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An inverse method for determining the elastic properties of thin layers using Love surface waves

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Estimation of the mechanical and geometrical parameters of thin coatings and surface layers in materials is of great practical importance in engineering and technology. Indeed, surface properties of many vital engineering components, such as turbine blades, pistons, or bearings, directly affect the longevity and safety of modern machinery. In this article, the authors present a novel inversion procedure for simultaneous determination of thickness, shear elastic constant, and density of thin coating layers in materials. The inversion procedure is based on measurements of the dispersion curve for surface acoustic waves of the Love type. The inverse problem is formulated as an optimization problem with the appropriately designed objective function, depending on the material parameters of the coating layer, ultrasonic frequency, and the experimental data, i.e. measured phase velocity of the surface Love wave. The minimization of the objective function provides three parameters of a thin layer, i.e. its thickness, shear elastic constant, and density. The proposed inverse method was checked experimentally for different layered structures, such as copper layer on steel substrate or ceramics-on-ceramics. The agreement between the results of calculations with the proposed inversion method and the experimental data was good.

Keywords: inverse problems; Love surface waves; elastic constants; acoustic wave dispersion; thin layers

1. Introduction

The mechanical properties of coatings deposited on a substrate and surface layers in graded materials are of crucial importance in the design and evaluation in modern engineering practice [1,2]. In fact, Young's modulus is the main mechanical parameter characterizing the elastic stiffness of the material. For example, it can be correlated with hardness and porosity [3], as well as with the wear and exploitation characteristics of the material [4,5]. Mechanical properties of thin films are also of primary importance for chip manufacturers in the electronic industry [6].

Traditional mechanical methods for characterization of the surface properties of materials are tedious, time consuming, and most importantly, destructive. For example, a small sample must be cut-off from the material in order for it to be examined by

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conventional metallurgical equipment. Employment of bulk and surface acoustic waves provide truly non-destructive tools in material characterization [7]. Ultrasonic waves are mechanical waves, whose propagation depends on mechanical properties of the material and geometrical structures of the sample. Thus, by measuring some wave parameters, one can try to determine characteristics of the material carrying the wave [8,9]. Since ultrasonic signals can be transformed to electrical signals, using, for example, piezoelectric effect, the ultrasonic signal can be easily digitized and sent to the computer for further processing. Therefore, ultrasonic methods can be implemented on a production line for an automatic, non-destructive control of industrial processes.

An important property of all surface waves is the fact that their amplitude decays practically to zero in a few wavelength from the guiding surface. Thus, by changing wave frequency, one can probe the subsurface profiles of the material. At the beginning, thin layers in materials were investigated with Rayleigh surface waves [10–12], which possess at least two perpendicular components of the mechanical displacement (shear vertical (SV) and longitudinal). Due to their inherent complexity, Rayleigh surface waves are rather difficult in practical applications, since no analytical solutions for Rayleigh waves are available, even in the material with isotropic properties. By contrast, Love surface waves have only one shear horizontal (SH) component of vibration and closed-form analytical solutions for Love surface waves do exist, even in anisotropic materials. However, it should be stressed that Love surface waves exist only in materials with a surface layer which is 'softer' than the substrate, i.e. when phase velocity of bulk acoustic waves in the layer is lower than that in the substrate. Moreover, Love surface waves are sensitive only to shear elastic properties of the surface layer and the substrate. Nevertheless, due to its simplicity, Love surface waves are very attractive for inverse problem applications, where one must calculate the corresponding direct problem solution many times. Love surface waves were used initially in geophysics to study mechanical properties of selected geological structures [13,14], since Love waves may accompany Rayleigh surface waves triggered by during earthquakes.

First attempts to use Love surface waves in inverse problems involved one-parameter inverse methods, which enabled the calculation of only one surface layer parameter, such as the thickness of the layer or its one elastic constant [9]. The parameter of the surface layer was deduced from measured dispersion curve for Love waves (wave velocity as a function of frequency). In this article, the authors propose a novel inverse method for simultaneous determination of three surface layer parameters, i.e. its thickness, shear elastic constant, and density. The following layered structures were studied in this article:

- thin ceramic layer on a ceramic substrate
- thin copper layer deposited electrolytically on a steel substrate.

Calculation of Love wave parameters (e.g., phase velocity, distribution of the wave amplitude with depth) for known *a priori* values of material parameters of the layer and substrate constitutes the direct problem. In this study, the direct problem was formulated and solved.

The inverse problem constitutes determination of unknown material parameters from the measured dispersion curves (phase velocity as a function of frequency) for Love waves. To solve the inverse problem, one has to perform the following steps:

- solve direct problem
- determine experimentally dispersion curves
- solve inverse problem.

In this article, the inverse problem was formulated and solved as an optimization problem. The objective function depending on the material parameters of the structure, frequency and experimental data (dispersion curves of the surface wave) was developed. The dispersion curves were measured in the computerized measuring set-up. Making use of the optimization methods, a minimum of the objective function was determined. This enabled the determination of the unknown mechanical parameters such as shear elastic coefficients and thickness of thin coating films. The elastic and geometrical parameters of thin films obtained from the inverse method were used as input data in the calculations of the direct problem. The dispersion curves resulting from the direct problem were compared with those measured experimentally. Good conformity between theoretical and experimental dispersion curves has been stated. This may justify the correctness of the inverse problem solution.

2. Direct Sturm–Liouville problem

Calculation of the dispersion curves and amplitude of a surface wave for the given values of elastic parameters of the surface layer and substrate forms a direct problem. The direct problem (direct Sturm–Liouville problem) describes the propagation of the Love wave in the layered media.

2.1. Love waves

The Love wave propagates in a semi-infinite layered structure, as shown in Figure 1. Here, an elastic isotropic layer is rigidly attached to an isotropic and elastic half-space. Mechanical vibrations of the SH surface wave are performed along the *y*-axis parallel to the propagation surface and perpendicularly to the direction of propagation z. The thickness of the layer is h. The problem considered is two-dimensional, having no variation along the *y* co-ordinate.



Figure 1. Geometry of a Love wave waveguide ($v_L < v_S$).

The mechanical displacement of the SH acoustic wave in the layer and substrate must satisfy the following wave equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial z^2} = \frac{1}{v_{L,S}^2} \frac{\partial^2 u}{\partial t^2}$$
(1)

where $v_{L,S}$ stands either for v_L or v_S . Here v_L and v_S are the velocities of bulk shear waves in the layer and substrate, respectively.

The time-harmonic mechanical displacement of the surface Love wave can be expressed as

$$u(x, z, t) = f(x) \cdot \exp[j(\omega t - \beta z)]$$
⁽²⁾

where f(x) describes the dependence of the wave amplitude on the depth x, $(-h < x < +\infty)$; $\beta = \omega/v$ is the wave number; ω is the angular frequency and v is the phase velocity of the Love wave.

Analytical formulas for the mechanical displacement of the Love wave are derived by substituting Equation (2) into Equation (1) and solving the resulting equation of motion for layer and substrate region, respectively.

The mechanical displacement of the Love wave in the layer $(-h < x \le 0)$ is the following:

$$u(x, z, t) = \{C_1 \sin[q(x+h)] + C_2 \cos[q(x+h)]\} \cdot \exp[j(\omega t - \beta z)]$$
(3)

where $q = \{\sqrt{(\frac{v}{v_L})^2 - 1}\} \cdot \beta$ and $v_L^2 = c_{44L}/\rho_L$. Here, c_{44L} and ρ_L are the shear elastic constant and density of the layer material, respectively. C_1 and C_2 are constants.

The mechanical displacement of the Love wave in the substrate (x > 0) is as follows:

$$u(x, z, t) = [C_3 \exp(-bx) + C_4 \exp(+bx)] \cdot \exp[j(\omega t - \beta z)]$$
(4)

where $b = \{\sqrt{1 - (\frac{v}{v_S})^2}\} \cdot \beta$, and $v_S^2 = c_{44S}/\rho_S$. Here, c_{44S} and ρ_S are the shear elastic constant and density of the substrate material, respectively. C_3 and C_4 are constants.

The amplitude f(x) of the surface Love wave should vanish for $x \to \infty$. At the interface (x = 0), the continuity condition for the mechanical displacement and shear stress must be satisfied. Moreover, at the free surface (x = -h), the shear stress is equal to zero. Therefore, the boundary conditions are in the form:

$$du/dx|_{x=-h} = 0 \tag{5}$$

$$c_{44L} du/dx|_{x=-0} = c_{44S} du/dx|_{x=+0}$$
(6)

$$u|_{x=-0} = u|_{x=+0} \tag{7}$$

$$u = 0 \text{ for } x \to \infty \tag{8}$$

Equations (3) and (4) along with the boundary conditions (5–8) constitute the mathematical model of the Love wave propagation in a layered structure.

2.1.1. Dispersion equation

The boundary conditions (5) and (8) imply $C_1 = 0$ and $C_4 = 0$. By substituting (3) and (4) into the boundary conditions (6) and (7) and setting the resulting determinant equal

to zero, we arrive at the following dispersion equation of the Love wave propagating in a layered half-space [15]:

$$\Omega = \tan\left\{\sqrt{\frac{v^2 \cdot \rho_L}{c_{44L}} - 1} \cdot \frac{\omega \cdot h}{v}\right\} - \frac{c_{44S}}{c_{44L}} \frac{\sqrt{1 - \frac{v^2 \cdot \rho_S}{c_{44S}}}}{\sqrt{\frac{v^2 \cdot \rho_L}{c_{44L}}} - 1} = 0$$
(9)

where *h* is the thickness of the surface layer; c_{44L} is the shear elastic constant of the layer; ρ_L is the density of the layer; ω is the angular frequency; *v* is the phase velocity of the Love wave; c_{44S} is the shear elastic constant of the substrate and ρ_S is the density of the substrate.

It can be shown from Equation (9) that the phase velocity of the Love wave depends on the elastic properties of the layered structure, thickness, and frequency.

The solution of the dispersion Equation (9) results in a series of discrete values of the Love wave velocity v_i , for a given value of frequency. Once the wave velocity v_i is known, the corresponding distribution $f_i(x)$ of the wave amplitude with depth x can be calculated from Equations (2)–(4). A set of pairs $\{v_i, f_i(x)\}$, where v_i is the surface wave velocity, and $f_i(x)$ the distribution of the wave amplitude with depth, constitutes the solution of the direct problem. The index i = 1 refers to the fundamental mode. Higher modes of Love waves are labelled with i > 1.

In this study, we have restricted our attention to the propagation of the fundamental mode of Love waves.

3. Experiment

The dispersion curves were measured in the computerized measuring set-up. In the set-up, the sending-receiving piezoelectric transducer is driven by the TB-1000 pulser-receiver computer card (Matec, USA). Love waves are excited by the plate transducer (1) attached to the waveguide face (Figure 2). The sending-receiving transducer (1) is excited to shear vibrations parallel to the waveguide surface and generates impulses of the Love wave that propagate along the waveguide surface. Theoretical and experimental analysis of the generation of SH surface waves by means of a plate transducer is presented in [16,17]. The Love wave impulse generated by the transducer is reflected in multiple ways between two opposite edges of the layered waveguide (Figure 2). The signals received by the transducer are amplified by the TB-1000 receiver and sent into the PDA-500 digitizer card (Signatec, USA). This card samples and digitizes the input analog signals. The accuracy of the



Figure 2. Waveguide (Cu on steel) of the Love wave. The shear surface wave is generated by the piezoelectric transducer plate (1) and propagates forth and back along the waveguide surface.



Figure 3. Measured dispersion curve of the Love wave in the layered structure Cu on steel.

measured velocity was estimated as 0.2%, i.e. $\pm 6 \text{ m s}^{-1}$. Measurements were carried out in the range from 0.5 to 10 MHz.

The phase velocity was determined by measuring the time of flight 'TOF' between two subsequent echoes of the ultrasonic surface wave travelling in the waveguide. The values of the time of flight 'TOF' were calculated using the cross-correlation method.

Figure 3 shows as an example the measured dispersion curve of the Love wave propagating in the layered structure Cu on steel from Figure 2.

3.1. Investigated structures

The measurements have been carried out on the following layered structures:

- (1) thin ceramic layer on a ceramic substrate;
- (2) thin copper (Cu) layer deposited electrolytically on a steel substrate (Figure 2).

The surface ceramic layer was a piezoelectric transducer depolarized ceramic plate glued to a piezoelectric transducer polarized ceramic substrate. The phase velocity of the bulk SH acoustic wave in the depolarized ceramics is lower than that in the polarized ceramics. This enables the propagation of Love waves in the considered layered ceramic structure.

Similarly, the phase velocity of the bulk SH acoustic wave in copper is lower than that in the steel substrate. Therefore, the Love wave can also be supported by the Cu layer deposited on the steel substrate.

4. Inverse problem

The inverse problem relies on the determination of unknown material parameters from the measured dispersion curves of SH surface waves (i.e. Love waves) propagating in the considered layered structure.

To solve the inverse problem, one has to carry out the following steps:

- (1) solve the direct problem;
- (2) determine experimentally the dispersion curves and
- (3) perform the inverse procedure.

In this article, the inverse problem was formulated and solved as an optimization problem [18] with properly defined objective function.

4.1. Objective function

The objective function is a measure of the distance between the mathematical model of the investigated object and the real object. The objective function Π depending on the material parameters of the structure, frequency, and experimental data (phase velocity of the surface Love wave) was introduced and defined as

$$\Pi = \sum_{j=1}^{N_e} \left| \Omega(h, c_{44L}, \rho_L, \omega_j, v_j, c_{44S}, \rho_S) \right|$$
(10)

where N_e is the number of experimental points; ω_j is the measured angular frequency; v_j is the measured phase velocity; h is a guess thickness of the layer; c_{44L} is a guess elastic constant of the coating layer; ρ_L is a guess density of the surface layer; c_{44S} is the shear elastic constant of the substrate (known '*a priori*') and ρ_S is the density of the substrate (known '*a priori*').

The design variables h, c_{44L}, ρ_L are arguments of the objective function Π and the quantities ω_j, v_j , and c_{44S}, ρ_S in Equation (10) are parameters. The optimized ones are the material parameters of the layer h, c_{44L}, ρ_L , whereas the material parameters of the substrate c_{44S}, ρ_S are given 'a priori'.

Making use of the optimization methods, a minimum of the objective function was determined. This enabled the determination of the optimum values for the unknown mechanical and geometrical parameters such as the elastic coefficient c_{44L} , density ρ_L , and thickness *h* of the thin coating layer. To minimize the considered objective function Π , the appropriate optimization procedures from the Mathcad[®] software package were employed.

The minimization problem was formulated mathematically as follows: minimize the objective function $\Pi(h, c_{44L}, \rho_L, \omega_j, v_j, c_{44S}, \rho_S)$ subject to linear constraints (i.e. (12), (15), (18), (21) or (24)). Employing the Mathcad package to solve the nonlinear minimization problem, the conjugate gradient method was used. In this Mathcad solving routine, guess initial values and constraints for the unknowns are required. The above-mentioned constraints reflected the real physical range of the optimized variables.

5. Determination of thin layers parameters

The minimization of the objective function subject to the given constraints results in the optimum values of unknown parameters (e.g. thickness, shear elastic constant of the surface layer).

Various numbers of parameters of the layer were extracted from the inverse method. We solved the inverse problem for three cases. In case 1, only thickness h is unknown.

Material	h	$c_{44} ({\rm Nm^{-2}})$	$ ho (\mathrm{kg}\mathrm{m}^{-3})$
Depolarized ceramics (layer)	200 μm	2.57E+10	7.5E+3
Polarized ceramics (substrate)	10 mm	3.95E+10	7.5E+3

Table 1. Exact material properties (thickness *h*, shear modulus c_{44} , and density ρ) of the investigated layered ceramics + ceramics structure.

In case 2, we assume that the thickness *h* and shear elastic constant c_{44L} are unknown, and in case 3, three parameters, i.e. the thickness *h*, shear elastic constant c_{44L} and density ρ_L are not known.

5.1. Ceramics + ceramics structure

5.1.1. Inversion of thickness h of ceramic layer $(c_{44L} \text{ and } \rho_L \text{ are given})$

Initial value:
$$h = 0 \,\mathrm{m}$$
 (11)

Constraints:
$$0 < h < 2E - 3 m$$
 (12)

Results from the inverse method:
$$h = 370 \,\mu m$$
 (13)

5.1.2. Inversion of thickness h and c_{44L} of ceramic layer (ρ_L is given)

Initial values:
$$h = 1E - 3 \text{ m}, c_{44L} = 0.3E + 10 \text{ N m}^{-2}$$
 (14)

Constraints:
$$0 < h < 2E - 3 \text{ m}$$
, $1.5E + 10 < c_{44L} < 3E + 10 \text{ N m}^{-2}$ (15)

Results from the inverse method: $h = 103 \,\mu\text{m}$ and $c_{44L} = 2.3\text{E} + 10 \,\text{Nm}^{-2}$ (16)

5.1.3. Comparison of the results obtained from the inverse method with the experiment

The exact values of the material parameters of the ceramics in both the layer and in the substrate (Table 1) were determined from the geometrical and ultrasonic measurements. The thickness was measured by micrometer screw, and the velocity of bulk shear acoustic waves was measured in the layer and substrate ceramics, respectively. The density of the ceramics is known from the producer catalogue.

The thickness $h = 370 \,\mu\text{m}$ resulting from the inverse method (Equation (13)) was substituted into the dispersion equation (10) as an input data in the calculations of the direct problem. Therefore, the phase velocity of the Love wave was calculated for several



Figure 4. Comparison of the experimental dispersion curve with that obtained from the inverse method (ceramics + ceramics structure).

values of frequency (theoretical dispersion curve). This theoretical dispersion curve was compared with the experimental dispersion curve (Figure 4). Very good conformity between the theoretical and experimental dispersion curves has been observed.

The inaccuracy when recovering the thickness of the ceramics layer may result from the technological processes used to fabricate the layered structure (surface ceramics layer on ceramics substrate). The surface ceramics layer was glued to the substrate and then polished to the final thickness. As a consequence, the real structure was instead a trilayered structure. The third glue layer has a non-uniform thickness and undefined elastic properties. This may result in the erroneous determination of the thickness of the surface ceramics layer. This case is an example of the difficulties in modelling the real structures.

5.2. Cu on steel structure

5.2.1. Inversion of thickness h of Cu layer (c_{44L} and ρ_L are given)

Initial value:
$$h = 0 \,\mathrm{m}$$
 (17)

Constraints:
$$0 < h < 2E - 3 m$$
 (18)

Results from the inverse method:
$$h = 541 \,\mu m$$
 (19)

Material	h	$c_{44} ({\rm N m^{-2}})$	$\rho (\mathrm{kg}\mathrm{m}^{-3})$
Cu (layer)	400 μm	3.93E+10	8.9E+3
Steel (substrate)	10 mm	7.99E+10	7.8E+3

Table 2. Exact material properties (thickness *h*, shear modulus c_{44} and density ρ) of the investigated layered structure Cu on steel.

5.2.2. Inversion of thickness h and c_{44L} of Cu layer (ρ_L is given)

Initial values:
$$h = 1E - 4m$$
, $c_{44I} = 3E + 10 N m^{-2}$ (20)

Constraints:
$$0 < h < 2E - 3m$$
, $3E + 10 < c_{44L} < 5E + 10 N m^{-2}$ (21)

Results from the inverse method:
$$h = 473 \,\mu\text{m}$$
 and $c_{44L} = 3.76\text{E} + 10 \,\text{N} \,\text{m}^{-2}$ (22)

5.2.3. Inversion of thickness h, c_{44L} and ρ_L of Cu layer

Initial values:
$$h = 1E - 3 \text{ m}$$
, $c_{44L} = 2E + 10 \text{ N m}^{-2}$, and $\rho_L = 8E + 3 \text{ kg m}^{-3}$ (23)

Constraints:
$$0 < h < 2E - 3 \text{ m}$$
, $3E + 10 < c_{44L} < 5E + 10 \text{ N m}^{-2}$, and
 $7E + 3 < \rho_L < 9E + 3 \text{ kg m}^{-3}$
(24)

Results from the inverse method: $h = 486 \ \mu\text{m}, \ c_{44L} = 3.83\text{E} + 10 \ \text{N} \ \text{m}^{-2}, \text{ and}$ $\rho_L = 9\text{E} + 3 \ \text{kg} \ \text{m}^{-3}$ (25)

5.2.4. Comparison of the results obtained from the inverse method with the experiment

The exact values of the material parameters of the copper layer and steel substrate (Table 2) were determined from the geometrical and ultrasonic measurements. The thickness was measured using a metallographic microscope, and the velocity of bulk shear acoustic waves was measured in the copper layer and steel substrate, respectively. The densities of copper and steel are known from physical tables.

Proceeding in a similar manner as in the case of the ceramics + ceramics layered structure, we compared the experimental dispersion curve to that obtained from the direct problem and calculated for the value of the thickness $h = 541 \,\mu\text{m}$ (Figure 5). This value of the thickness has resulted from the solution of the inverse problem (Equation (19)). Very good conformity between the theoretical and experimental dispersion curves has also been stated.

The difference between the theoretical (from the inverse method) and experimental thickness can be attributed to the properties of the technological properties of the Cu layer fabrication. The copper surface layer was deposited electrolytically on the steel substrate. From our metallographic observations it is evident that the obtained Cu surface layer has



Figure 5. Comparison of the experimental dispersion curve with that obtained from the inverse method (Cu + steel structure).

non-uniform thickness. Moreover, the structure of the surface Cu layer is porous and its contact with the steel substrate is not perfect.

6. Conclusions

A novel inverse method, employing Love surface waves for simultaneous determination of three surface layer parameters, i.e. its shear elastic constant, density and thickness, from measured dispersion curves, was developed. The proposed inverse method was then tested by ultrasonic measurements performed in selected surface structures.

Employing shear surface waves of the Love type for testing thin coating layers is more convenient than Rayleigh waves because the velocity of the Love wave depends only upon one shear elastic constant of the material. This greatly simplifies mathematical formulation of the resulting direct and inverse problems. As a consequence, the proposed inverse method provided numerical results in a few seconds on a standard personal computer (PC).

The direct problem was formulated analytically, providing a transcendental algebraic equation, which was solved numerically. Theoretical dispersion curves for the Love surface waves, propagating in the selected structures, were solutions of the direct problem.

The inverse problem was formulated as an optimization problem. Consequently, the objective function based on the dispersion equation was determined and minimized. The minimization problem was solved using the commercial Mathcad[®] software package.

The elastic and geometrical parameters obtained from the inverse method were used as input data in the calculations of the direct problem. Dispersion curves resulting from the direct problem were compared with those measured experimentally. Good conformity between theoretical and experimental dispersion curves has been stated. This may be evidence for the validity of the inverse method used for determining the mechanical properties of thin coating layers by means of SH surface waves of the Love type. In many papers [2,12,19], the agreement between the theoretical (resulting from the inverse method) and measured dispersion curves was treated as evidence for the correctness of the inverse method.

Many technological processes for the surface treatment (hardening, carbonizing, nitriding, implantation and diffusion) result in profiles (of the elastic properties) that vary with depth. For those types of profiles, the agreement between theoretical and experimental dispersion monotonically changing curves may provide evidence for the correctness of the inverse method.

For the structure Cu on steel the normalized distance between experimental and theoretical dispersion curves from Figure 5, using the Euclidean norm (Appendix), equals 1.3%. Similarly, for the structure ceramics-on-ceramics, the normalized distance between experimental and theoretical dispersion curves from Figure 4 is equal to 0.6%.

More detailed analysis describing quantitatively the distance between experimental and theoretical dispersion curves will be performed by the authors in future papers.

The presented measuring method and theoretical analysis can be also extended to the identification of the mechanical properties of other classes of modern materials such as composites, intermetallics, etc.

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Appendix: Definition of the distance between two vectors (functions)

A quantitative measure of the distance between two vectors (functions) can be defined mathematically using the concept of the 'norm' introduced by Polish mathematician S. Banach in the first half of the twentieth century. The distance 'd(f,g)' between two vectors 'f' and 'g' can be defined as: d(f,g) = ||f-g||, where: $|| \cdot ||$ is a norm, e.g., Euclidean norm. The normalized distance between two vectors 'Dist(f,g)' can also be expressed in percent (%), e.g., $\text{Dist}(f,g) = ||f-g|| / ||f|| \cdot 100\%$.