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# Analytical studying the group velocity of three-partial Love (type) waves in both isotropic and anisotropic media

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Impossibility to observe the non-dispersive Zakharenko type waves (ZTW) for the three-partial Love type waves (LTW3) is analytically shown for layered systems consisting of a layer on a substrate, in case either isotropic or anisotropic materials with the anisotropy factor $\alpha_f = (C_{44}C_{66} - C_{46}^2)^{1/2}/C_{44}$. The other solutions of new dispersive waves were also considered in addition to the LTW3-waves. The interesting structures Au/Muscovite and Au/Biotite were numerically investigated concerning the LTW3-waves. Monoclinic crystal Muscovite is likely for substrates with the speed $V_{t4} = (C_{44}/\rho)^{1/2} = 5053$ m/s and $\alpha_f \sim 2.08$ that gives $\beta_M = V_{t4}\alpha_f = 10{,}510$ m/s $\sim V_t^{[100]}$(Diamond) $= 12{,}800$ m/s. Possibility to find supersonic LTW-waves in piezoelectric crystals with $\beta \sim 20{,}000$ m/s is also discussed. Such the $\beta$ will be greater than the speed $V_l \sim 17{,}500$ m/s of the bulk longitudinal wave for Diamond. Also, the first- and second-order derivatives of the group velocity $V_g$, as well as the first-, second- and third-order derivatives of the phase velocity $V_{ph}$ were analytically obtained and shown in dependence on the layer thickness $kh$, where $k$ is the wavenumber in the wave propagation direction. The obtained results of the derivative calculations of the group velocity $V_g$ could be useful for finding inflexion points in dependence of the group delay time $\tau(kh) = L/V_g$ ($L$ is a gone distance) in dispersive delay lines, as well as for production automation of different filter and sensor on dispersive waves.

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## 1. Introduction

Since Love (1911) has discovered the surface acoustical waves polarised perpendicular to the sagittal plane in waveguides consisting of an isotropic layer on an isotropic substrate (figure 1), much work appeared concerning these classical three-partial Love waves (LW3). It is noted that both the $x_1$- and $x_3$-axes in the figure lie in the sagittal plane. Probably, the most famous works are the classical and excellent books (Farnell 1978, Dieulesaint and Royer 1980). The classical LW3-waves can propagate in layered systems consisting of both isotropic materials, as well as in crystals in the so-called highly-symmetric propagation directions. For crystals with monoclinic symmetries such as the point group symmetries $m$, 2, $2/m$, the waves will be the LTW3-waves with the elastic anisotropy factor (Maerfeld and Lardat 1969, Lardat *et al.* 1971) $\alpha_f = (C_{44}C_{66} - C_{46}^2)^{1/2}/C_{44}$. There can be $\alpha_f = 1$ for both

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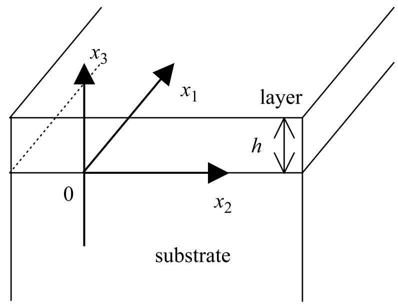


Figure 1. The layered system consisting of a layer on a substrate with the coordinate system.

isotropic materials and cubic crystals, and $\alpha_f = (C_{66}/C_{44})^{1/2}$ for most of the crystal symmetries, such as orthorhombic, tetragonal, trigonal and hexagonal. In the highly-symmetric directions, the LTW3-waves can propagate in structures, if the sagittal plane is perpendicular to an odd-order symmetry axis (Lardat *et al.* 1971, Farnell and Adler 1972, Farnell 1978).

Acoustic waves, such as dispersive Love type waves, are promising for sensors. When liquids come into contact with the propagating medium, there can be a dramatic loss reduction for appropriately rotated crystal cuts, allowing the shear-horizontal surface acoustic waves (SH-SAW) sensor to operate as a biosensor. Biosensors detect chemicals similar to chemical vapor sensors, but in liquids rather than vapor. Biosensors have already been fabricated using the SH-SAW sensors. Of all the known acoustic sensors for liquid sensing, sensors on the Love type waves has the highest sensitivity, according to Kovacs and Venema (1992). For instance, successful detection of anti-goat IgG using a SH-SAW with a polymer Love wave guide coating have been achieved in Gizeli *et al.* (1997), and a quartz Love wave sensor has been demonstrated as an ice sensor in Vellekoop and Jakoby (1999), see also Grate *et al.* (1993). The most popular crystal cuts and orientations for different applications are reviewed in Morgan (1991). For the other instance, different technical devices for signal processing can work on dispersive Love type waves, such as dispersive delay lines (Lardat *et al.* 1971). Therefore, investigation of group (phase) velocity of different dispersive waves must be useful.

The aim of the present theoretical work is to do investigations of the phase velocity $V_{\mathrm{ph}}$ of the LTW3-waves with the elastic anisotropy factor $\alpha_f$ and, therefore, of the group velocity $V_{\mathrm{g}}$ of the dispersive LTW3-waves for delay lines and sensors application that is still not done. This can be also useful for further investigations of the phase and group velocities of both the LTW7-waves, considering the piezoelectric effect, and the LTW5-waves in the layered systems consisting of two layers on a substrate. Bi-layer/substrate structures are more reach, in which, possibly, the non-dispersive five-partial Zakharenko type waves (ZTW5) can propagate within a dispersive mode of five-partial Love type waves (LTW5). The wave phenomenon called as the non-dispersive ZTW-waves can exist in many structures (Zakharenko 2005), where dispersive waves can propagate, and can be mathematically defined by the following formulas: $\mathrm{d}V_{\mathrm{ph}}/\mathrm{d}k = V_{\mathrm{g}}(\mathrm{d}V_{\mathrm{ph}}/\mathrm{d}\omega) = 0$, $\mathrm{d}V_{\mathrm{ph}}/\mathrm{d}k = (V_{\mathrm{g}} - V_{\mathrm{ph}})/k$ and $\mathrm{d}V_{\mathrm{ph}}/\mathrm{d}\omega = V_{\mathrm{ph}}(1 - V_{\mathrm{ph}}/V_{\mathrm{g}})/\omega$, where $V_{\mathrm{g}}$, $\omega$ and $k$ are the group velocity, angular frequency and wavenumber, respectively. The first relationship between the phase velocity derivatives shows that there is independence of the phase velocity $V_{\mathrm{ph}}$ on both the angular frequency $\omega$ and the wavenumber $k$. It is noted that dispersive waves are defined as dependence of the phase velocity $V_{\mathrm{ph}}$ on both the frequency $\omega$ and wavenumber $k$. It is also noted that the group velocity $V_{\mathrm{g}}$ cannot be equal to zero. The second and third formulae give clearance about where the situation $\mathrm{d}V_{\mathrm{ph}}/\mathrm{d}k = V_{\mathrm{g}}(\mathrm{d}V_{\mathrm{ph}}/\mathrm{d}\omega) = 0$ occurs. This occurs when the phase and group velocities are equal in dispersion relations for the wavenumber $k \neq 0$ ($k > 0$) and $k < \infty$. It is thought that phase (group) velocity investigations of dispersive waves can give more information on ZTW existence nature in each individual case.

The present theoretical investigations can be also useful for automation characterization of different technical devices, such as dispersive wave filters and sensors. The next two sections describe dispersion relations for both surface LTW3 and non-surface waves. Sections 4 and 5 relate to investigation of the LTW3 group velocity and its possible applications, respectively.

## 2. Theory and dispersion relations

The elastic constants, using enthalpy definition $H = E + PV$, where $E$ is the internal energy, and $P$ and $V$ are pressure and volume, respectively, are thermodynamically determined as:

$$C_{ijkl} = \frac{1}{V}\frac{\partial E}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}}, \tag{1}$$

where $\varepsilon_{ij}(\varepsilon_{kl})$ represents the Eulerian strain tensor. For each crystal symmetry there is its own corresponding independent components of the elastic constants tensor $C_{ijkl}$ that is perfectly described in the famous classical work by Nye (1989). The equation of motion in the tensor representation, which corresponds to propagating waves polarized perpendicular to the sagittal plane, results in the following equality:

$$(\mathrm{GL}_{22} - \rho\omega^2)U_2 = 0, \tag{2}$$

where the corresponding component of the Green–Christoffel (GL) tensor for a layer (the index $l$) and for a substrate (the index $s$) is written as:

$$\mathrm{GL}_{22}^{l} = k^2 C_{66}^{l} + \left(k_3^{l}\right)^2 C_{44}^{l} + 2kk_3^{l}C_{46}^{l} = \rho^{l}\omega^2,$$

$$\mathrm{GL}_{22}^{s} = k^2 C_{66}^{s} + \left(k_3^{s}\right)^2 C_{44}^{s} + 2kk_3^{s}C_{46}^{s} = \rho^{s}\omega^2, \tag{3}$$

where there is the following commonly-used equality $k_1^l = k_1^s = k$, as well as the projections $k_3^l$ and $k_3^s$ of the wavevector on the $x_3$-axis in figure 1. There are two roots for the first equation in equation (3):

$$k_3^{l(1,2)} = -\frac{C_{46}^{l}}{C_{44}^{l}}k \pm k_3, \quad \text{with} \quad k_3 = \alpha_f^l k\left[\left(\frac{V_{\mathrm{ph}}}{\beta^l}\right)^2 - 1\right]^{1/2} \quad \text{for} \quad V_{\mathrm{ph}} > \beta^l, \tag{4}$$

but

$$k_3^{l(1,2)} = -\frac{C_{46}^{l}}{C_{44}^{l}}k \pm \mathrm{j}\xi_3, \quad \text{with} \quad \xi_3 = \alpha_f^l k\left[1 - \left(\frac{V_{\mathrm{ph}}}{\beta^l}\right)^2\right]^{1/2} \quad \text{for} \quad V_{\mathrm{ph}} < \beta^l, \tag{5}$$

where $V_{\mathrm{ph}}$ is the phase velocity, $\alpha_f^l = (C_{66}^l C_{44}^l - C_{46}^{l2})^{1/2}/C_{44}^l$ is the elastic anisotropy factor and there is the propagating velocity $\beta^l = V_{t4}^l \alpha_{\mathrm{f}}^l$ with $V_{t4}^l = (C_{44}^l/\rho^l)^{1/2}$; $\mathrm{j} = (-1)^{1/2}$. In some highly-symmetric propagation directions, for example, in [100]-direction for cubic crystals, there is $C_{66} = C_{44}$ resulting in $V_{t4} = V_t$, where $V_t = (C_{66}/\rho)^{1/2}$ represents the speed of the bulk SH-wave. It is noted that the condition $C_{66}C_{44} > C_{46}^2$ is demanded for energy conservation, according to Lardat *et al.* (1971). Therefore, values of $\beta^2$ should be always positive. It was noted in Lardat *et al.* (1971) that there is $\beta < V_t$.

For the second equation in equation (3), the following two roots can be written for the substrate:

$$k_3^{s(1,2)} = -\frac{C_{46}^s}{C_{44}^s} k \pm \mathrm{j}\chi_3 \quad \text{with} \quad \chi_3 = \alpha_f^s k \left[1 - \left(\frac{V_{\mathrm{ph}}}{\beta^{\mathrm{s}}}\right)^2\right]^{1/2} \quad \text{for} \quad V_{\mathrm{ph}} < \beta^s. \tag{6}$$

This general condition for the phase velocity $V_{\mathrm{ph}} < \beta^s$ shows the existence of required positive values of the damping wavenumber $\chi_3$ for surface waves. In isotropic cases there is the following required condition $V_{\mathrm{ph}} < V_t^s$. However, in the case $V_{\mathrm{ph}} > \beta^s$ there are already the following roots:

$$k_3^{s(1,2)} = -\frac{C_{46}^s}{C_{44}^s} k \pm \zeta_3 \quad \text{with} \quad \zeta_3 = \alpha_f^s k \left[\left(\frac{V_{\mathrm{ph}}}{\beta^s}\right)^2 - 1\right]^{1/2} \quad \text{for} \quad V_{\mathrm{ph}} > \beta^s. \tag{7}$$

The boundary conditions (continuity of the corresponding displacement component $U_2$ at the interface between the layer and the substrate, at $x_3 = 0$ shown in figure 1, and continuity of the normal component of the stress tensor $\mathrm{ST}_{22}$ at $x_3 = 0$, as well as $\mathrm{ST}_{22} = 0$ at the free surface $x_3 = h$, where $h$ is the layer thickness) result in the following set of homogeneous equations:

$$\begin{aligned}
&f^s U_2^s - f^{l1} U_2^{l1} - f^{l2} U_2^{l2} = 0,\\
&f^s U_2^s \left[C_{44}^s k_3^s + C_{46}^s k\right] - f^{l1} U_2^{l1} \left[C_{44}^l k_3^{l1} + C_{46}^l k\right] - f^{l2} U_2^{l2} \left[C_{44}^l k_3^{l2} + C_{46}^l k\right] = 0,\\
&f^{l1} U_2^{l1} \left[C_{44}^l k_3^{l1} + C_{46}^l k\right] \exp\left(\mathrm{j}k_3^{l1} h\right) + f^{l2} U_2^{l2} \left[C_{44}^l k_3^{l2} + C_{46}^l k\right] \exp\left(\mathrm{j}k_3^{l2} h\right) = 0.
\end{aligned} \tag{8}$$

There are so-called weight coefficients $f^s$, $f^{l1}$ and $f^{l2}$ in equation (8). Expanding the boundary conditions determinant BCD3 formed from equation (8), the following dispersion relation appears for the case (4):

$$\chi_3 h = a k_3 h \tan(k_3 h) \quad \text{with} \quad a = \frac{C_{44}^l}{C_{44}^s}. \tag{9}$$

The phase velocity $V_{\mathrm{ph}}$ of the LTW3-waves can be readily found from the following functions $\omega(k_3)$ and $k(k_3)$, taking $b = b_1 = [1 - (\beta^l/\beta^s)^2]^{1/2}$:

$$\omega(k_3) = \frac{V_t^l}{b_1} \frac{\alpha_f^l}{\alpha_f^s} \left[k_3^2 \left(\frac{\alpha_f^s}{\alpha_f^l}\right)^2 + \chi_3^2\right]^{1/2};$$

$$k(k_3) = \frac{1}{b_1 \alpha_f^s} \left[k_3^2 \left(\frac{V_t^l}{V_t^s}\right)^2 + \chi_3^2\right]^{1/2}. \tag{10}$$

It is clearly seen in equations (9) and (10) that the LTW3-waves can exist, if the following condition $\beta^l < V_{\mathrm{ph}} < \beta^s$ is full-filled owing to a required real value of $b_1 > 0$. It is noted that the phase ($V_{\mathrm{ph}}$) and group ($V_{\mathrm{g}}$) velocities are defined by the following well-known formulae:

$$V_{\mathrm{ph}} = \frac{\omega}{k} \quad \text{and} \quad V_{\mathrm{g}} = \frac{\mathrm{d}\omega}{\mathrm{d}k}. \tag{11}$$

The phase and group velocities for the LTW3-waves are shown in figure 2(a) for the instance structures, such as Au/Muscovite and Au/Biotite consisting of Au-layer on substrates of Muscovite and Biotite (named for the Biot of French physicist). Figure 2(b) shows the phase velocity (three modes) for the second possible dispersive solutions of equations (9) and (10) giving dispersive waves for negative values of $\tan(k_3 h > 0)$. Two other existence possibilities of dispersive solutions will be discussed in the next section. The LTW3 displacements $U_2$ along the $x_2$-axis in figure 1 for the anisotropic case can be calculated for the layer and substrate with the following formulas:

$$\begin{aligned} U_2 &= U_0 \frac{\cos[k_3(x_3 - h)]}{\cos(k_3 h)} \exp\left[ j\left( k_1 x_1 - \frac{C^l_{46}}{C^l_{44}} k_1 (x_3 - h) - \omega t \right) \right] \quad \text{for} \quad 0 \le x_3 \le +h, \\ U_2 &= U_0 \exp(\chi_3 x_3) \exp\left[ j\left( k_1 x_1 - \frac{C^s_{46}}{C^s_{44}} k_1 x_3 - \omega t \right) \right] \quad \text{for} \quad x_3 \le 0. \end{aligned} \tag{12}$$

It is noted that $U_0$ and $t$ in equation (12) represent the so-called weight coefficient and time, respectively. It is clearly seen that the displacements in equation (12) for anisotropic case have an oscillating term in the exponent argument in both a layer and a substrate for monoclinic crystals with $C_{46} \neq 0$. For the other crystal symmetries, the displacements behave similar to the displacement behavior of the classical LW3-waves in layered system, consisting of isotropic materials. Figure 3 shows the LTW3 displacement behavior for the structure Au/Biotite.

The dispersion relation (9) is likely to both isotropic and anisotropic cases with the elastic anisotropy factor $\alpha_{\mathrm{f}}$, which is included in both the wavenumbers $\chi_3$ and $k_3$. It is clearly seen in the dispersion relation (9) that $+k_3$ and $-k_3$ are equivalent, because positive values of the damping wavenumber $\chi_3$ will be always required for surface waves in the taken coordinate system shown in figure 1 (values of the $x_3$-axis are negative in the substrate). However, there can be $\tan(k_3 h) < 0$ in equation (9), therefore, $\chi_3 < 0$, that does not give wave damping towards depth of the substrate for non-surface dispersive waves.

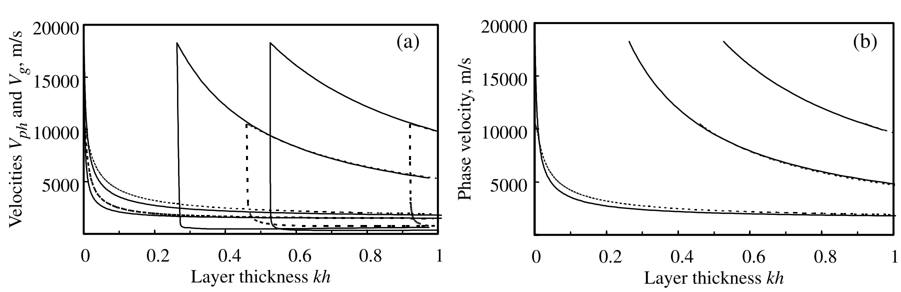


Figure 2. (a) The phase (normal lines) and group (bold) velocities for three modes of dispersive LTW3-waves for the layered systems: Au/Biotite (solid) and Au/Muscovite (dashed); (b) the phase velocity for three modes of dispersive non-surface waves for the layered systems: Au/Biotite (solid lines) and Au/Muscovite (dashed lines).

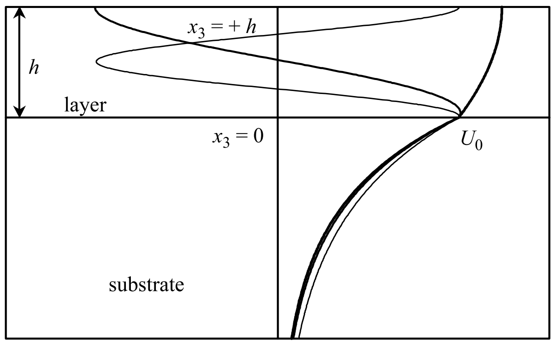


Figure 3. The displacements behaviour for three modes of dispersive LTW3-waves for the layered system Au/Biotite with $h = 1\ \mu$m.

The layered systems studied for the LTW3-waves shown in figure 2(a) were chosen, because Gold possesses the slowest speed $V_t^l$ ~1526 m/s among crystals listed in table 1 and monoclinic crystal Muscovite has the fastest velocity equivalent $\beta_M \sim 10{,}510$ m/s due to a great anisotropy factor $\alpha_f \sim 2.08$. This gives the lowest relationship $\beta^l/\beta^s \sim 0.145$ among the other structures in table 1. It is noted that the velocity $\beta_M$ is only 22% less than the speed $V_t^{[100]} \sim 12{,}800$ m/s of the bulk SH-wave for Diamond. The LTW3 existence condition $V_t^l < V_t^s$ changes into the condition $\beta^l < \beta^s$ for monoclinic materials. It is noted that Muscovite can be characterized as crystal possessing "hexagonal" symmetry in addition to the class $2/m$ of the monoclinic prismatic symmetry, according to Aleksandrov and Prodaivoda (2000). Some promising crystals for Acoustoelectronics, such as Biotite ($K(Mg,Fe)_3 AlSi_3 O_{10} \times (OH,F)_2$) and Phlogopite ($KMg_3 Si_3 AlO_{10} \times (OH,F)_2$), were carefully left in "hexagonal" symmetry in Aleksandrov and Prodaivoda (2000) due to missing of more safety information about the elastic properties of the crystals. However, there are on-line crystallographic data, which give monoclinic symmetry for both Biotite and Phlogopite. It is noted that the presence of the elastic constant $C_{46}$ does not change significantly the anisotropy factor $\alpha_f$, because absolute value of $C_{46}$ is one order less than that of both $C_{44}$ and $C_{66}$. It is noted that there can be $C_{44} \ll C_{66}$ and $C_{44} \gg C_{66}$ (table 1). Hence, even for monoclinic crystals there can be taken $\alpha_f \sim (C_{66}/C_{44})^{1/2}$. Therefore, the following characteristics for Biotite were used in calculations: $V_{t4} \sim 5018$ m/s, $\alpha_f \sim 3.639$ and $\beta \sim 18{,}260$ m/s. And for Phlogopite there are $V_{t4} \sim 5117$ m/s, $\alpha_f \sim 3.618$ and $\beta \sim 18{,}512$ m/s. It is clearly seen that the velocity $\beta$ for both materials is significantly greater than the speed $V_l \sim 17{,}500$ m/s for Diamond. Diamond is used in technical devices in order to operate in GHz-frequency range. However, Diamond is very expensive and does not possess the piezoelectrical effect. Also, suitable layered systems for the classical LW3-waves with $a < 1$ and $a > 1$ are Au/Si, Au/GaAs ($a \sim 0.774$), Ag/GaAs and Cu/GaAs ($a \sim 1.226$) in table 1. Layered systems, such as Ag/Diopsite and Coesite/Jadeite are also suitable for the LTW3-wave existence.

## 3. The other dispersive wave solutions

This section describes possible existence of the other dispersive waves in addition to the dispersive waves (figure 2(b)) discussed in the previous section. They represent new types of

Table 1. Some different materials and layered systems are suggested. Material constants of the cubic crystals were taken from Blistanov *et al.* (1982). Material constants of monoclinic crystals (point group symmetry 2/*m*) were taken from the corresponding references noted in the first column (Aleksandrov *et al.* 2000). In the last column there is $\beta = V_t$ for cubic crystals.

| *Material* | *Density* $\rho$ *(kg/m³)* | $C_{66}$, ($C_{44}$, $C_{46}$), $10^{10}$ *(N/m²)* | $\alpha_f$ | *Velocity,* $V_t$ *and* $\beta$ *(m/s)* | *Layered system (layer/substrate)* | $a = C^l_{44}/C^s_{44}$ | $\beta^l/\beta^s$ |
|---|---|---|---|---|---|---|---|
| GaAs | 5316 | 5.94 | 1.0 | 3343 | Au/Si | 0.578 | 0.261 |
| Si | 2328 | 7.96 | 1.0 | 5847 | Si/GaAs | 1.340 | 1.749 |
| Ge | 5327 | 6.70 | 1.0 | 3547 | Ge/GaAs | 1.128 | 1.061 |
| Au | 19754 | 4.60 | 1.0 | 1526 | Au/GaAs | 0.774 | 0.457 |
| Ag | 10534 | 4.61 | 1.0 | 2092 | Ag/GaAs | 0.774 | 0.626 |
| Cu | 8936 | 7.52 | 1.0 | 2901 | Cu/GaAs | 1.266 | 0.868 |
| Diopside (Levien *et al.* 1979)<br>($CaMgSi_2O_6$) | 3290 | 6.60<br>(7.40, 0.73) | 0.939 | 4479<br>(4207) | Ag/Diopside | 0.623 | 0.497 |
| Jadeite (Kandelin and Weidner 1988)<br>($NaAlSi_2O_6$) | 3330 | 9.40<br>(8.80, 1.30) | 1.023 | 5313<br>(5435) | Coesite/Jadeite | 0.770 | 0.759 |
| Coesite (Weidner and Carleton 1977)<br>($SiO_2$) | 2920 | 5.88<br>(6.78, 1.0) | 0.920 | 4487<br>(4126) | Si/Hedenbergite | 1.174 | 1.417 |
| Hedenbergite (Kandelin and Weidner 1988)<br>($CaFeSi_2O_6$) | 3550 | 6.0<br>(5.50, −1.0) | 1.029 | 4111<br>(4228) | Cu/Muscovite | 4.558 | 0.276 |
| Muscovite (Vaugham 1986)<br>($KAl_2(Si_3Al)O_{10}(OH,F)_2$) | 2820 | 7.20<br>(1.65, −0.32) | 2.080 | 5053<br>(10510) | Au/Muscovite | 2.788 | 0.145 |
| Epidote (Ryzhova *et al.* 1966)<br>($Ca_2(Fe^{+++},Al)_3(SiO_4)_3(OH)$) | 3400 | 7.95<br>(3.91, −0.23) | 1.425 | 4836<br>(6889) | Au/Epidote | 1.177 | 0.222 |

dispersive waves. They exist in the case when the values of the damping wavenumber $\chi_3$ for the substrate are negative. This occurs for the case (5), where there is the following dispersion relation:

$$\chi_3 h = -a\xi_3 h \tanh(\xi_3 h). \tag{13}$$

It is clearly seen in equation (13) that there is $\chi_3 h < 0$, because there is $\tanh(\xi_3 h > 0) > 0$. Therefore, for the case of equations (5), (6) and (13), which represents existence of the other possible solutions of dispersive waves with the polarization, like the one of the LTW3-waves (perpendicular to the sagittal plane), and taking $b = b_1 = [1 - (\beta^l/\beta^s)^2]^{1/2}$ or $b = b_2 = j[(\beta^l/\beta^s)^2 - 1]^{1/2}$, the suitable phase velocities can be calculated from the following dependencies:

$$\omega(\xi_3) = \frac{V_t^l}{b}\frac{\alpha_f^l}{\alpha_f^s}\left[-\xi_3^2\left(\frac{\alpha_f^s}{\alpha_f^l}\right)^2 + \chi_3^2\right]^{1/2}; \quad k(\xi_3) = \frac{1}{b\alpha_f^s}\left[-\xi_3^2\left(\frac{V_t^l}{V_t^s}\right)^2 + \chi_3^2\right]^{1/2}. \tag{14}$$

It is noted that the phase velocity $V_{\text{ph}}$ should be positive real. Therefore, for imaginary values of $b_2$ in equation (14) there should be negative values under square roots.

For the cases (5), (13) and (14) there are two possibilities to find solutions of dispersive waves. The first possibility represents the case $\beta^l < \beta^s$, therefore, there is $b = b_1 = [1 - (\beta^l/\beta^s)^2]^{1/2}$. Here, values under square roots in equation (14) should be positive real, in order to have positive real functions $\omega(\xi_3)$ and $k(\xi_3)$. This gives two inequalities for analyzing:

$$B^2\tanh^2(\xi_3 h) - 1 \geq 0 \quad \text{and} \quad B^2\tanh^2(\xi_3 h) - \left(\frac{\beta^l}{\beta^s}\right)^2 \geq 0 \quad \text{with} \quad B = a\frac{\alpha_f^l}{\alpha_f^s}, \tag{15}$$

from which it is clearly seen that there is as follows: $B\tanh(\xi_3 h) \geq 1$ and $B\tanh(\xi_3 h) \geq \beta^l/\beta^s$. Because $\beta^l < \beta^s$, it is necessary and enough to treat only the first inequality. It is well-known that the hyperbolic tangent is confined between zero and unity for $\xi_3 h > 0$. Finally, the following requirements for solutions existence can be written for such dispersive waves:

$$\beta^l < \beta^s \quad \text{and} \quad B \geq 1. \tag{16}$$

In this case, the phase velocity $V_{\text{ph}}$ starts with its minimum value of $V_{\text{ph}} = 0$ for $\xi_3 h > 0$. It is noted that for $B = 1 + \delta$ with $\delta \to 0$, the phase velocity $V_{\text{ph}}$ will start with $V_{\text{ph}} = 0$ for $\xi_3 h \to +\infty$. Such dispersive solutions exist in the following $\xi_3 h$-, $kh$- and $V_{\text{ph}}$-ranges:

$$\begin{aligned}
&\text{Arctanh}(1/\text{B}) \leq \xi_3 h \leq +\infty;\\
&\frac{1}{b\alpha_f^s}\text{Arctanh}(1/B)\left[-\left(\frac{V_t^l}{V_t^s}\right)^2 + \left(\frac{a}{B}\right)^2\right]^{1/2} \leq kh(\xi_3 h) \leq +\infty;\\
&0 \leq V_{\text{ph}} \leq \beta^l\left[\frac{B^2 - 1}{B^2 - (\beta^l/\beta^s)^2}\right]^{1/2}.
\end{aligned} \tag{17}$$

It is clearly seen in equation (17) that there is the phase velocity $V_{\mathrm{ph}} < \beta^{l}$. It is noted that there is here only single mode of such dispersive waves.

The second possibility represents the case $\beta^{l} > \beta^{s}$, for which there are imaginary values of $b = b_2 = \mathrm{j}[(\beta^{l}/\beta^{s})^2 - 1]^{1/2}$. Therefore, values under square roots in the dispersion relation (14) should be negative real, in order to have positive real values of the functions $\omega(\xi_3)$ and $k(\xi_3)$. Thus, inequality equation (15) can be written as:

$$B^2\tanh^2(\xi_3 h) - 1 \leq 0 \quad \text{and} \quad B^2\tanh^2(\xi_3 h) - \left(\frac{\beta^l}{\beta^s}\right)^2 \leq 0. \tag{18}$$

Inequalities in equation (18) give the following requirements for dispersive waves solutions: $\beta^{l} > \beta^{s}$ and $B\tanh(\xi_3 h) \leq 1$. It is also noted that here there is only single mode of such dispersive waves. It is obvious that the phase velocity $V_{\mathrm{ph}}$ starts with $V_{\mathrm{ph}} = \beta^{s}$ at $\xi_3 h = 0$ and decreases to zero:

$$0 \leq \xi_3 h \leq \mathrm{Arctanh}(1/B);$$

$$0 \leq kh(\xi_3 h) \leq \frac{1}{b\alpha_f^s}\mathrm{Arctanh}(1/B)\left[-\left(\frac{V_t^l}{V_t^s}\right)^2 + \left(\frac{a}{B}\right)^2\right]^{1/2}; \quad \beta^s \geq V_{\mathrm{ph}} \geq 0. \tag{19}$$

The phase velocities for dispersive solutions of the other possible cases of equations (17) and (19) are shown in figure 4(a) and (b), respectively. The insertions in figure 4 show that there can be $\mathrm{j}\omega$ and $\mathrm{j}k$ for the real $V_{\mathrm{ph}}$ giving energy dissipation due to the imaginary frequency, as well as $\mathrm{j}\omega$ and $k$ for the imaginary $V_{\mathrm{ph}}$. The displacements behaviour for the cases (17) and (19) can be found in both layer and substrate as follows:

$$U_2 = U_0\frac{\cosh[\xi_3(x_3 - h)]}{\cosh(\xi_3 h)}\exp\left[\mathrm{j}\left(k_1 x_1 - \frac{C_4^l}{C_{44}^l}k_1(x_3 - h) - \omega t\right)\right] \quad \text{for} \quad 0 \leq x_3 \leq +h,$$

$$U_2 = U_0\exp(-\chi_3 x_3)\exp\left[\mathrm{j}\left(k_1 x_1 - \frac{C_{46}^s}{C_{44}^s}k_1 x_3 - \omega t\right)\right] \quad \text{for} \quad x_3 \leq 0 \quad \text{and} \quad \chi_3 < 0. \tag{20}$$

Layered systems with $a > 1$ and $\beta^{l} < \beta^{s}$ are likely to the other dispersive wave existence of the case (17). For instance, both the LTW3-waves and the other dispersive waves of the case (17) for $B = a\alpha_f^l/\alpha_f^s > 1$ can exist in the structures Cu/Muscovite, Au/Muscovite and Au/Epidote. For dispersive wave existence of the case (19), there is no condition for $a$, which can exist in layered systems with the condition $\beta^{l} > \beta^{s}$ giving impossibility for LTW3-wave existence. For example, the structures Si/Hedenbergite and Si/GaAs studied in figure 4(b) do not give the existence possibility for the LTW3-waves, but they are suitable for the wave existence of the case (19).

It is thought that new dispersive waves shown in figure 4(a) and (b) can be surface waves, if one root in equation (6) with negative imaginary part will be taken for $\chi_3 h < 0$, as well as non-surface waves in the case when one root in equation (6) with positive imaginary part will be taken for $\chi_3 h < 0$. It is noted that for the LTW3-waves, one root in equation (6) with negative imaginary part is taken for $\chi_3 h > 0$. Displacements behaviour for the non-surface waves of the cases (17) and (19) are drown in figure 5. It is noted that the piezoelectrical effect or an additional layer can cause some changes in dispersion relations of the dispersive waves of the cases in equations (17) and (19), like occurs for LTW3-waves. It is also noted that the new dispersive waves become the bulk SH-wave for the substrate at the layer thickness

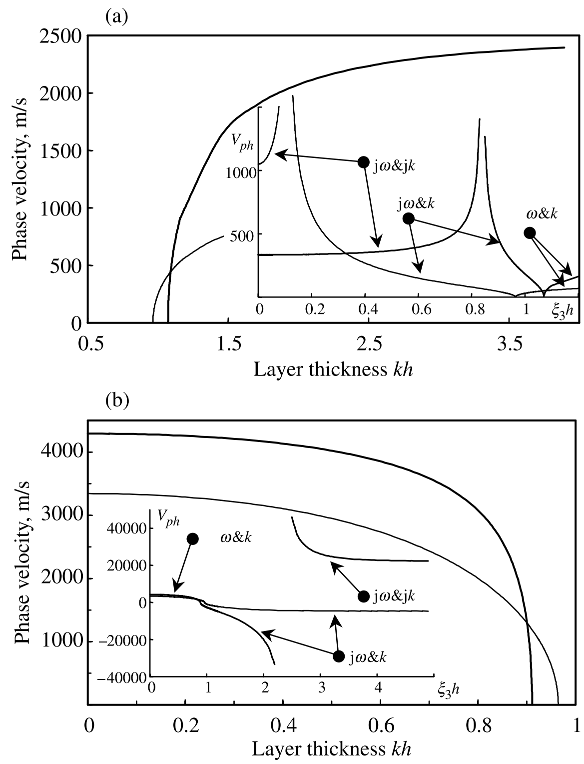


Figure 4. The phase velocity $V_{\mathrm{ph}}$ for the other solutions of dispersive waves for two possible cases: (a) equation (17) for the structures Au/Muscovite (normal line) and Cu/GaAs (bold line); (b) equation (19) for the structures Si/GaAs (normal line) and Si/Hedenbergite (bold line). The corresponding insertions show the dependencies $V_{\mathrm{ph}}(\xi_3 h)$.

$h \to 0$. The same there is for both the surface Bleustein–Gulyaev (BG) wave (Bleustein 1968, Gulyaev 1969) and the LTW3-waves, which become the bulk SH-wave for the piezoelectric constants $e_{ijk} \to 0$ and $h \to 0$, respectively, showing the hybridization between the bulk SH-wave and wave of the electrical potential in the BG wave and the one between two bulk SH-waves of two layers in the LTW3-waves. It is possible that the new dispersive waves will be

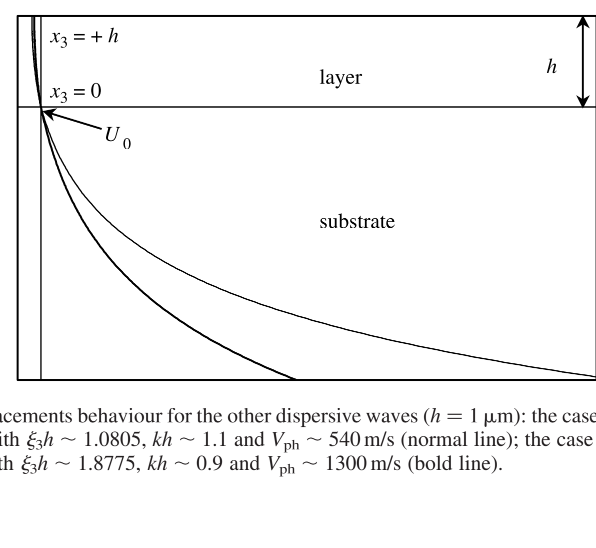


Figure 5. The displacements behaviour for the other dispersive waves ($h = 1$ μm): the case of equation (17) for the structure Cu/GaAs with $\xi_3 h \sim 1.0805$, $kh \sim 1.1$ and $V_{\mathrm{ph}} \sim 540$ m/s (normal line); the case of equation (19) for the structure Si/GaAs with $\xi_3 h \sim 1.8775$, $kh \sim 0.9$ and $V_{\mathrm{ph}} \sim 1300$ m/s (bold line).

also used in dispersive wave technical devices, if they will be studies more widely for this purpose. Therefore, the next section studies only the group velocity of the LTW3-waves, which are widely used in filters and sensors on dispersive waves.

## 4. Investigation of the LTW3 group velocity

The velocities $V_{\mathrm{g}}$ and $V_{\mathrm{ph}}$ are the most important characteristics for different technical devices. There is unique behavior of the group velocity $V_{\mathrm{g}}$ for different dispersive waves, for example, for Love (type) waves. The group velocity of classical Love waves has one extreme point already in layered systems, consisting of an isotropic layer on an isotropic substrate. In addition, some characteristics, such as inflexion points, are also important to be known for filters, such as dispersive delay lines. Finding inflexion points of the group velocity $V_{\mathrm{g}}$ with the well-known techniques “paper-and-pencil” is, probably, inconvenient and imprecise for theoretical study and not suitable for experimental characterization of different devices on dispersive waves. It is also noted that production of different devices on dispersive SAW increases continuously requiring process automation. Therefore, methods for automation characterization of devices on dispersive waves must be developed. Indeed, in addition to piezoelectric materials, non-piezoelectric materials for dispersive wave devices are also used, which can be even more preferable.

The group velocity $V_{\mathrm{g}}$ can be calculated by taking derivatives from equation (10). This gives the following:

$$\frac{\mathrm{d}\omega h}{\mathrm{d}k_3 h} = \left(\frac{\beta^l}{\alpha_f^s b}\right)^2 \frac{1}{\omega h(k_3 h)}\left[k_3 h\left(\frac{\alpha_f^s}{\alpha_f^l}\right)^2 + \chi_3 h\frac{\mathrm{d}\chi_3 h}{\mathrm{d}k_3 h}\right];$$

$$\frac{\mathrm{d}kh}{\mathrm{d}k_3 h} = \left(\frac{1}{\alpha_f^s b}\right)^2 \frac{1}{kh(k_3 h)}\left[k_3 h\left(\frac{V_t^l}{V_t^s}\right)^2 + \chi_3 h\frac{\mathrm{d}\chi_3 h}{\mathrm{d}k_3 h}\right]. \tag{21}$$

In equation (21), there appears the following first-order derivative of the damping wavenumber $\chi_3 h$ for the substrate from the non-dimensional value of the wavenumber $k_3 h$ for the layer:

$$\frac{\mathrm{d}\chi_3 h}{\mathrm{d}k_3 h} = a\left[\tan(k_3 h) + \frac{k_3 h}{\cos^2(k_3 h)}\right]. \tag{22}$$

It is clearly seen that the first-order derivative in equation (22) goes to infinity as $1/\cos^2(x)$ at $k_3 h = n\pi/2$, where $n = 1, 3, 5, \ldots, N$.

The group velocity $V_{\mathrm{g}}$ can be readily obtained from equations (21) and (22):

$$V_{\mathrm{g}} = \frac{\mathrm{d}\omega h}{\mathrm{d}k_3 h}\Big/\frac{\mathrm{d}kh}{\mathrm{d}k_3 h} = \frac{\mathrm{d}\omega}{\mathrm{d}k} \tag{23}$$

and from the well-known formula taken from Zakharenko (2005):

$$V_{\mathrm{g}} = V_{\mathrm{ph}} + kh\frac{\mathrm{d}V_{\mathrm{ph}}}{\mathrm{d}kh}, \tag{24}$$

where the functions $V_{\mathrm{ph}}(kh)$ and $\mathrm{d}V_{\mathrm{ph}}(kh)/\mathrm{d}(kh)$ should be known. The phase and group velocities of the LTW3-waves are shown in figure 2(a). It is clearly seen that the phase velocity $V_{ph}(kh)$ does not have extreme points in the figure. However, the group velocity $V_g(kh)$ has minimum in each mode.

The first-order derivative of the group velocity $dV_g/dkh$ can be found from this expression:

$$\frac{dV_g}{dkh} = \left(\frac{dkh}{dk_3h}\right)^{-2}\left[\frac{d^2\omega h}{d(k_3h)^2} - V_g\frac{d^2kh}{d(k_3h)^2}\right] \tag{25}$$

where the group velocity $V_g$ and the first-order derivative $dkh/dk_3h$ are taken from equations (23) and (21), respectively. Two second-order derivatives in equation (25) are given in the Appendix by formulae (A.1) and (A.2). The first-order derivatives of the phase and group velocities are shown in figure 6 for the structures Au/Muscovite and Au/Biotite, which were calculated with formulae (24) and (25), respectively. It is clearly seen in figure 6 that the first-order derivatives change significantly more rapidly at $kh \to 0$ than the corresponding velocities in figure 2(a) at the same $kh$. This feature can be used for sensitivity improvements of different biological/chemical sensors for sensing smaller amount of chemical elements.

It is noted that it is impossible to observe non-dispersive ZTW in any dispersive mode of the LTW3-waves in both isotropic and anisotropic cases. This is so, because both the frequency $\omega h$ and the wavenumber $kh$ in equation (10) depend on the non-dimensional value of $k_3h$ possessing neither extreme points, except $k_3h = 0, \pi, 2\pi, \ldots$, giving corresponding mode beginning. The first-order derivative $dV_{ph}(kh)/dkh$ shown in figure 6 supports the conclusion of the impossibility existence for the non-dispersive ZTW-waves in any dispersive LTW3 mode. Probably, the non-dispersive ZTW-waves can usually exist in lowest-order modes of different types of dispersive waves, such as dispersive Bleustein–Gulayev (BG) waves (Liu *et al.* 2003) or dispersive Rayleigh type waves (RTW) (Zhang *et al.* 2001, Zakharenko 2005). It is thought that the dispersive BG-waves can be treated as the LTW lowest-order mode representing the LTW first type, which can only exist in piezoelectrics. The higher-order modes of the LTW-waves correspond to the second type. It is also thought that all LTW3 modes relate to the second type. From this view point, a RTW lowest-order mode representing the first type of dispersive RTW waves is usually confined between the non-dispersive RTW wave for a substrate and the one for a layer. However, higher-order modes of the second type of dispersive RTW waves are usually confined

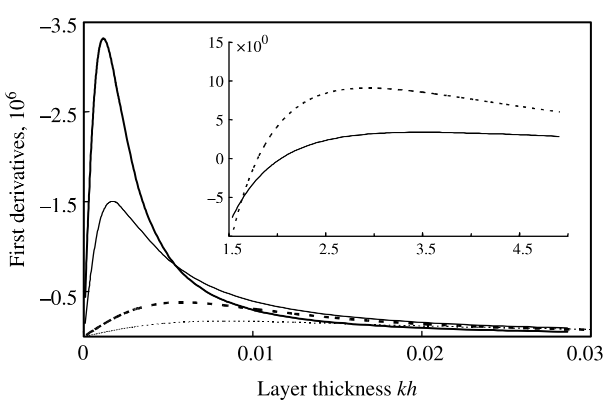


Figure 6. The first-order derivatives of both the phase (normal lines) and group (bold) velocities for the first mode of dispersive LTW3-waves for the structures: Au/Biotite (solid) and Au/Muscovite (dashed). The insertion shows the group velocity derivatives.

between the speed $V_t$ of the corresponding bulk transverse wave for a substrate and the one for a layer. Probably, the non-dispersive ZTW-waves cannot exist in some modes of the second type of dispersive RTW-waves. However, this is not obvious. For example, non-dispersive ZTW-waves can split some higher-order modes of Lamb type waves in anisotropic plates (Solie and Auld 1973, Parygin *et al.* 2000, Anisimkin 2004). Therefore, phase velocity of different types of dispersive waves must be investigated.

The second-order derivatives of the phase and group velocities are shown in figure 7 for the structures Au/Muscovite and Au/Biotite. In order to calculate the second-order derivative of the group velocity $V_g$, the following formula is required:

$$\begin{aligned}\frac{d^2V_g}{d(kh)^2} = &-2\left(\frac{dkh}{dk_3h}\right)^{-4}\frac{d^2kh}{d(k_3h)^2}\left[\frac{d^2\omega h}{d(k_3h)^2} - V_g\frac{d^2kh}{d(k_3h)^2}\right]\\ &+\left(\frac{dkh}{dk_3h}\right)^{-3}\left[\frac{d^3\omega h}{d(k_3h)^3} - \frac{d^2kh}{d(k_3h)^2}\frac{dV_g}{dk_3h} - V_g\frac{d^3kh}{d(k_3h)^3}\right],\end{aligned} \tag{26}$$

where the first-order derivative of the group velocity $dV_g/d(k_3h)$ is given in the Appendix along with the other higher-order derivatives, see formulae (A.3)–(A.6). The second- and third-order derivatives of the phase velocity $V_{ph}$ can be calculated with the following formulae taken from Zakharenko (2005):

$$\frac{d^2V_{ph}}{d(kh)^2} = \frac{1}{kh}\left[\frac{dV_g}{dkh} - 2\frac{dV_{ph}}{dkh}\right]; \tag{27}$$

$$\frac{d^3V_{ph}}{d(kh)^3} = \frac{1}{kh}\left[\frac{d^2V_g}{d(kh)^2} - 3\frac{d^2V_{ph}}{d(kh)^2}\right]. \tag{28}$$

To take the first-, second- and third-order derivatives of the phase velocity $V_{ph}$, as well as the first- and second-order derivatives of the group velocity $V_g$, is enough for many cases, in order to characterize some technical devises, for example, dispersive delay lines and SAW sensors. However, already taking higher-order derivatives of the group velocity $V_g$ even for the classical LW3-waves represents more complicated theoretical investigations, which can

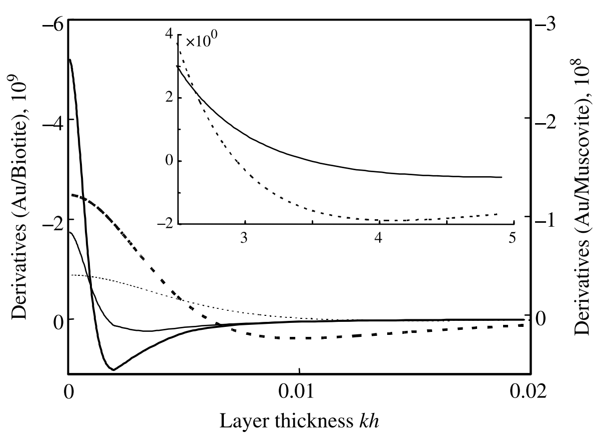


Figure 7. The second-order derivatives of both the phase (normal lines) and group (bold) velocities for the first mode of dispersive LTW3-waves for the structures: Au/Biotite (solid) and Au/Muscovite (dashed). The insertion shows the group velocity derivatives.

be followed in the future in the case of necessity. It is obvious that for the extreme points problem, it is more convenient to deal with the signs " + " and " − " in the corresponding first-order derivatives of the velocities $V_{\mathrm{ph}}$ and $V_{\mathrm{g}}$ rather than to directly calculate or to measure the velocities (figure 8). It is thought that measurements of the first-order derivatives of the velocities could improve measurements of the velocities for weakly-dispersive waves. Also, it is possible in the future to graphically show dependencies of the damping wavenumber $\chi_3 h(k_3 h)$ and its derivative equation (24), as well as the higher-order derivatives (A.2) and (A.6) given in the Appendix, similar to the case of the classical LW3 waves investigated in Dieulesaint and Royer (1980), where the dependence $\chi_3 h(k_3 h)$ was originally shown.

## 5. Delay line applications

The obtained results of calculations of the first- and second-order derivatives of the group velocity $V_{\mathrm{g}}$ could be useful for finding inflexion points in dependence of the group delay time $\tau = L/V_{\mathrm{g}}$ on the non-dimensional value of $kh$ in dispersive delay lines (Lardat *et al.* 1971), around which the time $\tau$ has a linear dependence:

$$\frac{\mathrm{d}\tau}{\mathrm{d}kh} = -\frac{L}{V_{\mathrm{g}}^2}\frac{\mathrm{d}V_{\mathrm{g}}}{\mathrm{d}kh} \quad \text{and} \quad \frac{\mathrm{d}^2\tau}{\mathrm{d}(kh)^2} = 2\frac{L}{V_{\mathrm{g}}^3}\left(\frac{\mathrm{d}V_{\mathrm{g}}}{\mathrm{d}kh}\right)^2 - \frac{L}{V_{\mathrm{g}}^2}\frac{\mathrm{d}^2V_{\mathrm{g}}}{\mathrm{d}(kh)^2}, \tag{29}$$

where $L$ is a gone distance, and $V_{\mathrm{g}}$, $\mathrm{d}V_{\mathrm{g}}/\mathrm{d}kh$ and $\mathrm{d}^2V_{\mathrm{g}}/\mathrm{d}(kh)^2$ are defined by formulas (24), (25) and (26), respectively, calculated in the previous section. Therefore, at the inflexion points, the following condition should be full-filled:

$$\left(\frac{\mathrm{d}V_{\mathrm{g}}}{\mathrm{d}kh}\right)^2 = \frac{V_{\mathrm{g}}}{2}\frac{\mathrm{d}^2V_{\mathrm{g}}}{\mathrm{d}(kh)^2} \tag{30}$$

Figure 9 shows calculations of the inflexion points using the condition (30). As it is shown in the figure, there are two such points for the structure Au/Biotite, which are readily found. Therefore, many acoustic wave characteristics can be readily found by a robot managed by a special software written for this purpose, with which it can characterize dispersive wave filters and sensors.

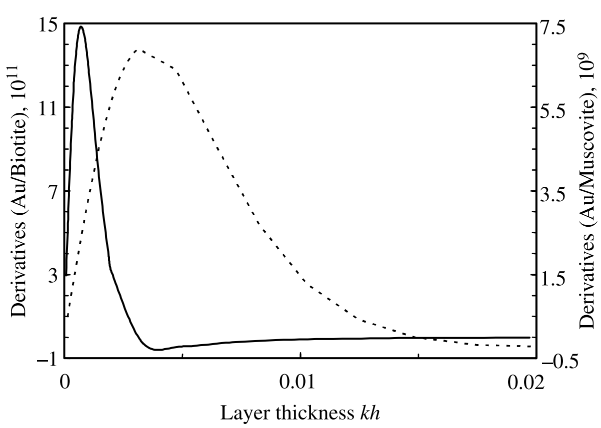


Figure 8. The third-order derivatives of the phase velocity $V_{\mathrm{ph}}$ for the first mode of dispersive LTW3-waves for the layered systems: Au/Biotite (solid line) and Au/Muscovite (dashed line).

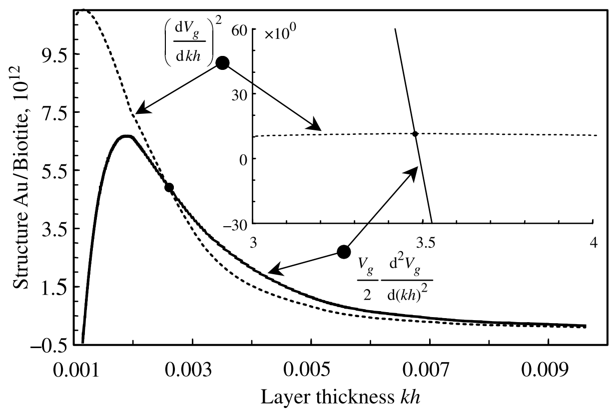


Figure 9. The inflexion points shown by two crossing points from equation (30) for delay line applications on dispersive LTW3-waves for the structure Au/Biotite.

Also, the first- and second-order derivatives of the group velocity $V_g$ from the values of $\omega h$ given in the Appendix by formulae (A.7)–(A.9) can be readily calculated by the same way, because they should be known for some characteristics of different technical devices. It is clearly seen in the Appendix formulae that investigation of the group velocity dependence $V_g(\omega h)$ represents more complicated case than that of the dependence $V_g(kh)$. However, this is more convenient for experimentalists, who work with the dependence $V_g(\omega h)$, but not with the $V_g(kh)$.

## 6. Conclusion

The present theoretical investigations took particularly care of showing existence of different dispersive wave solutions for waves polarized perpendicular to the sagittal plane in layered systems, consisting of a layer on a substrate, including crystal anisotropy. Different possibilities of dispersive wave existence were theoretically treated, one of them represents the LTW3-waves. The other possible solutions for the cases of equations (17) and (19) represent new dispersive waves. Some suitable layered systems for each treated case were listed in the table. As the general purpose, two interesting structures, such as Au/Muscovite and Au/Biotite, were numerically investigated concerning the LTW3-waves. Such layered systems could be convenient for some technical devices, for which there are requirements of a great dispersion and fast propagating velocities. It was found that the propagating velocity $\beta$ of Muscovite is only 22% less than the speed $V_t$(Diamond) $\sim$ 12,800 m/s. It is well-known that Diamond, being very expensive, is all the same used for technical devices in order to work in a GHz-frequency range, see the recent patents (United States Patent 5343107 1994). Hopefully, Muscovite (Biotite, Phlogopite) single crystals will be not expensive compared with Diamond. It is thought that piezoelectric crystals with the $\beta \sim$ 20,000 m/s being greater than the speed $V_l \sim$ 17,500 m/s for Diamond can exist.

Also, in the present theoretical investigations, the delay line characteristics, such as the delay time $\tau = L/V_g$, were instantly studied, because the dependence $\tau(kh)$ possesses a linear behavior around inflexion points. For this purpose, the derivatives $dV_g/dkh$ and $d^2V_g/d(kh)^2$ must be obtained. In order to calculate the derivatives of the group velocity $V_g$, it is necessary to obtain the first-, second- and third-order derivatives of the phase velocity $V_{ph}$ that was also carried out in the present work. It is emphasized that this can be used for all-round automation of filter and sensor production, such as dispersive delay lines or sensors on the LTW-waves. The same investigations of the group velocity can be done for Lamb type waves in the future.

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## Appendix. The derivatives

Two second-order derivatives in equation (25) are given as follows:

$$\frac{\mathrm{d}^2\omega h}{\mathrm{d}(k_3h)^2} = -\frac{1}{\omega h}\left\{\left(\frac{\mathrm{d}\omega h}{\mathrm{d}k_3h}\right)^2 - \left(\frac{\beta^l}{\alpha_f^s b}\right)^2\left[\left(\frac{\alpha_f^s}{\alpha_f^l}\right)^2 + \left(\frac{\mathrm{d}\chi_3h}{\mathrm{d}k_3h}\right)^2 + \chi_3h\frac{\mathrm{d}^2\chi_3h}{\mathrm{d}(k_3h)^2}\right]\right\};$$
$$\frac{\mathrm{d}^2kh}{\mathrm{d}(k_3h)^2} = -\frac{1}{kh}\left\{\left(\frac{\mathrm{d}kh}{\mathrm{d}k_3h}\right)^2 - \left(\frac{1}{\alpha_f^s b}\right)^2\left[\left(\frac{V_t^l}{V_t^s}\right)^2 + \left(\frac{\mathrm{d}\chi_3h}{\mathrm{d}k_3h}\right)^2 + \chi_3h\frac{\mathrm{d}^2\chi_3h}{\mathrm{d}(k_3h)^2}\right]\right\}, \tag{A.1}$$

where the second-order derivative of the damping wavenumber $\chi_3 h$ for the substrate from the wavenumber $k_3 h$ for the layer represents the following dependence:

$$\frac{\mathrm{d}^2\chi_3h}{\mathrm{d}(k_3h)^2} = \frac{2a}{\cos^2(k_3h)}[1 + k_3h\tan(k_3h)]. \tag{A.2}$$

The first-order derivative of the group velocity $V_\mathrm{g}$ can be calculated numerically from the following equations:

$$\frac{\mathrm{d}V_\mathrm{g}}{\mathrm{d}k_3h} = \left(\frac{\mathrm{d}kh}{\mathrm{d}k_3h}\right)^{-1}\left[\frac{\mathrm{d}^2\omega h}{\mathrm{d}(k_3h)^2} - V_\mathrm{g}\frac{\mathrm{d}^2kh}{\mathrm{d}(k_3h)^2}\right]. \tag{A.3}$$

The more complicated expression for the second-order derivative of the group velocity $V_\mathrm{g}$ is given by the following formula:

$$\frac{\mathrm{d}^2V_\mathrm{g}}{\mathrm{d}(k_3h)^2} = -\left(\frac{\mathrm{d}kh}{\mathrm{d}k_3h}\right)^{-2}\frac{\mathrm{d}^2kh}{\mathrm{d}(k_3h)^2}\left[\frac{\mathrm{d}^2\omega h}{\mathrm{d}(k_3h)^2} - V_\mathrm{g}\frac{\mathrm{d}^2kh}{\mathrm{d}(k_3h)^2}\right]$$
$$+\left(\frac{\mathrm{d}kh}{\mathrm{d}k_3h}\right)^{-1}\left[\frac{\mathrm{d}^3\omega h}{\mathrm{d}(k_3h)^3} - V_\mathrm{g}\frac{\mathrm{d}^3kh}{\mathrm{d}(k_3h)^3} - \frac{\mathrm{d}V_\mathrm{g}}{\mathrm{d}k_3h}\frac{\mathrm{d}^2kh}{\mathrm{d}(k_3h)^2}\right]. \tag{A.4}$$

In formulas equations (A.3) and (A.4), the following third-order derivatives are defined as follows:

$$\frac{\mathrm{d}^3\omega h}{\mathrm{d}(k_3h)^3} = -\frac{1}{\omega h}\left\{3\frac{\mathrm{d}\omega h}{\mathrm{d}k_3h}\frac{\mathrm{d}^2\omega h}{\mathrm{d}(k_3h)^2} - \left(\frac{\beta^l}{\alpha_f^s b}\right)^2\left[3\frac{\mathrm{d}\chi_3h}{\mathrm{d}k_3h}\frac{\mathrm{d}^2\chi_3h}{\mathrm{d}(k_3h)^2} + \chi_3h\frac{\mathrm{d}^3\chi_3h}{\mathrm{d}(k_3h)^3}\right]\right\};$$
$$\frac{\mathrm{d}^3kh}{\mathrm{d}(k_3h)^3} = -\frac{1}{kh}\left\{3\frac{\mathrm{d}kh}{\mathrm{d}k_3h}\frac{\mathrm{d}^2kh}{\mathrm{d}(k_3h)^2} - \left(\frac{1}{\alpha_f^s b}\right)^2\left[3\frac{\mathrm{d}\chi_3h}{\mathrm{d}k_3h}\frac{\mathrm{d}^2\chi_3h}{\mathrm{d}(k_3h)^2} + \chi_3h\frac{\mathrm{d}^3\chi_3h}{\mathrm{d}(k_3h)^3}\right]\right\}, \tag{A.5}$$

where the third-order derivative $\mathrm{d}^3(\chi_3 h)/\mathrm{d}(k_3 h)^3$ can be readily obtained from this equality:

$$\frac{\mathrm{d}^3\chi_3h}{\mathrm{d}(k_3h)^3} = \frac{4a\tan(k_3h)}{\cos^2(k_3h)}[1 + k_3h\tan(k_3h)] + \frac{2a}{\cos^2(k_3h)}\left[\tan(k_3h) + \frac{k_3h}{\cos^2(k_3h)}\right]. \tag{A.6}$$

The first- and second-order derivatives of the group velocity $V_{\mathrm{g}}$ from the values of $\omega h$ are calculated as the following functions:

$$\frac{\mathrm{d}V_{\mathrm{g}}}{\mathrm{d}\omega h} = \frac{1}{V_{\mathrm{g}}}\frac{\mathrm{d}V_{\mathrm{g}}}{\mathrm{d}kh} = 2\frac{V_{\mathrm{g}}}{V_{\mathrm{ph}}}\frac{\mathrm{d}V_{\mathrm{ph}}}{\mathrm{d}\omega h} + \omega h\left(\frac{V_{\mathrm{g}}}{V_{\mathrm{ph}}}\right)^2\frac{\mathrm{d}^2V_{\mathrm{ph}}}{\mathrm{d}(\omega h)^2}; \tag{A.7}$$

$$\begin{aligned}\frac{\mathrm{d}^2V_{\mathrm{g}}}{\mathrm{d}(\omega h)^2} = {} & \left[2\frac{V_{\mathrm{g}}}{V_{\mathrm{ph}}} + \left(\frac{V_{\mathrm{g}}}{V_{\mathrm{ph}}}\right)^2\right]\frac{\mathrm{d}^2V_{\mathrm{ph}}}{\mathrm{d}(\omega h)^2} + \omega h\left(\frac{V_{\mathrm{g}}}{V_{\mathrm{ph}}}\right)^2\frac{\mathrm{d}^3V_{\mathrm{ph}}}{\mathrm{d}(\omega h)^3} \\ & + 2\left[\frac{\mathrm{d}V_{\mathrm{ph}}}{\mathrm{d}\omega h} + \omega h\frac{V_{\mathrm{g}}}{V_{\mathrm{ph}}}\frac{\mathrm{d}^2V_{\mathrm{ph}}}{\mathrm{d}(\omega h)^2}\right]\frac{\mathrm{d}}{\mathrm{d}\omega h}\left(\frac{V_{\mathrm{g}}}{V_{\mathrm{ph}}}\right),\end{aligned} \tag{A.8}$$

where there is the following first-order derivative:

$$\frac{\mathrm{d}}{\mathrm{d}\omega h}\left(\frac{V_{\mathrm{g}}}{V_{\mathrm{ph}}}\right) = \frac{1}{V_{\mathrm{ph}}^2}\left[\frac{\mathrm{d}V_{\mathrm{g}}}{\mathrm{d}\omega h}V_{\mathrm{ph}} - \frac{\mathrm{d}V_{\mathrm{ph}}}{\mathrm{d}\omega h}V_{\mathrm{g}}\right]. \tag{A.9}$$