCD2 behavior of cases 1, 3, and relevant listed in table 1 with more complicated cases 2, 4, 6, and 8 shown in figure 6b. It is clearly seen that the BCD2 for direction [101] equals to zero at the velocity  $V_{ph0}$ . Figure 7 shows the velocity  $V_t$  of the bulk acoustic wave (BAW) using different

crystal cuts for both  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{GeO}_{20}$  as well as the found solutions  $V_{ph0}$  in direction [101].



**Figure 7.** The speeds  $V_t$  of the bulk SH-waves in dependence on the propagation directions from [100] to [001] for cubic piezoelectric crystals  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{GeO}_{20}$

The complete mechanical displacement  $U_2^\Sigma$  and electrical potential  $\varphi^\Sigma$  are written in the plane wave form as follows, using suitable eigenvalues and eigenvectors of obtained  $V_{ph}$ :

$$\begin{aligned}
 U_2^\Sigma &= \sum_{p=1,2} F^{(p)} U_2^{0(p)} \exp[jk(n_1 x_1 + n_3^{(p)} x_3 - V_{ph} t)] \\
 \varphi^\Sigma &= \sum_{p=1,2} F^{(p)} \varphi^{0(p)} \exp[jk(n_1 x_1 + n_3^{(p)} x_3 - V_{ph} t)] \quad (35)
 \end{aligned}$$

The weight functions  $F^{(1)}$  and  $F^{(2)}$  are readily determined from equation (34) and show the following relationship:

$$F^{(1)} = -F^{(2)} \quad (36)$$

because two equal eigenvalues  $n_3^{(1)} = n_3^{(2)}$  give the same eigenvectors  $\{U_2^{0(1)}, \varphi^{0(1)}\}$  and  $\{U_2^{0(2)}, \varphi^{0(2)}\}$ .

It is obvious that the weight factors  $F^{(1)} = -F^{(2)}$  in equation (36) will zero the complete mechanical displacement  $U_2^\Sigma$  and electrical potential  $\varphi^\Sigma$  in equation (35). That means that the  $V_{ph0}$  solution in equation (30) is always obtained and represents a “latent” possibility concerning SAW existence in piezoelectric cubic monocrystals, supplementing the opinion of Gulyaev written in Ref. [10]. Hence, there is a possibility to change boundary conditions that can be achieved by a mass loading in order to apply some additional perturbation to the surface of a cubic crystal for finding SAWs. Therefore, the following sections relate to studying dispersive SAWs in various layered structures consisting of cubic piezoelectrics.

## CHAPTER IV. Boundary Conditions for SH-waves in Layered Systems

Mass loading such as with a thin film on the free surface of a monocrystal significantly complicates the problem of finding SAWs, and one deals here with the layered system shown in figure 1. Therefore, boundary conditions for SH-waves must be written for two sides of the layer: the layer-substrate interface at  $x_3 = 0$  (see figure 1) and the layer-vacuum interface at  $x_3 = h$ . It is obvious that equality of the mechanical displacements  $U_2$  along the  $x_2$ -axis must be at  $x_3 = 0$  ( $U_2^S = U_2^L$ ) where

$$U_2^S = \sum_{S(p)} F^{S(p)} U_2^{S(p)} \quad \text{and} \quad U_2^L = \sum_{L(p)} F^{L(p)} U_2^{L(p)} \quad (37)$$

Here the superscripts  $S$  and  $L$  are for the substrate and layer, respectively. The second condition on the stress tensor normal component  $\tau_{32}$  at  $x_3 = 0$  requires continuity resulting in  $\tau_{32}^S = \tau_{32}^L$ , where

$$\begin{aligned} \tau_{32}^S &= \sum_{S(p)} F^{S(p)} \left[ C_{44}^S k_3^{S(p)} U_2^{S(p)} + (e_{14}^S k_1 + e_{34}^S k_3^{S(p)}) \phi^{S(p)} \right] \\ \tau_{32}^L &= \sum_{L(p)} F^{L(p)} \left[ C_{44}^L k_3^{L(p)} U_2^{L(p)} + (e_{14}^L k_1 + e_{34}^L k_3^{L(p)}) \phi^{L(p)} \right] \end{aligned} \quad (38)$$

Two electrical boundary conditions at  $x_3 = 0$  require continuity of the normal component  $D_3$  of the electrical displacements ( $D_3^S = D_3^L$ ) where

$$\begin{aligned} D_3^S &= \sum_{S(p)} F^{S(p)} \left[ (e_{36}^S k_1 + e_{34}^S k_3^{S(p)}) U_2^{S(p)} - \epsilon_{33}^S k_3^{S(p)} \phi^{S(p)} \right] \\ D_3^L &= \sum_{L(p)} F^{L(p)} \left[ (e_{36}^L k_1 + e_{34}^L k_3^{L(p)}) U_2^{L(p)} - \epsilon_{33}^L k_3^{L(p)} \phi^{L(p)} \right] \end{aligned} \quad (39)$$

as well as continuity of the electrical potential ( $\phi^S = \phi^L$ ) where

$$\phi^S = \sum_{S(p)} F^{S(p)} \phi^{S(p)} \quad \text{and} \quad \phi^L = \sum_{L(p)} F^{L(p)} \phi^{L(p)} \quad (40)$$

At the free surface  $x_3 = h$  there is a single mechanical boundary condition  $\tau_{31}^L = 0$ , where

$$\tau_{32}^L = \sum_{L(p)} F^{L(p)} \left[ C_{44}^L k_3^{L(p)} U_2^{L(p)} + (e_{14}^L k_1 + e_{34}^L k_3^{L(p)}) \phi^{L(p)} \right] \times \exp(jk_3^{L(p)} h) \quad (41)$$

as well as one electrical boundary condition, according to Ref. [29]:

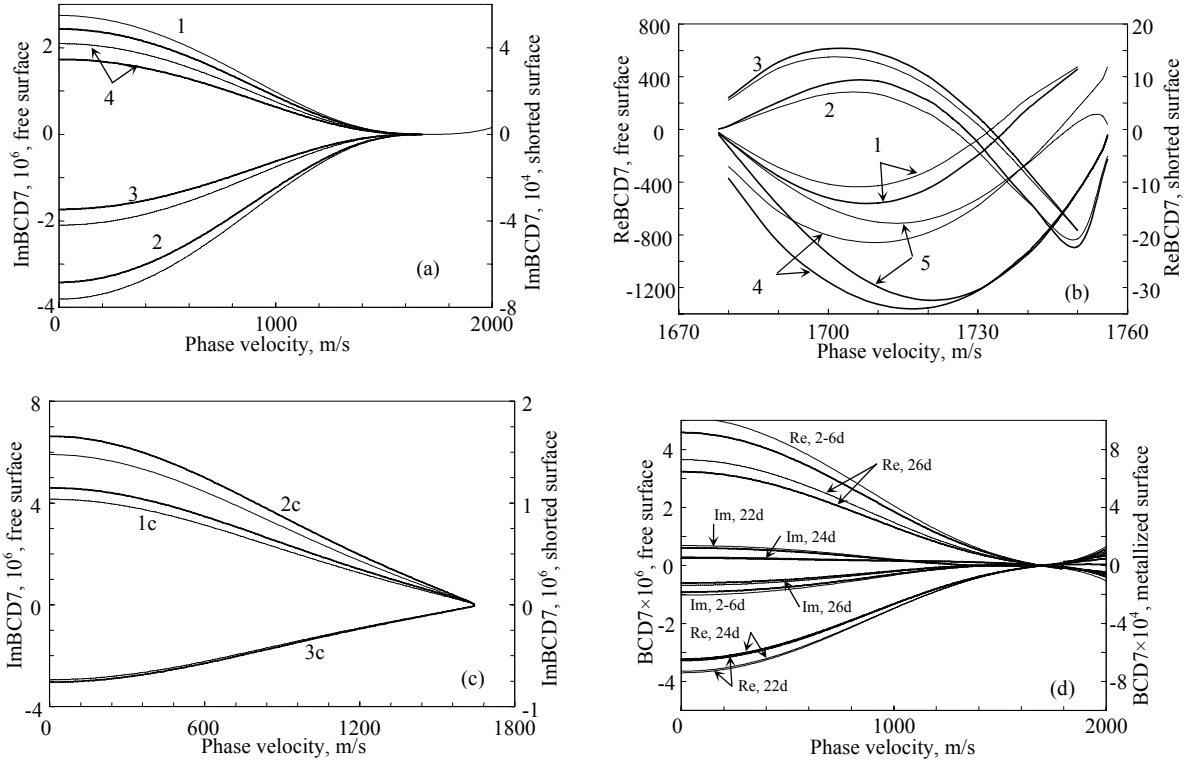
$$D_3^{Lf} = \sum_{L(p)} F^{L(p)} \left[ (e_{36}^L k_1 + e_{34}^L k_3^{L(p)}) U_2^{L(p)} - (\epsilon_{33}^L k_3^{L(p)} - jk_1 \epsilon_0) \phi^{L(p)} \right] \times \exp(jk_3^{L(p)} h) \quad (42)$$

In equations (37) – (42), the index  $p$  runs from 1 to 2 for the substrate and from 1 to 4 for the layer.

The boundary-condition determinant can be readily formed using equations (37) – (42), which will be used for finding SH-SAWs. Such SAWs propagate in the layer by damping towards the substrate depth. Also, SAW propagation in piezoelectrics can be coupled with the electrical potential, which can be found in a vacuum and keeps all information about the propagating SAWs. It is thought that the electrical potential amplitude should decrease in a vacuum from the layer free surface. Accounting all partial displacement components  $F^{S(p)}$  in the substrate and electrical one  $F^{(0)}$  in a vacuum in addition to the components  $F^{L(p)}$  for the layer, the resulting waves will be seven-partial. Therefore, the studied boundary-condition determinant (BCD) will be called below seven-order BCD7.

Structures consisting of a layer on a substrate have an additional parameter such as the layer thickness  $h$  complicating theoretical investigations of wave existence. Therefore, it is natural to choose a constant value of  $h$ . The non-dimensional value of  $kh$  is commonly used, where  $k$  is the wavenumber in wave propagation direction. Various propagation directions and various layered systems are analyzed in figure 8 for the same value of  $kh = 1$ , using the strong piezoelectric cubic crystals  $\text{Bi}_{12}\text{SiO}_{20}$

and  $\text{Bi}_{12}\text{GeO}_{20}$ . Note that the bulk SH-wave speed for  $\text{Bi}_{12}\text{SiO}_{20}$  is lower than that for  $\text{Bi}_{12}\text{GeO}_{20}$ . For instance, in direction [101], they are as follows:  $V_t^S = V_t(\text{Bi}_{12}\text{SiO}_{20}) \sim 1756.104$  m/s and  $V_t^G = V_t(\text{Bi}_{12}\text{GeO}_{20}) \sim 1760.575$  m/s.



**Figure 8.** The comparison of BCD7 behaviors in dependence on the  $V_{ph}$  at  $kh = 1$  for the cases of free surface (thick lines) and surface metallization (thin lines). (a) Propagation direction [101]: “1”, “2”, “3”, “4”, and “5” label the layered systems such as the layer of  $\text{Bi}_{12}\text{SiO}_{20}$ (case 7 in table 1) on the substrate of  $\text{Bi}_{12}\text{GeO}_{20}$ (case 3 in table 1),  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{SiO}_{20}(7)$ ,  $\text{Bi}_{12}\text{GeO}_{20}(3)/\text{Bi}_{12}\text{SiO}_{20}(7)$ ,  $\text{Bi}_{12}\text{GeO}_{20}(3)/\text{Bi}_{12}\text{SiO}_{20}(3)$ , and  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$ , respectively, which are the same for (b) showing  $V_{ph}$ -range  $V_{ph0} < V_{ph} < V_t$  for purely imaginary roots in direction [101]; (c) propagation direction [100] with “1c”, “2c”, and “3c” being for the layered systems  $\text{Bi}_{12}\text{SiO}_{20}(1)/\text{Bi}_{12}\text{GeO}_{20}(5)$ ,  $\text{Bi}_{12}\text{SiO}_{20}(1)/\text{Bi}_{12}\text{SiO}_{20}(5)$ , and  $\text{Bi}_{12}\text{GeO}_{20}(5)/\text{Bi}_{12}\text{SiO}_{20}(1)$ ; (d) combinations of the other cases listed in table 1: “22d”, “24d”, “26d”, and “2-6d” are for the structures  $\text{Bi}_{12}\text{SiO}_{20}(2)/\text{Bi}_{12}\text{GeO}_{20}(2)$ ,  $\text{Bi}_{12}\text{SiO}_{20}(2)/\text{Bi}_{12}\text{GeO}_{20}(4)$ ,  $\text{Bi}_{12}\text{SiO}_{20}(2)/\text{Bi}_{12}\text{GeO}_{20}(6)$ , and  $\text{Bi}_{12}\text{SiO}_{20}(2)/\text{Bi}_{12}\text{SiO}_{20}(6)$



It is possible to suggest that some surface waves can be found possessing the  $V_{ph} < V_t^S$  because  $V_t^S < V_t^G$ . Concerning propagation direction [101] in the layered systems shown in figures 8a and 8b, some solutions of BCD7 can be obtained for different electrical boundary conditions (free surface and surface metallization) only in the  $V_{ph}$ -range:  $V_{ph0} < V_{ph} < V_t^S$ . The solutions correspond to new dispersive SH-SAWs, because surface Bleustein-Gulyaev wave cannot exist in piezoelectric cubic crystals. The interesting case is the layered systems consisting of the  $\text{Bi}_{12}\text{SiO}_{20}$ -layer on the  $\text{Bi}_{12}\text{SiO}_{20}$ -substrate with different polarities (cases 3 and 7 in table 1) in which the new dispersive SH-SAWs can be also found. It is thought that this situation can be found as a defect of crystal growth.

The following section discusses dispersion relations for the new SH-SAWs propagating in direction [101] of various layered structures. It is clearly seen in figures 8a, 8c, and 8d that the BCD7 has large values for small  $V_{ph}$  in all possible layered systems, and possible solutions can be obtained only when the  $V_{ph}$  approaches the speed  $V_t$  of bulk SH-wave. However, any solutions of surface waves were not revealed when the propagation direction corresponds to direction [100] for both the cubic crystals, for which the BCD7 behaviors are shown in figure 8c. The same negative result was obtained for the propagation directions and layered systems shown in figure 8d. Indeed, for the other cases 2, 4, 6, and 8 listed in table 1, the real and imaginary parts of complex BCD7 shown in figure 8d change their sign at different  $V_{ph}$  for all possible structures consisting of the studied cubic crystals. Also, an existence possibility of dispersive SAWs, using propagation directions [101] and [100] for a layer and substrate, respectively, was not verified assuming that these two-layer structures are more complicated. Such investigations can be readily carried out in the future by the same method analyzing BCD7 behaviors, if such problems will be highlighted for possible applications.

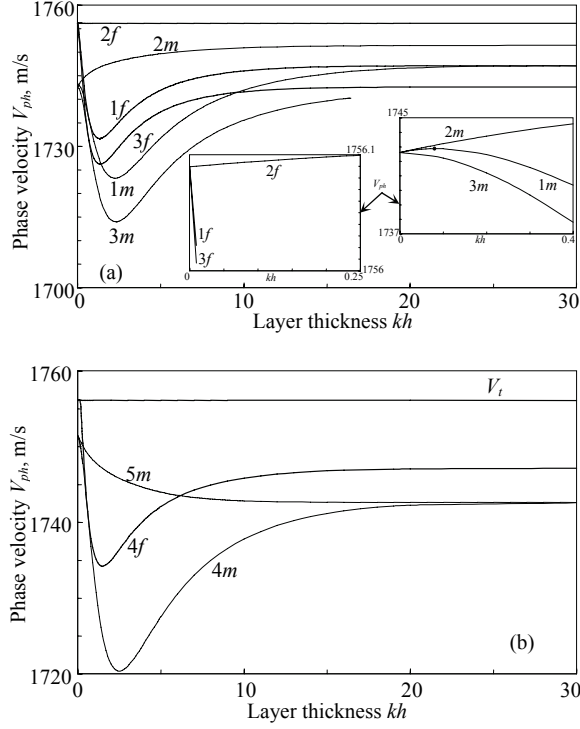
## CHAPTER V. Numerical Results and Discussions

It is thought that dispersion relations representing dependencies  $V_{ph}(kh)$  are the most important characteristic of dispersive waves. It is obvious that the problem of finding of SH-waves in layered systems, using an additional parameter such as the layer thickness  $h$ , is richer concerning possible obtained results. Figure 9 – showing dispersion relations for SH-waves propagating in piezoelectric cubic crystals – supports such statement, because it is thought that the new dispersive SH-SAWs can be observed in an array of various layered systems.

Figure 9a introduces results for several layered systems with the  $\text{Bi}_{12}\text{SiO}_{20}$ -substrate, whereas figure 9b introduces additional results for two possible configurations with the  $\text{Bi}_{12}\text{GeO}_{20}$ -substrate. SH-waves propagate in direction [101] or relevant (see cases 3 and 7 in table 1) for both a layer and substrate in all the cases, using the electrical boundary conditions of free and shorted surfaces to receive more information about the new dispersive waves.

It is clearly seen in figures 9a and 9b that the new SH-SAWs possess the single mode in each case with the following condition for the phase velocity  $V_{ph} < V_t(\text{Bi}_{12}\text{SiO}_{20}) < V_t(\text{Bi}_{12}\text{GeO}_{20})$ . Also, such peculiarities as the non-dispersive Zakharenko waves [30] corresponding to all the extreme points of the phase velocity  $V_{ph}$  versus the non-dimensional value of  $kh$  are clearly seen in figure 9. Therefore, the existence of such type of the non-dispersive waves at these points in suitable layered structures allows utilization of the structures instead of monocrystals in different SAW technical devices. This was also discussed in Ref. [30]. Note that two extreme points of the function  $V_{ph}(kh)$  can be found in figure 9. This is similar to the in-plane-polarized Rayleigh type waves studied in Ref. [31], in which two non-dispersive Zakharenko type waves can be also found.

Using the  $\text{Bi}_{12}\text{SiO}_{20}$ -substrate, the following layered systems in figure 9a can be discussed:



**Figure 9.** The dispersion relations in various layered systems consisting of the cubic crystals  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{GeO}_{20}$ . (a) The  $\text{Bi}_{12}\text{SiO}_{20}$ -substrate was used: “ $1f$ ”, “ $2f$ ”, and “ $3f$ ” are for the case of free surface and the layered systems  $\text{Bi}_{12}\text{GeO}_{20}$ (case 7 in table 1)/ $\text{Bi}_{12}\text{SiO}_{20}$ (case 3 in table 1),  $\text{Bi}_{12}\text{GeO}_{20}$ (3)/ $\text{Bi}_{12}\text{SiO}_{20}$ (3), and  $\text{Bi}_{12}\text{SiO}_{20}$ (7)/ $\text{Bi}_{12}\text{SiO}_{20}$ (3), respectively; “ $1m$ ”, “ $2m$ ”, and “ $3m$ ” are for the case of surface metallization and the corresponding layered systems. The left and right insertions show the mode beginnings with the single point denoting the first non-dispersive Zakharenko wave. (b) The  $\text{Bi}_{12}\text{GeO}_{20}$ -substrate was used: “ $4f$ ” and “ $4m$ ” are for the layered system  $\text{Bi}_{12}\text{SiO}_{20}$ (3)/ $\text{Bi}_{12}\text{GeO}_{20}$ (7), and “ $5m$ ” is for  $\text{Bi}_{12}\text{SiO}_{20}$ (3)/ $\text{Bi}_{12}\text{GeO}_{20}$ (3). The non-dispersive Zakharenko waves correspond to extreme points of the function  $V_{ph}(kh)$

1) The first structure consists of the  $\text{Bi}_{12}\text{GeO}_{20}$ -layer rotated according to case 7 in table 1 on the  $\text{Bi}_{12}\text{SiO}_{20}$ -substrate using case 3 in the table. Here, the  $V_{ph}$  for the free-surface electrical condition starts with the SAW velocity  $V_{ph}^{f0}(\text{Bi}_{12}\text{SiO}_{20}) \sim$

1756.0896 m/s [32, 37]  $< V_t(\text{Bi}_{12}\text{SiO}_{20}) \sim 1756.104$  m/s, comes to the minimum value of  $\sim 1731.650$  m/s at  $kh \sim 1.336$ , and approaches the non-dispersive interfacial-wave velocity  $\sim 1747.138$  m/s [37] for a large value of  $kh$  ( $kh \rightarrow \infty$ ). However, the different  $V_{ph}$ -behavior occurs for the shorted-case mode, which begins with the velocity  $V_{ph}^{m0}(\text{Bi}_{12}\text{SiO}_{20}) \sim 1742.609$  m/s [32, 37] at zero  $kh$  and approaches the same value of  $\sim 1747.138$  m/s [37] for  $kh \rightarrow \infty$ . The  $V_{ph}$  has the maximum value of  $\sim 1742.870$  m/s at small  $kh \sim 0.08$  shown by the point in the right insertion in figure 9a and the minimum value of  $\sim 1723.242$  m/s at  $kh \sim 2.26$ . It is thought that all the  $V_{ph}$  extreme points can be readily found in experiments by a method based on sign evaluation of the derivative  $dV_{ph}/dkh$ . This was also discussed in Ref. [18].

2) For the  $\text{Bi}_{12}\text{GeO}_{20}(3)/\text{Bi}_{12}\text{SiO}_{20}(3)$  structure, the free-surface case  $V_{ph}$  originating with the  $V_{ph}^{f0}$  at zero  $kh$  increases and reaches  $V_t(\text{Bi}_{12}\text{SiO}_{20})$  at  $kh \sim 0.27$ . This is shown in the left insertion in figure 9a. The same qualitative behavior occurs for the shorted-case mode, which originates with the SAW velocity  $V_{ph}^{m0}(\text{Bi}_{12}\text{SiO}_{20}) \sim 1742.609$  m/s [32, 37] at  $kh = 0$  and increases to the SAW velocity  $V_{ph}^{m1}(\text{Bi}_{12}\text{GeO}_{20}) \sim 1751.469$  m/s [32, 37].

3) Probably, the most interesting configuration is  $\text{Bi}_{12}\text{SiO}_{20}(7)/\text{Bi}_{12}\text{SiO}_{20}(3)$ , in which the same material is used for both the layer and substrate applying two possible polarities (possible defect of crystal growth). Indeed, here there occurs the open-surface mode beginning with the velocity  $V_{ph}^{f0}$  at  $kh = 0$ , and the  $V_{ph}$  achieves the velocity  $V_{ph}^{m0}$  for  $kh \rightarrow \infty$ . The minimum  $V_{ph}$  has the value of  $\sim 1726.235$  m/s at  $kh \sim 1.37$ . It is natural that the metallized-surface mode also starts with the velocity  $V_{ph}^{m0}$  at zero  $kh$ . Notwithstanding, it does not return to the  $V_{ph}^{m0}$  interrupting at  $kh \sim 16.379$ . The minimum  $V_{ph}$ -value for this interrupted mode is  $\sim 1713.989$  m/s at  $kh \sim 2.32$ .

The following reverse configurations with the  $\text{Bi}_{12}\text{GeO}_{20}$ -substrate shown in figure 9b can be also analyzed:

4) For the  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  configuration with  $V_t(\text{layer}) < V_t(\text{substrate})$ , the free-surface mode in figure 9b commences with  $V_{ph} = V_t(\text{Bi}_{12}\text{SiO}_{20})$  at  $kh \sim 0.159$ , but not at zero  $kh$ . That gives the “silence”  $kh$ -zone for the waves. With increase in  $kh$ , the  $V_{ph}$  runs through the minimum value of  $\sim 1734.207$  m/s at  $kh \sim 1.49$ . For large values of  $kh > 30$ , the  $V_{ph}$  approaches the interfacial-wave velocity  $\sim 1747.138$  m/s [37] also calculated for the  $\text{Bi}_{12}\text{GeO}_{20}(7)/\text{Bi}_{12}\text{SiO}_{20}(3)$  structure. The shorted-surface mode originates with  $V_{ph}(kh = 0) = V_{ph}^{m1}$  and, going through the minimum value of  $\sim 1720.372$  m/s at  $kh \sim 2.5$ , returns up to the velocity  $V_{ph}^{m0}$  for  $kh \rightarrow \infty$ .

5) A free-surface mode does not exist for the  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$  configuration. However, the single mode for the shorted-surface case begins with the velocity  $V_{ph}^{m1}$  at zero  $kh$  and decreases to the velocity  $V_{ph}^{m0}$  for  $kh \rightarrow \infty$ . Note that the mode behavior is reverse to that for the reverse configuration:  $\text{Bi}_{12}\text{GeO}_{20}(3)/\text{Bi}_{12}\text{SiO}_{20}(3)$ .

It is thought that the  $\text{Bi}_{12}\text{GeO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  structure will have similar dispersion relations obtained for the  $\text{Bi}_{12}\text{GeO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  structure. Concerning the studied different structures, it is obvious that each structure is unique that can be useful in defectoscopy of grown crystals and interface inspection of two-layer structures.

For comparison, Ref. [9] particularly discusses a similar case when the layer and the substrate are identical  $\text{LiNbO}_3$  of class 3 m, except that they are polarized in opposite directions. Here, the phase velocities  $V_{f0}$  and  $V_{s0}$  for the surface electrically free and shorted conditions, respectively, were also obtained when the layer is in the absence of initial stresses. In Ref. [9], dispersive BG-waves were calculated in the layered piezoelectric  $\text{LiNbO}_3$ -structure possessing a single mode. Their results show that for a given value of  $kh$ , the phase velocity of the free-surface case is higher than that of electrically shorted case. Also, in the limit of  $kh \rightarrow 0$  the wave mode tends to the surface BG-wave in a piezoelectric half-space with the phase velocities  $V_{f0} \sim 4538$  m/s for the free-surface case and  $V_{s0} \sim 4203$  m/s for the shorted-surface condition.

With increasing the value of  $kh$  from zero, the velocities  $V_{f0}$  and  $V_{s0}$  rapidly decrease to their minimum  $V_{ph}$ -values corresponding to the non-dispersive Zakharenko type waves. With increasing the value of  $kh$  to 3, the velocities  $V_{f0}$  and  $V_{s0}$  asymptotically tend to 4202 m/s.

The non-dispersive Zakharenko waves [30], representing extreme points of the function  $V_{ph}(kh)$  in dispersion relations for dispersive waves, can be described by the following formulas, using the following formula  $d(u/v)/dx = (vdu/dx - udv/dx)/v^2$  which is well-known as Leibniz's formula:

$$\frac{dV_{ph}}{dkh} = V_g \frac{dV_{ph}}{d\omega h} = 0 \quad (43)$$

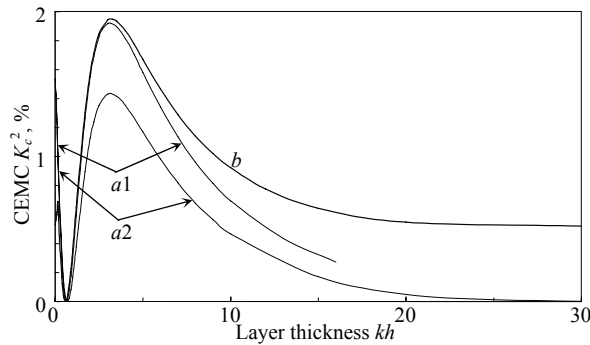
$$\frac{dV_{ph}}{dkh} = \frac{1}{kh} (V_g - V_{ph}) \quad (44)$$

$$\frac{dV_{ph}}{d\omega h} = \frac{V_{ph}}{\omega h} \left( 1 - \frac{V_{ph}}{V_g} \right) \quad (45)$$

The relationship (43) between the  $V_{ph}$ -derivatives shows that there is independence of the  $V_{ph}$  on both the angular frequency  $\omega$  and the wavenumber  $k$  in the same  $k$ - $\omega$ -domain with  $V_g \neq 0$ . The formulas (44) and (45) clarify that formula (43) is satisfied when the phase and group velocities are equal in dispersion relations for the wavenumber  $k \neq 0$  and  $k < \infty$ . It is thought that the case of  $V_g = V_{ph} \rightarrow 0$  ( $V_g = V_{ph} = 0$ ) represents the Bose-Einstein condensation (BEC). It is possible to show that for the BEC near zero, the following relationship  $V_g \sim 2V_{ph}$  ( $V_g = 2V_{ph}$ ) occurs for a free quasi-particle propagating in a vacuum. Therefore, the BEC as dispersive waves can correspond to inflection points of both the  $V_g$  and  $V_{ph}$ .

It is possible to evaluate the coefficient of electromechanical coupling (CEMC)  $K_c^2$  of the new dispersive SH-SAWs for some interesting layered systems, for which the dispersion relations are shown in figure 9. For the  $\text{Bi}_{12}\text{SiO}_{20}(7)/\text{Bi}_{12}\text{SiO}_{20}(3)$  structure with different polarities shown in figure 10, the  $K_c^2$  approaches the maximum value of  $\sim 2\%$  at  $kh \sim 4$  to 5. Note that the  $\text{Bi}_{12}\text{SiO}_{20}(7)/\text{Bi}_{12}\text{SiO}_{20}(3)$  and  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{SiO}_{20}(7)$  structures show the same dispersion relations, and

therefore, the same dependencies  $K_c^2(kh)$ . It is also noted that the  $K_c^2$  is interrupted for the structures at  $K_{c0}^2$  ( $kh_c \sim 16.378$ )  $\sim 0.27\%$  due to the mode interruption at  $kh_c$  for the case of surface metallization. When the  $\text{Bi}_{12}\text{SiO}_{20}$ -layer is substituted by the  $\text{Bi}_{12}\text{GeO}_{20}$ -layer with the same polarity to form the structure  $\text{Bi}_{12}\text{GeO}_{20}(7)/\text{Bi}_{12}\text{SiO}_{20}(3)$  with  $V_t(\text{Bi}_{12}\text{GeO}_{20}) > V_t(\text{Bi}_{12}\text{SiO}_{20})$ , the  $K_c^2$  has the maximum value slightly larger than  $1.43\%$  and smaller than  $K_c^2(kh \rightarrow 0) \sim 1.54\%$ , and approaches zero already at  $kh = 30$ . This can manifest that the new dispersive SH-SAWs at large values of  $kh > 30$  behave as waves propagating in non-piezoelectric crystals with zero  $K_c^2$ . This occurs as soon as the  $V_{ph}$  for the case reaches the interfacial-wave velocity  $V_{in1} \sim 1747.138$  m/s [37] which is unique for the structure. The value of  $V_{in1}$  is significantly larger than both values of  $V_t^{[100]}(\text{Bi}_{12}\text{SiO}_{20}) \sim 1643$  m/s and  $V_t^{[100]}(\text{Bi}_{12}\text{GeO}_{20}) \sim 1668$  m/s. Omitting the piezoelectric effect in the calculations for direction [101], one can also find that  $V_t^{[101]} = V_t^{[100]}$ .



**Figure 10.** The coefficient of electromechanical coupling (CEMC)  $K_c^2$  (%) calculated with formula (46) for the layered systems such as  $\text{Bi}_{12}\text{SiO}_{20}$ (case 7 in table 1)/ $\text{Bi}_{12}\text{SiO}_{20}$ (case 3 in table 1),  $\text{Bi}_{12}\text{GeO}_{20}(7)/\text{Bi}_{12}\text{SiO}_{20}(3)$ , and  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  denoted by “a1”, “a2”, and “b”, respectively

However, treating the reverse configuration to  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$ , namely when the  $\text{Bi}_{12}\text{SiO}_{20}$ -substrate is substituted by the  $\text{Bi}_{12}\text{GeO}_{20}$ -one to form the  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{SiO}_{20}(7)$  structure, the  $K_c^2$  also achieves the maximum value of  $\sim 2\%$  at  $kh \sim 4$  to  $5$ . In this  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  structure in which several modes of Love type waves can also exist from  $kh = 0$  to  $kh = 200$ , the  $K_c^2$  approaches some

relatively small value of 0.5% for a large value of  $kh > 30$  (see figure 10). That indicates some coupling with the electrical potential and can be used in addition to the modes of the Love waves. It is clearly seen in the figure that in these three calculated cases, the  $K_c^2$  equals to zero at  $kh \sim 0.5$  to  $0.7$ .

The CEMC shown in figure 10 was calculated for the single modes of the new dispersive SH-SAWs with the following well-known formula:

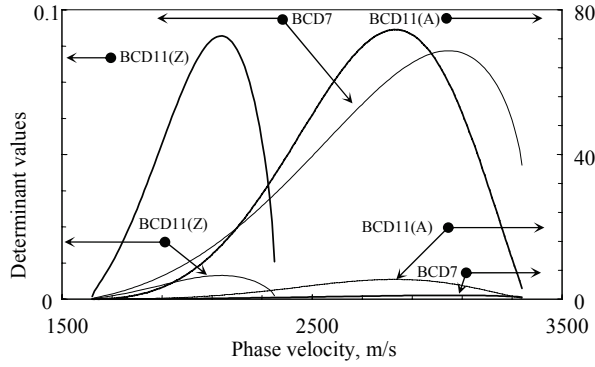
$$K_c^2 = 2 \frac{V_f - V_m}{V_f} \quad (46)$$

where  $V_f$  and  $V_m$  are the velocities for the free and metallized surfaces, respectively. It is noted that the  $K_c^2$  for the other configurations shown in figure 9 was not calculated, because the velocities for the cases of free surface are equal to the speed  $V_t^S = V_t(\text{Bi}_{12}\text{SiO}_{20})$  or are slightly below  $V_t^S$  at small values of  $kh$ . That can mean disappearance of SAW dispersive modes. Note that characteristics of the new non-dispersive SAW propagating in the monocrystals such as  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{SiO}_{20}$  were investigated in Ref. [32].

The layered structures, consisting of piezoelectric cubic crystals GaP and GaAs, can be readily fabricated, for example, see the work [33] on properties of interface and relaxation properties of grown GaP/GaAs structures by chemical beam epitaxy. The production technology of the structures is continuously improved. The crystals are widely used to fabricate multi-layered structures such as photonic crystals and superlattices. It is thought that they are also suitable for study of a possible existence of the new dispersive SAWs propagating in layered structures like GaP/GaAs. Also, it is noted that GaAs is used as a substrate material, for instance, in the layered structure ZnO/GaAs [34], which are currently of a great interest for design of integrated SAW filters. Indeed, GaP can be also used as a substrate material. In addition to thin films made from hexagonal ZnO and cubic ZnS possessing low toxicity and being inexpensive and easily obtained, thin films made from the cubic crystal ZnTe (see table 2) can be also used in layered structures for various



applications. Also, these materials have continuously attracted attention as potentially useful active optoelectronic materials.



**Figure 11.** The  $\text{Re}(\text{BCD11})$  behavior for the multi-layered structures GaAs/GaP/GaAs (see “A”) and ZnTe/GaP/GaAs (see “Z”) in dependence on the  $V_{ph}$ , using both electrical boundary conditions of free surface (thick lines) and surface metallization (thin lines). Here there is  $V_{ph0}(\text{GaP}) < V_{ph} < V_t(\text{GaAs})$  for GaAs/GaP/GaAs and  $V_{ph0}(\text{GaP}) < V_{ph} < V_t(\text{ZnTe})$  for ZnTe/GaP/GaAs (see table 2). The following parameters were set:  $kh = 1$ ,  $h_1/h = 1$  and  $h_2/h = 3$  where  $h_1$  is the layer thickness for the first layer (GaP) and  $h_2$  is the one for the second layer (GaAs or ZnTe). For comparison, the  $\text{Re}(\text{BCD7})$  behavior for the GaP/GaAs structure with  $kh = 1$  is also shown

Therefore, any existence of the new dispersive SAWs was verified in such layered systems as GaP/GaAs, GaAs/GaP, ZnTe/GaAs, and GaAs/ZnTe. It is thought that the new dispersive SAWs cannot be found in such layered systems and in some multi-layered structures (see figure 11) consisting of the weak piezoelectrics. Note that for some layered structures consisting of the weak piezoelectrics listed in table 2, the velocity  $V_{SAW}$  listed in the table is also found for very small values of  $kh \sim 10^{-5}$ . Notwithstanding, these SAW solutions cannot be found already at  $kh \sim 10^{-4}$ . Also, it is possible to investigate the new SAW existence in layered systems consisting of

non-cubic crystals by studying suitable propagation directions, in which the surface Bleustein-Gulyaev waves cannot exist. Ref. [35] discusses some cases when the surface BG-waves cannot exist in crystals of hexagonal class 622 and tetragonal class 422. Therefore, theoretical investigations concerning non-cubic crystals can be reported in the future.



## CHAPTER VI. Love Type Waves

Concerning the existence of the seven-partial Love type waves (LTW7) propagating in the configuration of the  $\text{Bi}_{12}\text{SiO}_{20}$ -layer on the  $\text{Bi}_{12}\text{GeO}_{20}$ -substrate, the LTW7 several modes are shown in figure 12 for two possible cases such as normal polarity for  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$  and different polarity for  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$ , using different electrical boundary conditions. It was found that the first non-shorter-case LTW7-mode for  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$  begins with some velocity  $V_1 \sim 1760.565$  m/s slightly lower than the speed  $V_t(\text{Bi}_{12}\text{GeO}_{20}) \sim 1760.575$  m/s. Note that the velocity difference  $\Delta V = V_t - V_1 \sim 10$  mm/s is significant, because the calculation accuracy was set about  $1 \mu\text{m/s}$ . It is thought that the unshorted-case LTW7-modes for  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  start with the second mode as shown in figure 12, and the first mode looks like it can only start outside the positive values of  $kh$ . This can mean that it does not exist similar to the first shorter-case LTW7-modes for both the  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$  and  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  structures. The beginnings of the all existing modes in the  $kh$ -range  $0 < kh < 200$  are listed in table 3. It is clearly seen in the table that the higher-order mode beginnings for  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$ , starting with the second modes of shorter and non-shorter cases, are shifted towards the smaller values of  $kh$  with the constant  $kh_s$  such as  $kh_s \sim 12$  relative to the corresponding those for  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$ .

It is also obvious, using both figure 12 and table 3, that a shorter-case mode starts at a smaller value of  $kh$  in comparison with a corresponding original  $kh$ -value of non-shorter-case mode providing the usual relationship  $V_{s1}/V_{f1} < 1$ . Here,  $V_{s1}$  and  $V_{f1}$  are the velocities for shorter and non-shorter cases at the same suitable value of  $kh_1$ , at which both modes exist. This indicates that all the LTW7 modes are very sensitive to an external perturbation applied to the free surface, which is widely used for sensor applications. It is also noted that the unusual behavior of the LTW7 lowest-order mode of the shorter case is shown by the empty points in figure 12 for

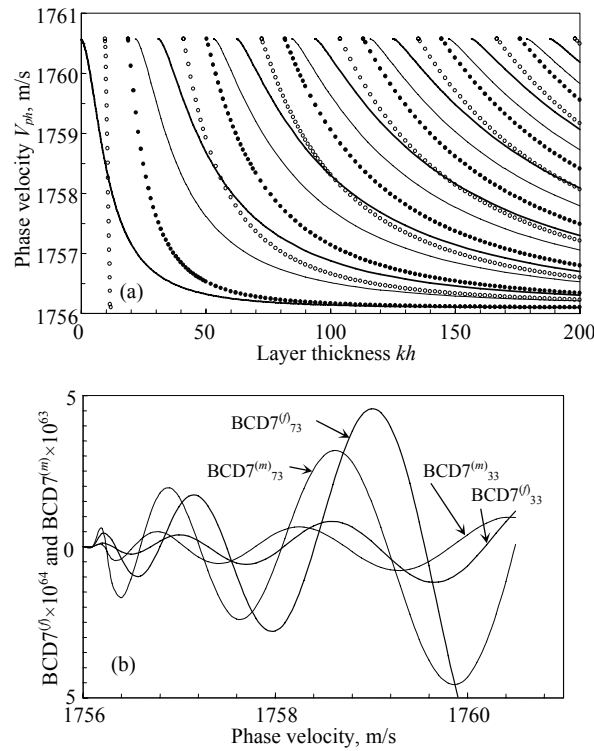
$\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$ . The mode starts with the velocity  $V_t(\text{Bi}_{12}\text{GeO}_{20})$  at some  $kh_0 \sim 9.61$  and achieves the bulk SH-wave velocity  $V_t(\text{Bi}_{12}\text{SiO}_{20})$  already at  $kh \sim 11.7$ .

**Table 3.** The  $kh$ -positions of mode beginning for various layered systems

Mode number	$\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$ , free surface	$\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$ , metallized surface	$\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$ , free surface	$\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$ , metallized surface
1	0.0	-	-	-
2	30.88	21.63	18.88	9.61
3	62.30	53.05	50.30	41.05
4	93.72	84.47	81.72	72.47
5	125.14	115.89	113.14	103.89
6	156.56	147.31	144.56	135.31
7	187.98	178.73	175.98	166.73

It is also possible to discuss that a large  $kh$ -“silence” zone occurs for both the electrical boundary conditions in the  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  structure, see figure 12. It is natural that for very large values of  $kh$ , the first mode of the unshorted case and all the higher-order modes of the treated cases approach the speed  $V_t(\text{Bi}_{12}\text{SiO}_{20}) \sim 1756.104$  m/s. It was also found that each following mode is equally distant from the corresponding previous mode with the  $kh$ -step:  $kh_{s0} \sim 31.42$ , excluding the unusual modes such as the first mode starting at  $kh = 0$  and the shorted-case mode starting at  $kh_0 \sim 9.61$  for the  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  structure listed in table 3. For comparison, the paper [36] by Kessenikh *et al.* discusses LTW7 propagation in layered systems, consisting of an isotropic layer on a transversely-isotropic substrate of classes 6, 4, 6 mm, 4 mm, 622, and 422. In Ref. [36], they introduced the dynamic CEMC  $K_D^2$  depending on the non-dimensional value of  $kh$ . They also discussed the possible cases when the  $K_D^2$  sign is positive or negative, as well as when the  $K_D^2$  sign

is changed at some critical  $kh$  with increase in the value of  $kh$ . Applying their theoretical results to the studied layered systems in this paper, it is possible to discuss that the  $K_D^2$  is different for the  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$  and  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  structures, because the first non-shorter LTW7-mode for  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$  begins with  $V_1 < V_t(\text{Bi}_{12}\text{GeO}_{20})$  and, because there is the  $kh$ -“silence” zone for the LTW7 propagating in the  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  structure. Note that the “silence” zone also occurs for the new SH-SAWs propagating in the  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$  structures.



**Figure 12.** (a) The LTW7 several modes. The thick and thin lines represent the cases of free and metallized surfaces, respectively, for the layered systems consisting of the layer of  $\text{Bi}_{12}\text{SiO}_{20}$  (case 3 in table 1) on the substrate of  $\text{Bi}_{12}\text{GeO}_{20}$  (case 3 in table 1). The filled and empty cycles represent the cases of free and metallized surfaces for  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(7)$ . (b) The boundary-condition determinants (BCD7) at  $kh = 200$ : “ $f$ ” and “ $m$ ” are for the free and metallized surfaces, and “33” and “73” are for the layered systems  $\text{Bi}_{12}\text{SiO}_{20}(3)/\text{Bi}_{12}\text{GeO}_{20}(3)$  and  $\text{Bi}_{12}\text{SiO}_{20}(7)/\text{Bi}_{12}\text{GeO}_{20}(3)$



## CONCLUSION

These theoretical investigations of SH-SAW existence in piezoelectric cubic crystals when the SAWs propagate in direction [101] perpendicular to an even-order symmetry axis of a piezoelectrics demonstrated the following results:

the surface Bleustein-Gulyaev waves cannot exist in piezoelectric cubic monocrystals that confirms Gulyaev's statement recently written in Ref. [10]. Indeed, the new surface SH-waves called the ultrasonic surface Zakharenko waves (USZWs) can propagate in cubic piezoelectrics [32] and cubic piezomagnetics [38], which differ from the surface Bleustein-Gulyaev waves;

the new dispersive SH-SAWs can be found in various layered structures consisting of a layer on a substrate, for instance, in strong piezoelectrics such as  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{GeO}_{20}$ ;

it is thought that such dispersive SH-SAWs cannot be solidly revealed in the layer-on-substrate structures using weakly-piezoelectric cubic crystals such as GaAs, GaP, and ZnTe. The existence of the new SH-SAW was also verified by studying multi-layered structures consisting of the weak piezoelectrics: GaAs/GaP/GaAs and GaAs/GaP/ZnTe.

Also, surface SH-waves propagating in direction [100] were not found studying various layer-on-substrate structures consisting of  $\text{Bi}_{12}\text{SiO}_{20}$  and  $\text{Bi}_{12}\text{GeO}_{20}$ , as well as in the other directions listed in table 1 for both materials. This indicates that propagation direction [101] is unique concerning the new SH-SAW existence, using different electrical boundary conditions of free surface and surface metallization for strong piezoelectric cubic crystals.

The seven-partial Love type wave (LTW7) can also exist in the  $\text{Bi}_{12}\text{SiO}_{20}/\text{Bi}_{12}\text{GeO}_{20}$  layered system with  $V_t(\text{Bi}_{12}\text{GeO}_{20}) > V_t(\text{Bi}_{12}\text{SiO}_{20})$  and in the same structures with the other possible polarity at the layer-substrate interface. It is thought that the polarity phenomenon as an interfacial defect can be readily distinguished in manufactured layered structures. Also, it was found that the LTW7



mode beginnings for the neighbour modes are equidistant from each other. It was also found that the LTW7 phase velocity is very sensitive to any change in the crystal polarity (different electrical boundary conditions). This can be used for filter and sensor applications.

The theoretical investigations of the two-layer systems described in this work can be also applied to layered systems consisting of cubic piezomagnetics, because piezoelectrics and piezomagnetics can be described in the same way following Ref. [43]. However, the magnetoelectrical effect must be accounted when a piezoelectrics and a piezomagnetics are used to create piezoelectric/piezomagnetic laminated composites. Some works on the subject are cited in Refs. [43-57]. It is also worth noting that the recent book in Ref. [57] acquaints theoreticians and experimentalists with several new shear-horizontal surface acoustic waves (SH-SAWs) in piezoelectromagnetics of class 6 mm.

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