# COMPUTATIONS OF THE ACOUSTIC-WAVES PROPAGATION-PARAMETERS AND THE SUBSEQUENT ELASTIC CONSTANTS DERIVATION IN A SINGLE LAYER ON A SUBSTRATE

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*The aim of this article is to present a phenomenon of acoustic waves propagation in a single layer on a semi-infinite substrate from the classical theory of elasticity point of view, and recall the description of this phenomenon by G. W. Farnell and E. L. Adler issued in 1972. Additionally, the purpose is to provide tutorial-type, step-by-step scheme for the numerical algorithm, using matrix formalism, in order to calculate frequencies, velocities and polarizations of different acoustic modes propagating within a layer. It was shown how from these calculations elastic constants of materials can be derived from fittings into dependencies between velocities and acoustic wave-vectors. The approach presented is related to Brillouin light scattering (BLS) experiments. The BLS experiments provide information about acoustic modes frequencies, velocities and wave-vectors, thus supporting the fitting procedure by reduction number of the unknown parameters.*

*Keywords: Elastic constants, Thin layers, Sezawa and Rayleigh waves, Brillouin light scattering*

## 1. INTRODUCTION

About 50 years ago, in the extensive monograph Physical Acoustics edited by Mason and Thurston, in the 9th volume, the chapter by G. W. Farnell and E. L. Adler under the title *Elastic Wave Propagation in Thin Layers* was published [1]. The chapter addressed many physical aspects of the acoustic waves propagation in thin layered structures. The approach based on the classical theory of elasticity providing many details about types of possible acoustic excitations concentrating on the description of a single layer attached to a semi-infinite substrate. It was discussed there how acoustic waves are influenced by a layer thickness, densities of materials, and eventually by the piezoelectricity. To compare those past times achievements with actual development, in the field of thin layers elasticity, it can be said that the situation is similar to that with Newton's laws of a motion which are still in use in solving practical problems despite there were invented long time ago. However, an important advantage of the current situation is that the Farnel and Adler formalism can now be easily employed on quite fast computers became available for everybody. This makes possible to write own code suited for own needs, using multi-parameter fitting in order to obtain information about elastic properties.

In the current paper three types of crystallographic symmetries will be analyzed: the isotropic, the cubic, and the hexagonal. The mathematical formulation will be given in the matrix form as the eigen-problem for the acoustic waves motion. The formalism strictly addresses BLS spectroscopy of acoustic waves in thin films. The reason for this is the BLS method is a directional one. It means that in the experiments the waves can be sensed in a given in-plane direction. Thus, after subsequent sample rotations information about in-plane anisotropies and crystallographic symmetries can be deduced.

The paper consists of eight parts, including this introduction, and four appendixes (A-D). We start with the classical equation of motion for an acoustic wave in a continuous medium followed by presentation of possible solutions of the equation. Next, after use of boundary conditions for the top-surface and for the layer-substrate interface the problem is presented in a matrix form or, in other words, is reduced to the eigen-problem of the acoustic wave propagation in a single-layer on a semi-infinite substrate. From that moment we usually take advantage from information about waves frequencies and wave-vectors obtained from the Brillouin light scattering (BLS) experiments. This leads to the final stage of the elastic constants determination. The subsequent titles of chapters are informative enough, so there is no need to describe their contents more detailed. As we would like to outline only the method we exclude piezoelectricity of materials.

The scientific content of the paper is restricted to acoustic waves propagating in a thin layer with velocities which are smaller than the slowest bulk transverse acoustic waves propagating inside a material of a substrate. To deal with the case when a layer is faster than the substrate the different type of calculations have to be carried out. This will be a topic of a next paper.

## 2. EQUATION OF MOTION. HOMOGENEOUS EQUATIONS IN A HOMOGENEOUS LAYER

The starting point for the solution of the problem is the second Newton's law of motion written in the tensor formalism,namely*

$$T_{ij,j} = \rho \ddot{u}_i , \tag{1}$$

where the strain tensor is the linearly dependent on the deformation

$$T_{ij,j} = c_{ijkl} S_{kl,j} . \tag{2}$$

In other words, the strain tensor-components $T_{ij,j}$ are linear combinations of the deformations $S_{kl,j}$ with the elastic constants $c_{ijkl}$ being the proportionality constants.

## 3. THE EQUATION OF MOTION SOLUTION INTHE FORM OF PARTIAL WAVES

The assumed solution for the acoustic-waves motion in a thin layer should include following types of parameters: the angular wave-frequency $\omega$ and the wave-vector $\chi$ at the given position $r = [x, y, z]$, both $\omega$ and $\chi$ coupled together into the time-dependent wave-phase $\chi \cdot r - \omega t$ , next, the vector of polarization $\gamma$ , the amplitude *b* (in general the imaginary quantity), and the most important for the acoustics of layers, the undersurface wave-amplitude-changes expressed by the folbwings:

$$u = \gamma e^{i(\chi_x x + \chi_z h - \omega t)} , \tag{3a}$$

or

$$u = \gamma e^{ik\,h\,b} e^{i(kx - \omega t)} , \tag{3b}$$

where in Eq. 3b the factor responsible for the amplitude modifications was extracted from the phase, $\chi = [k, 0, k \cdot b]$ is the acoustic wave vector, and *k* is the acoustic in-plane wave vector derived from the BLS geometry. From the above results the assumed frame of reference for the acoustic waves motion. Thus, the wave-vector $\chi$ has no *y* in-plane component, has the *x* in-plane component parallel to the direction of propagation, and the out-of-plane *z*-component influenced by the layer thickness *h* (Fig. 1).

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*The equation is written along the Einstein's summation rule. Thus, a repeated subscript means summation over this subscript going (here) from 1 to 3 (due to 3-dimensionality of space), while, a comma before a subscript means a spatial derivative. For example, the first component ($\rho \ddot{u}_1$) of the right hand-side of Eq. 1 equals: $T_{1j,j} = T_{11,1} + T_{12,2} + T_{13,3} = \partial T_{11} / \partial x + \partial T_{11} / \partial y + \partial T_{11} / \partial z$

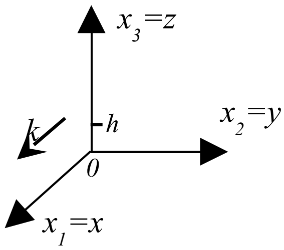


Fig. 1. A frame of reference needed for the description of acoustic waves guided in the *x* direction, in the layer of thickness *h,* with the in-plane wave-vector component *k*.

However, the total solution of the wave-propagation problem should take into the account boundary conditions imposed on a top layer-surface as well as on the interface between a layer and a substrate. From that results following expressions for the total solution composed from partial ones:

$$u_j = \left[ \sum_n C_n \gamma_j^{(n)} \exp\left(ikb^{(n)}h\right) \right] \cdot \exp\left[ik(x - \mathrm{v}t)\right], \text{ n=1..8,} \tag{4a}$$

for the layer, and

$$u_j = \left[ \sum_m C_m \gamma_j^{(m)} \exp\left(ikb^{(m)}h\right) \right] \cdot \exp\left[ik(x - \mathrm{v}t)\right], \text{ m=a, b, c, d,} \tag{4b}$$

for the substrate, where the *j* subscript numerates the three spatial components of the wave amplitude $u = [u_x, u_y, u_z]$ ($x \leftrightarrow 1, y \leftrightarrow 2, z \leftrightarrow 3$), and where v is the acoustic wave speed. The coefficients $C_n$ and $C_m$ assure of the displacements and stresses continuity at the free surface and at the interface between the layer and the substrate. The *b* in the above expressions is the unit-less parameter. It measures, for a given partial wave, the wave-amplitude into the direction normal to the surface direction. The one important point in the above derivations should be underlined - we do not use the unit vector $|\chi| = 1$, but that vector which contains components derived from the BLS geometry of scattering, namely

$$\chi = [\chi_x = k, \chi_y = 0, \chi_z = k \cdot b] \ . \tag{5}$$

4. THE EQUATION OF MOTION AS THE EIGEN-PROBLEM

In the next step of calculations we have to transform the equation of motion (Eq. 1) into the linear algebra problem. To do that all the wave amplitudes (Eqs. 3a-3b) and dependencies between strains and deformations (Eq. 2) have to be substituted into Eq. 1. Thank to this we obtain the set of following linear equations

$$c_{ijkl} \chi_j \chi_l u_k = \mathrm{v}^2 \rho u_k \delta_{ik} \ , \tag{6}$$

which can be written for the every wave component $u_k$. This algebraic system of homogeneous equations creates the eigen-problem, which admits non-null solutions only if the determinant is equal to zero:

$$\left| c_{ijkl}\chi_j\chi_l - \mathrm{v}^2\rho\delta_{ik} \right| = 0 . \tag{7}$$

More simply, the above equation can written as follows

$$\left| Q_{ik} - X\delta_{ik} \right| = 0 , \tag{8}$$

where $Q_{ik} = c_{ijkl}\chi_j\chi_l$ is the characteristic matrix* written in an open form as

$$Q_{ik} = \begin{bmatrix} c_{55}k^2b^2 + 2c_{15}\,k^2b + k^2c_{11} & c_{45}k^2b^2 + \left(c_{14}+c_{56}\right)k^2b + k^2c_{16} & c_{35}k^2b^2 + \left(c_{13}+c_{55}\right)k^2b + k^2c_{15} \\ c_{45}k^2b^2 + \left(c_{14}+c_{56}\right)k^2b + k^2c_{16} & c_{44}k^2b^2 + 2c_{46}k^2\,b + k^2c_{66} & c_{34}k^2b^2 + \left(c_{36}+c_{45}\right)k^2b + k^2c_{56} \\ c_{35}k^2b^2 + \left(c_{13}+c_{55}\right)k^2b + k^2c_{15} & c_{34}k^2b^2 + \left(c_{36}+c_{45}\right)k^2b + k^2c_{56} & c_{33}k^2b^2 + 2c_{35}\,k^2b + k^2c_{55} \end{bmatrix}, \tag{9}$$

where we used the simplified 11-> 1, 22-> 2, 33-> 3, 23-> 4, 13-> 5, 12-> 6 notations for the elastic constants $c_{ik}$. As for the every eigen-problem applied in physics the eigen-values and eigen-vectors possess appropriate interpretation. Thus, an eigen-vector informs about the polarization components of a partial wave, while the eigen-value $X$ inform about a speed and/or frequency of the wave.

## 5. THE Z-COMPONENT OF THE ACOUSTIC WAVE VECTOR

Usually, in solving the bulk-acoustics problem the $X = \rho\mathrm{v}^2$ eigen-value is treated as an unknown quantity. For the thin layers however, this quantity is directly accessible form the BLS experiment. In the experiment the dependencies between amplitudes of waves and a depth in the layered structure are not accessible. This is why, in a next step, we should solve Eq. 7 with the $\chi_z$ vector-component being the unknown quantity. Thank to this we can obtain the $\chi_z = \chi_z\left(\chi_x, c_{ijkl}, \mathrm{v}, \rho\right)$ dependencies, or similarly, we solve the equation of motion in respect to the *b's* in order to obtain the $b = b\left(\chi_x, c_{ijkl}, \mathrm{v}, \rho\right)$ dependences. Obviously, both steps are equivalent as the simple $\chi_z = kb$ relation is evident.

Next, taking again the $\left| c_{ijkl}\chi_j\chi_l - \mathrm{v}^2\rho\delta_{ik} \right| = 0$ equation, substituting to it the $\chi_z = \chi_z\left(\chi_x, c_{ijkl}, \mathrm{v}, \rho\right)$ or $b = b\left(\chi_x, c_{ijkl}, \mathrm{v}, \rho\right)$ expressions, we obtain equation with clearly

*This is elastic part of the (4x4) matrix which, with the exclusion of electric phenomena due to the piezoelectricity of material, thus, possesses here the (3x3) dimension.

visible polarization vectors $\gamma(\chi_x, c_{ijkl}, \mathrm{v}, \rho)$ for a given partial wave. This is visible below (Eq. 10).

$$\begin{bmatrix} & c_{ijkl}\chi_j\chi_l - \mathrm{v}^2\rho\delta_{ik} & \end{bmatrix} \cdot \begin{bmatrix} \gamma_x \\ \gamma_y \\ \gamma_z \end{bmatrix} = 0 . \tag{10}$$

6. THE MATRIX OF BOUNDARY CONDITIONS

The problem seems to be still unsolved due to unknown partial waves amplitudes $C_n$ (Eq. 4a) and $C_m$ (Eq. 4b), but importantly, due to the lack of fitting to the measured acoustic velocities.

In the previous chapters we outlined method of solutions for speeds and polarizations of acoustic waves. Now, the boundary conditions must be imposed in order to calculate C's amplitudes and to determine elastic constants from the fitting. The boundary conditions have the form of homogeneous algebraic equations for the layer and the substrate and can be represented by the following matrix-form equation:

$$\begin{bmatrix} & G_{ik} \quad (12x12) & \end{bmatrix} \times \begin{pmatrix} C_a \\ C_1 \\ C_2 \\ C_b \\ C_3 \\ \ldots \\ C_c \\ C_d \end{pmatrix} = 0 \tag{11}$$

In the Mason and Thurston monograph [1] all the possible (twelve) boundary conditions are ordered as follows*:

<u>A. Mechanical transverse</u>:

1) continuity of the transverse displacement at the interface ($u_2^{(l)} = u_2^{(s)}$ at *z=0*),

2) continuity of the transverse shear stress at the interface ($T_{32}^{(l)} = T_{32}^{(s)}$ at *z=0*),

3) vanishing of the transverse shear stress at the free surface ($T_{32}^{(l)}$ at *z=h*),

* We will keep this order in followed derivations, however please keep in mind that the order of *C's*, in the columnar matrix of Eq. 11, is correlated with the boundary conditions list, below. Please, keep in mind also that C's subscripts (1…8) and (a, b, c, d) are exactly the same as those from Eqs. 4a-4b.

B. Electrical:

4) continuity of the normal component of the electrical displacement at the interface ($D_3^{(l)} = D_3^{(s)}$ at $z=0$),

5) continuity of the electrical potential at the interface ($\phi^{(l)} = \phi^{(s)}$ at $z=0$),

6) continuity of the normal component of the electrical displacement at the free surface ($D_3^{(l)} = k\varepsilon_0\phi^{(l)}(h)$, and $D_3^{z>h} = -\varepsilon_0(\partial\phi^{z>h}/\partial z)$ with $\phi^{z>h} = \phi^{(l)}(h)\exp[-k(z-h)]$),

C. Mechanical sagittal:

7) continuity of the longitudinal displacement at the interface ($u_1^{(l)} = u_1^{(s)}$ at $z=0$),

8) continuity of the vertical displacement at the interface ($u_3^{(l)} = u_3^{(s)}$ at $z=0$),

9) continuity of the sagittal shear stress at the interface ($T_{31}^{(l)} = T_{31}^{(s)}$ at $z=0$),

10) continuity of the vertical compressional stress at the interface ($T_{33}^{(l)} = T_{33}^{(s)}$ at $z=0$),

11) vanishing of the sagittal shear stress at the free surface ($T_{31}^{(l)} = 0$ at $z=h$),

12) vanishing of the vertical compressional stress at the free surface ($T_{33}^{(l)} = 0$ at $z=h$).

Thus, those twelve boundary conditions yield twelve equations. Just from that results number of $C_n$ and $C_m$ coefficients (comp. again Eqs. 4a-4b); in a general case the eight $C_n$ coefficients for a layer and the four $C_m$ coefficients for a substrate. It is also convenient to present a graphical equivalence of Eq. 11 and the above list of the boundary conditions in order to show positions of terms responsible for different types of acoustic excitations guided in the layer (Fig. 2).

*Boundary conditions* ↓ / *Order of C's amplitudes* ↵

| | *m=a* | *n=1* | *n=2* | *m=b* | *n=3* | *n=4* | *n=5* | *n=6* | *n=7* | *n=8* | *m=c* | *m=d* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | L | L | L | 0 | 0 | 0 | | | | | | |
| 2 | L | L | L | 0 | 0 | 0 | | | | | | |
| 3 | 0 | L | L | 0 | 0 | 0 | | | | | 0 | 0 |
| 4 | 0 | 0 | 0 | | | | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0 | 0 | 0 | | | | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 | 0 | | | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | | | | 0 | 0 | 0 | RS | RS | RS | RS | RS | RS |
| 8 | | | | 0 | 0 | 0 | RS | RS | RS | RS | RS | RS |
| 9 | | | | 0 | 0 | 0 | RS | RS | RS | RS | RS | RS |
| 10 | | | | 0 | 0 | 0 | RS | RS | RS | RS | RS | RS |
| 11 | 0 | | | 0 | 0 | 0 | RS | RS | RS | RS | 0 | 0 |
| 12 | 0 | | | 0 | 0 | 0 | RS | RS | RS | RS | 0 | 0 |

Fig. 2. Graphical representation of the boundary condition matrix $G_{ik}$ equivalent to Eq. 11. Regions responsible for electrical phenomena are in grey. A part of determinant describing Love modes is marked by 'L' symbol, while a part responsible for Rayleigh and Sezawa modes is marked by the 'RS' symbol. At some places the matrix-elements always equal zero. Both the order of the boundary conditions and the order of the C's amplitudes were adopted from [1].

However, for the problem with the electrical part omitted ($m=b$, $n=3$, 4 omitted – compare the electrical boundary conditions 4 through 6) the problem is reduced for the 9x9 $[G_{ik}]$ matrix (see Appendix D). For example, for the cubic layer on the hexagonal substrate it equals to*

$$\begin{bmatrix} -\gamma_2^{(n)} & \cdots & \gamma_2^{(m)} & \cdots \\ c_{44(l)}b^{(n)}\gamma_2^{(n)} & \cdots & c_{44(s)}b^{(m)}\gamma_2^{(m)} & \cdots \\ c_{44(l)}b^{(n)}\gamma_2^{(n)}\exp\left(ikb^{(n)}h\right) & \cdots & 0 & \cdots \\ -\gamma_1^{(n)} & \cdots & \gamma_1^{(m)} & \cdots \\ -\gamma_3^{(n)} & \cdots & \gamma_3^{(m)} & \cdots \\ -c_{44(l)}b^{(n)}\gamma_1^{(n)} - c_{44(l)}\gamma_3^{(n)} & \cdots & c_{44(s)}b^{(m)}\gamma_1^{(m)} + c_{44(s)}\gamma_3^{(m)} & \cdots \\ -c_{11(l)}b^{(n)}\gamma_3^{(n)} - c_{12(l)}\gamma_1^{(n)} & \cdots & c_{13(s)}\gamma_1^{(m)} + c_{33(s)}b^{(m)}\gamma_3^{(m)} & \cdots \\ \left(c_{44(l)}b^{(n)}\gamma_1^{(n)} + c_{44(l)}\gamma_3^{(n)}\right)\exp\left(ikb^{(n)}h\right) & \cdots & 0 & \cdots \\ \left(c_{11(l)}b^{(n)}\gamma_3^{(n)} + c_{12(l)}\gamma_1^{(n)}\right)\exp\left(ikb^{(n)}h\right) & \cdots & 0 & \cdots \end{bmatrix}. \quad (12)$$

$$n = 1,2,5,6,7,8, \qquad m = a,c,d$$

Next, going more into the specific situation, for the system with only Rayleigh and Sezawa modes (the in-plane polarized Love modes don't exist or are decoupled from the Rayleigh and Sezawa modes in that case) the $[G_{ik}]$ matrix simplifies to the 6x6 matrix ($m=a$, $n=1$, 2 indexes for Love modes are omitted in this case).

The G-matrix mathematical-treatment is again narrowed to the linear algebra problem. This is why, keeping in mind that the final purpose of our calculations is to derive elastic constants for the layered structure from fittings to the data obtained experimentally, the $\det[G]= 0$ equation should be is solved along with Eq. 11 - for given set of physical and geometrical properties ($\rho$, $c_{ijkl}$, $h$) of the structure, and for the values of $k$ obtained from the scattering geometry. Thus, the $\det[G] = 0$ equation, as a matter of fact, has the only speed as an unknown parameter, thus, the equation roots give the dispersion relations $v_{computed}(k) = \omega/k$ for all the acoustic modes. These roots can be found looking for the minima of $\det[G]$ expression as the function of speeds v.

Summarizing; in a general case from the following condition

$$\det\begin{bmatrix} & & \\ & G_{ik} \quad (12x12) & \\ & & \end{bmatrix} = 0 \quad (13)$$

*We changed order of rows and columns in the $|G_{ik}|$ determinant in comparison to original description by Farnell and Adler [1], however as it is known, the value of determinant does not change after such modifications. The *C's* positions in the columnar matrix (comp. Eq. 11) also have to be changed accordingly.

elastic constants of the structure and dispersion relations can be determined. Additionally, in a case of nonpiezoelectric materials, used for a layer and for a substrate, from the following equation

$$\begin{bmatrix} & & \\ & G_{ik} \quad (6x6) & \\ & & \end{bmatrix} \times \begin{pmatrix} C_5 \\ C_6 \\ C_7 \\ C_8 \\ C_c \\ C_d \end{pmatrix} = 0 \tag{14}$$

$$n = 5,6,7,8 \qquad m = c,d$$

the $C$'s amplitudes for the Rayleigh and Sezawa waves can be determined, while the Love modes amplitudes can be obtained from the following matrix equation

$$\begin{bmatrix} & & \\ & G_{ik}\,(3x3) & \\ & & \end{bmatrix} \times \begin{pmatrix} C_1 \\ C_2 \\ C_a \end{pmatrix} = 0 . \tag{15}$$

$$n = 1,2, \qquad m = a$$

Eventually, if the Sezawa and Rayleigh modes are not decoupled from the Love modes we have to use Eq. 11 against Eqs. 14-15. Thus, from Eqs. 14-15 or Eq. 11 the values of all the $C$-amplitudes can be found, apart from an arbitrary overall multiplicative factor (the excitation amplitude of the modes). In other words the $C$-amplitudes determine the shape of the displacement field of a given mode.

Summarizing again this step of calculation, it can be said, that the elements of the G-matrix are dependent on:

- the physical properties (mass density ρ and elastic constants ($c_{ijkl}$) of the layer(s),
- the geometrical properties (thickness $h$) of the layer(s),
- the acoustic-wave propagation direction $\chi_x = k$ (the $\chi_z = kb$ is known from the eigen-equation of $Q$-matrix),
- the acoustic-wave speed v.

7. FITTING ELASTIC CONSTANTS

As it was yet written, the velocities of acoustic waves from the previous chapter, are function of $k$, and depend parametrically on the density, the elastic constants and the thickness (ρ, $c_{ijkl}$, $h$):

$$\mathrm{v} = \mathrm{v}_{computed}(k, \rho, c_{ijkl}, h). \quad (16)$$

Doing in this final stage the fitting we should do the followings [3]:

- select a subset of parameters - typically the $c_{ijkl}$ of the layer,
- assume definition of a mesh of values of these parameters,
- identify the most probable values by the common least squares fitting procedure to minimize the $[\Sigma(\mathrm{v}_{computed} - \mathrm{v}_{measured})^2]$ expression.

As an example consider hypothetical situation when experimental BLS data do not ensure us if we dealt with an isotropic or a hexagonal film deposited onto the well known isotropic substrate.

In terms of the elements of the tensor of elastic constants $c_{ij}$, the isotropy of the layer implies (here we uses simplified, 2-indexed description of elastic constants – see explanation below Eq. 9): $c_{11} = c_{22} = c_{33}$, $c_{12} = c_{13} = c_{23}$, $c_{44} = c_{55} = c_{66} = (1/2)(c_{11} - c_{12})$, and all the others $c_{ij} = 0$, meaning that the tensor is fully determined by two independent values (typically taken as $c_{11}$ and $c_{44}$).

In hexagonal symmetry of the layer the equalities $c_{11} = c_{22}$, $c_{13} = c_{23}$, $c_{44} = c_{55}$, $c_{66} = (1/2)(c_{11} - c_{12})$ hold true, but the eventual film anisotropy allows that $c_{33} \neq c_{11} = c_{22}$, $c_{12} \neq c_{13} = c_{23}$, $c_{44} = c_{55} \neq c_{66}$, meaning that full determination of the tensor requires five independent values – these can be taken as: $c_{11}$, $c_{33}$, $c_{12}$, $c_{13}$ and $c_{44}$. Computations in the hexagonal symmetry can be performed starting with isotropic properties, identified by $c_{33} = c_{11}$, $c_{13} = c_{12}$, $c_{44} = (1/2)(c_{11} - c_{12})$ equations, and then, relaxing these equalities, treating $c_{33}$, $c_{13}$ and $c_{44}$ as additional free parameters, beside $c_{11}$ and $c_{12}$.

The possibility of finding the five elastic constants depends on the sensitivity of the computed velocities to their values. As it was written in previous chapters, for given values of the substrate properties the computed velocities of the acoustic modes are functions of the film properties (mass density $\rho$, thickness $h$, several independent elastic constants $c_{ij}$), of the wave-vector k and of the mode (the branch of the dispersion relation), which can be indicated by a mode index $j$: $\mathrm{v}_j = \mathrm{v}_j(k, \rho, c_{ij}, h)$.

The sensitivity function of a computed speed $\mathrm{v}_j$ to a given parameter $p$ can be estimated by the partial derivative $\partial \mathrm{v}/\partial p$, numerically computed as $\Delta \mathrm{v}/\Delta p$, or better by the logarithmic derivative $\partial(\log \mathrm{v})/\partial(\log p)$, numerically computed as $(\Delta \mathrm{v}/\mathrm{v})/(\Delta p/p)$. Then, we have to sample the velocities $\mathrm{v}_j$ at a discrete set of wave-vectors $\mathrm{k}^*$. Thus, we can compute a mode specific sensitivity to parameter $p$ as

* in-plane acoustic wave vector

$$\frac{1}{N_k}\sum_k \frac{\Delta v_j(k)/v_j(k)}{\Delta p(k)/p(k)} \tag{17}$$

These sensitivities to a given parameter (one of the $c_{ij}$) often turn out to be numerically of the same order for the various modes (although in some cases they have opposite signs for different modes). It is therefore reasonable to compute a global sensitivity

$$\frac{1}{N_j}\cdot\frac{1}{N_k}\sum_j\sum_k \frac{\Delta v_j(k)/v_j(k)}{\Delta p(k)/p(k)}. \tag{18}$$

For example, for a hypothetical case, these global sensitivity indexes can have the following values:

Tab. 1. Numerical sensitivity of elastic constants, treated as free parameters, to the experimental data fitting.

| parameter | $C_{11}$ | $C_{12}$ | $C_{44}$ | $C_{13}$ | $C_{33}$ |
|---|---|---|---|---|---|
| sensitivity | 0.24 | ~ 0 | 0.11 | 0.07 | 0.16 |

Firstly, these values are not high - they mean that a 1% change of $c_{11}$ causes a change of velocity of 0.24%, and a 1% change of $c_{13}$ causes a change of velocity of only 0.07%; they show that $c_{11}$ and $c_{33}$ are likely to be better determined, since they have the higher sensitivities, while $c_{12}$ cannot be determined, since the velocities of the acoustic modesare insensitive to its value.

Secondly, the null sensitivity to $c_{12}$ is not surprising, since $c_{12}$ gives the $T_1$ stress component due to the $S_2$ strain component $T_1 = c_{12} S_2$ , but in the acoustic modes being probed $S_2$ is always null: axes have $z=x_3$ normal to the surface, and $x=x_1$ in the surface and directed along the propagation direction, such that the displacement is proportional to $C(z)exp[i(kx - \omega t)]$ and has no dependence on $y=x_2$. Taking into account the null sensitivity to $c_{12}$, the fit of the computed dispersion relations to the measured ones is performed with four free parameters, leaving $c_{12}$ fixed at the value found by the isotropic approximation to the analyzed data.

The global sensitivity can be evaluated also for the other parameters involved in the computation of $v_j = v_j(k,\rho,c_{ij},h)$. For the properties of a substrate such sensitivity is not relevant, since in practice largely accepted values of mass densities and elastic properties can be adopted from literature data (for example for silicone). Similarly, the wave-vector $k$ is determined with good precision by the scattering geometry. Instead, the film mass density $\rho$ and thickness $h$ can be measured by other methods, like XRD, and might be affected by uncertainties, whose effects can be assessed by the sensitivity indexes. Such indexes can sometimes equal to higher values than those of the elastic constants global sensitivities. For example for the heavy layerwhich less stiff than the substrate (silicon) we can obtain

Tab. 2. Numerical sensitivity of the layer density and the layer thickness, treated as free parameters, to the experimental data fitting.

| parameter | ρ | *h* |
|---|---|---|
| sensitivity | 0.49 | 0.40 |

This is not surprising: the stiffness of the acoustic modes comes mainly from the substrate, the stiffness of the film being only minor, while the inertia of the acoustic mode comes mainly from the film. A change of the film elastic constants modifies only a minor contribution to stiffness, while a change of its density or thickness modifies the major contribution to inertia, and has a larger effect.

These sensitivities must be kept in mind. A change of 1% of the film density causes a change of velocities similar to that induced by a change of 2-4 % of the elastic constants. This means that a 1% error in the measurement of density or thickness causes an error of 2-4 % of the elastic constants. Importantly, the sensitivities can be treated as criterion in order to distinguish crystallographic symmetry of the film: lower values of the elastic constants sensitivities leading to better fitting to the experimental dispersion relations $\mathrm{v}_j = \mathrm{v}_j(k, \rho, c_{ij}, h)$ enable the choice between isotropic and/or different symmetries identification.

8. FINAL REMARKS

The main aim of present efforts relied on fitting of the calculated acoustic modes speeds to experimental data obtained in Brillouin light scattering experiments. Besides this we could conclude about crystallographic symmetries of the layer guiding the modes. Finally, it was possible to obtain values of elastic constants from the fitting using boundary condition. In Fig. 3 a typical example of the fitting to experimental BLS data is given. Points are surrounded by uncertainties which are much smaller to be visible within the figure scale.

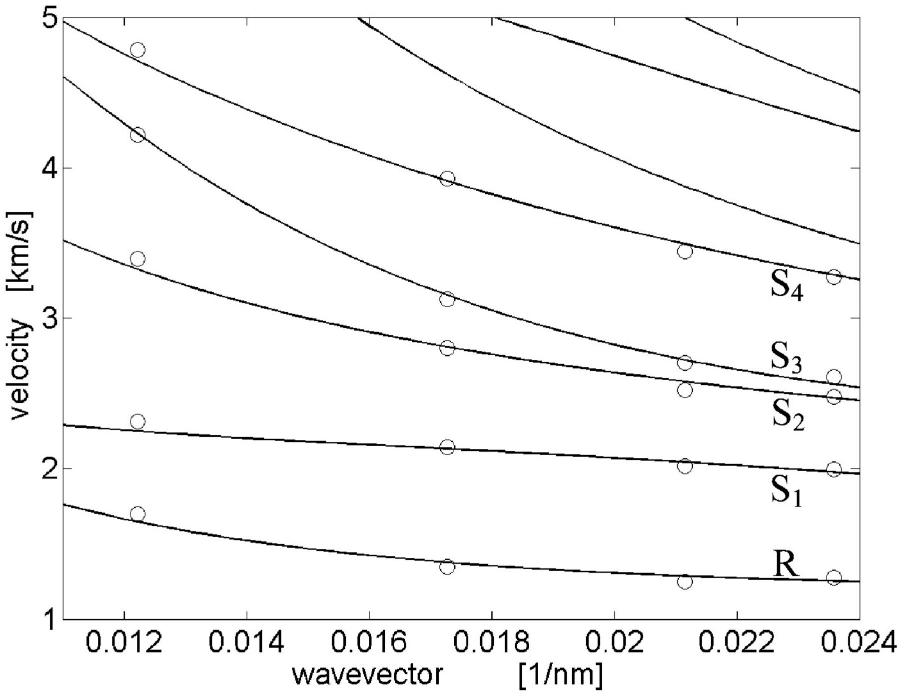


Fig. 3. Dependencies between velocities and the wave-vector for the Rayleigh mode (R) and Sezawa modes ($S_{1...4}$) guided in a thin slow layer deposited onto a faster substrate.

It is a hope of authors that provided analysis of thin layers elasticity associated with the guided acoustic modes will support the large community of solid state scientists, especially those who are not familiar with the Brillouin light scattering.

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*In the book "Brillouin spectroscopy in crystal lattices", eigen-problems for isotropic, cubic and hexagonal symmetries have been presented [2]. However, the calculations were done for unit wave-vectors $|\chi|=1$. The results from book can be transformed for the $\chi = [\chi_1 = k, \chi_2 = 0, \chi_3 = k \cdot b]$ approach if the every eigen-value will be multiplied by the $k^2$, while in the every solution for b's the $X$ (eigen-value) will be substituted by $X/k^2$ in order to obtain $\chi_z$. In the Appendixes the calculations for the $Q_{ik}$ matrix elements , the $X$ eigen-values, the $\gamma$ eigen-vectors, and the $\chi_z$ components ($b$-amplitudes) for the isotropic, cubic and hexagonal symmetries are provided.