Determination of the elastic properties of thin layers and graded materials using generalized Love waves

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Abstract. The elastic properties of coatings and graded materials are very important in the design and evaluation for engineering purposes. It is well known that the velocity of the ultrasonic surface waves propagating in the layered structures and graded materials is strongly dependent on the elastic properties of the medium. Thus, by using an appropriate inverse algorithm, the elastic properties can be deduced from the measured phase velocity dispersion curves (dependence of velocity on frequency) of the surface wave.

In this study we applied generalized shear surface waves (i.e., generalized Love waves) to investigate the elastic parameters of the layered media and graded materials. Generalized Love waves posses only one component of the mechanical displacement what is an advantage. Due to this reason, the mathematical description of the propagation of generalized Love waves is simpler than that using Rayleigh waves.

In this article an inversion procedure for determining the elastic and geometrical parameters of thin coating layers from the measured dispersion curves of ultrasonic shear surface waves (i.e., Love waves) is presented. The inverse problem is formulated as an optimization problem with appropriately developed objective function. The objective function depends on the material parameters of the coating layer, frequency, and experimental data (phase velocity of the surface Love wave). The minimization of the objective function leads to a set of the optimum mechanical parameters of the thin layers (e.g., thickness, shear elastic constants). Good conformity between the experimental dispersion curves and those resulting from the inverse method can prove the correctness of the proposed inverse procedure.

Keywords: inverse problems, Love waves, elastic constants, acoustic wave dispersion, thin layers, graded materials

1. Introduction

The elastic properties of coatings and graded materials are very important in the design and evaluation for engineering purposes [1,2]. E.g., Young's modulus is a main mechanical parameter that characterises the elastic stiffness of material. It is correlated with hardness and porosity [3] and determines also wear and exploitation characteristics [4,5]. Mechanical characterisation of thin films is a main issue especially in the microelectronic industry [6].

Classical mechanical methods for measuring elastic properties of thin films are tedious, time consuming and destructive. To overcome these discrepancies ultrasonic methods that use bulk and surface acoustic waves have been introduced.

Ultrasonic waves are mechanical waves and their parameters depend on the mechanical and micro-structural properties of materials where these waves propagate. Ultrasonic methods for investigation of the material properties are non-destructive methods [7]. This is a main advantage of the ultrasonic methods in relation to the mechanical methods used for investigation of the mechanical properties of materials. Moreover, ultrasonic methods can be computerised. Due to this reason, ultrasonic methods can be employed directly on the production line for measuring the mechanical parameters of materials.

It is well known that the velocity of the ultrasonic surface waves propagating in the layered structures is strongly dependent on the elastic properties of the media. Thus, by using an appropriate inverse algorithm, the elastic properties can be deduced from the measured phase velocity dispersion curves (relationship between the phase velocity and the frequency) of the ultrasonic surface wave [8,9].

In this study we applied shear horizontal surface waves (i.e., Love waves) to investigate the elastic parameters of thin coating films. Love shear surface waves can propagate in a layered structure in which the phase velocity of bulk shear acoustic waves in a layer is lower than that in a substrate.

Till present, Rayleigh surface waves have been used to investigate mechanical properties of thin surface layers [10-12]. Love waves were used mostly to evaluate the mechanical properties of layers in geoacoustics [13,14]. Rayleigh surface waves posses two components of mechanical displacement (shear vertical SV and longitudinal). By contrast, Love waves posses only one SH (shear horizontal) component of the mechanical displacement what is an advantage. Due to this reason, the mathematical description of the propagation of Love waves is simpler than that using Rayleigh waves.

The energy of Love waves is concentrated in the vicinity of the surface. The penetration depth of Love waves depends on frequency. Therefore, they are particularly useful to determine the profiles of the mechanical properties of non-homogeneous graded materials e.g., thin films deposited on an elastic substrate.

In this paper, the theoretical and experimental investigations have been carried out on the following layered structure: thin copper (Cu) layer deposited electrolytically on a steel substrate

Calculation of the surface 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 relies on the determination of unknown material parameters from the measured dispersion curves (i.e., dependence of phase velocity on frequency) of the elastic surface waves (e.g., Love waves).

In the present paper the inverse problem was formulated and solved as an optimisation problem. The objective function depending of 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 computerised measuring set-up. Making use of the optimisation 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 obtained from the inverse method elastic and geometrical parameters of thin films were used as input data in the calculations of the direct problem. Resulting from the direct problem dispersion curves were compared with those measured experimentally. Good conformity between theoretical and experimental dispersion curves has been stated. This can 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 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 shown in Fig.1. Here, an elastic isotropic layer is rigidly attached to an isotropic and elastic half-space. Mechanical vibrations of the shear horizontal surface wave are performed along the y axis parallel to the surface. The Love wave propagates along the z direction. The thickness of the layer is h.
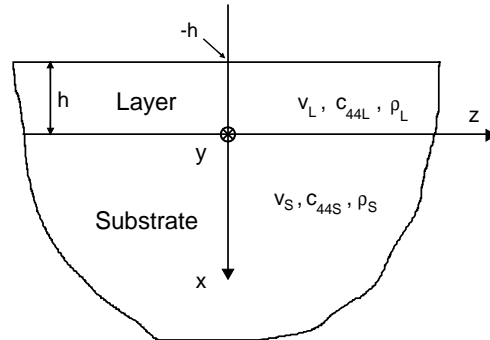

Fig.1. Geometry of a Love wave waveguide ($v_L < v_S$).

2.1.1. Dispersion equation

Using the appropriate boundary conditions, we arrive at the following dispersion equation of the Love wave propagating in a layered half-space [15]:

$$\Omega = \tan\left\{\sqrt{\left(\frac{v}{v_L}\right)^2 - 1} \cdot \beta h\right\} - \frac{c_{44S}}{c_{44L}} \frac{\sqrt{1 - \left(\frac{v}{v_S}\right)^2}}{\sqrt{\left(\frac{v}{v_L}\right)^2 - 1}} = 0 \qquad (1)$$

where: v is the phase velocity of the Love wave, v_L is the bulk shear wave velocity in the layer, v_S is the bulk shear wave velocity in the substrate, $\beta = \omega/v$ is the wave number ω is the angular frequency, c_{44S} is the shear elastic constant of the substrate, c_{44L} is the shear elastic constant of the layer material.

It can be shown from Eq.1, that the phase velocity of the Love wave depends on the elastic properties of the layered structure, thickness and frequency.

Solution of the dispersion equation (1) 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. 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 by $i>1$.

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

3. Experiment

The dispersion curves were measured in the computerised measuring set-up. In the set-up, the sending–receiving piezoelectric transducer is driven by the TB-1000 pulser–receiver computer card (Matec, USA). The Love wave impulse generated by the transducer is reflected in multiple ways between two opposite edges of the layered waveguide (Fig. 2).
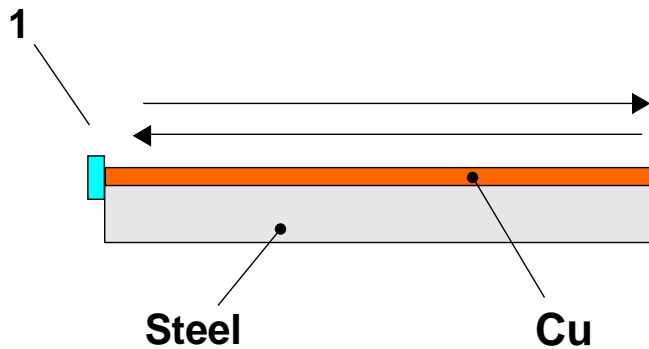

Fig.2. Waveguide (Cu on steel) of the Love wave. Shear surface wave is generated by the piezoelectric transducer (1) and propagates forth and back along the waveguide surface.

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 digitises the input analog signals. The accuracy of the measured velocity equals 0.1% i.e., 3 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. The values of time of flight "TOF" were calculated using the cross-correlation method.

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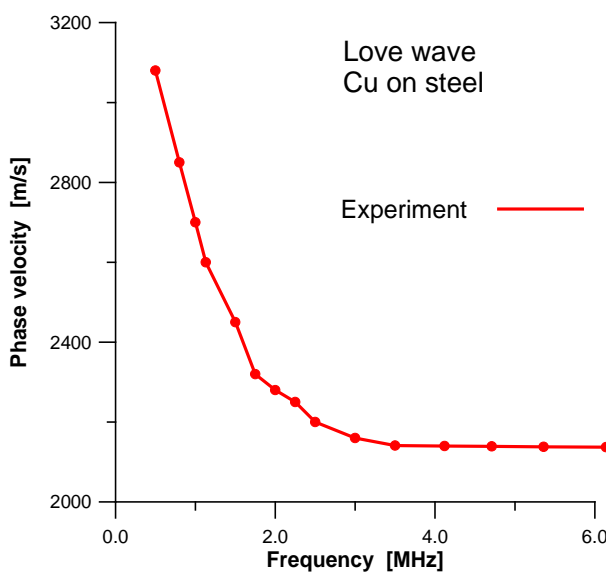

Fig.3. Measured dispersion curve of the Love wave in the layered structure Cu on steel.

3.1. Investigated structures

The measurements have been carried out on the following layered structure: thin copper (Cu) layer deposited electrolytically on a steel substrate, see Fig.3.

The phase velocity of the bulk SH acoustic wave in copper is lower than that in the steel substrate. Therefore, the Love wave can 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 shear horizontal 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
3) perform the inverse procedure

In this paper, the inverse problem was formulated and solved as an optimisation problem [16] 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 depending on the material parameters of the structure, frequency, and experimental data (phase velocity of the surface Love wave) was introduced and defined as:

$$\Pi = \sum_{j=1}^{N_e} \left| \Omega\!\left(h,\, c_{44L},\, \rho_L,\, \omega_j,\, v_j\right) \right| \qquad (2)$$

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.

Making use of the optimisation 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} and thickness h of the thin coating layer. To minimise the considered objective function Π the appropriate optimisation procedures from Mathcad® computer program were employed.

5. Determination of thin layers parameters

Minimisation 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. 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. Cu on steel structure

5.1.1. Inversion of thickness h of Cu layer

Initial value: $h = 0$ m (3), Constraints: $0 < h < 2\text{e-}3$ m (4).

Results from the inverse method: $h = 541$ μm (5).

5.1.2. Inversion of thickness h and c$_{44L}$ of Cu layer

Initial values: $h = 1\text{e-}4$ m, $c_{44L} = 3\text{e+}10$ N m^{-2} (6). Constraints: $0 < h < 2\text{e-}3$ m, $3\text{e+}10 < c_{44L} < 5\text{e+}10$ N m^{-2} (7).

Results from the inverse method: $h = 473$ μm, and $c_{44L} = 3.76\text{e+}10$ N m^{-2} (8).

5.1.3. Inversion of thickness h, c$_{44L}$ and ρ$_L$ of Cu layer

Initial values: $h = 1\text{e-}3$ m, $c_{44L} = 2\text{e+}10$ N m^{-2}, $\rho_L = 8\text{e+}3$ kg m^{-3} (9). Constraints: $0 < h < 2\text{e-}3$ m, $3\text{e+}10 < c_{44L} < 5\text{e+}10$ N m^{-2} , $7\text{e+}3 < \rho_L < 9\text{e+}3$ kg m^{-3} (10).

Results from the inverse method: $h = 486$ μm, $c_{44L} = 3.83\text{e+}10$ N m^{-2}, and $\rho_L = 9\text{e+}3$ kg m^{-3} (11)

5.1.4. Verification

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

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

Material	h	c_{44} [N m^{-2}]	ρ [kg m^{-3}]
Cu (copper) (layer)	400 μm	3.93e+10	8.9e+3
Steel (substrate)	10 mm	7.99e+10	7.8e+3

We compared the experimental dispersion curve to that obtained from the direct problem and calculated for the value of the thickness $h =$ 541 μm, see Fig.4. This value of the thickness has resulted from the solution of the inverse problem (Eq.5). Very good conformity of the theoretical and experimental dispersion curves has also been stated.
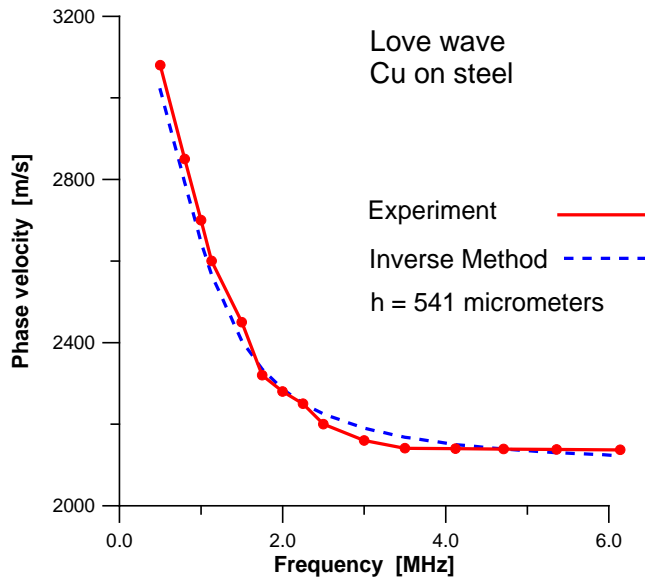

Fig.4. Comparison of the experimental dispersion curve with that obtained from the inverse method (Cu + steel structure).

The discrepancies between measured values of thickness and that resulting from the inverse method can be explained by the technological properties of the fabrication processes used to produce the layered structures. The copper surface layer was deposited electrolitycally on the steel substrate. In the present paper, we assumed that the considered layered structures consist of two layers (coating + substrate). In reality, this assumption is only an approximation, and the investigated structures can be trilayer or even multilayer.

6. Conclusions

A new inverse method employing Love waves to extract the elastic and geometrical properties of thin layers from the measured dispersion relations was established. To the authors' knowledge, the application of Love waves for determining the mechanical properties of thin coating layers is a novelty. The usefulness of the ultrasonic method employing Love waves to investigate the elastic and geometrical properties of thin coating layers has been stated.

Employing shear surface waves (i.e., Love waves) for testing thin coating layers is more convenient than Rayleigh waves because the velocity of the Love wave depends upon only one elastic constant. This simplifies significantly the solution of the direct and inverse problem.

The direct problem was formulated and solved analytically. Theoretical dispersion curves were obtained.

The inverse problem was formulated as an optimisation problem. Consequently, the objective function based on the dispersion equation was determined and minimised.

The obtained from the inverse method elastic and geometrical parameters were used as input data in the calculations of the direct problem. Resulting from the direct problem dispersion curves were compared with those measured experimentally. Good conformity between theoretical and experimental dispersion curves has been stated. This can evidence for the validity of the inverse method used for determining the mechanical properties of thin coating layers by means of shear horizontal surface waves of the Love type.

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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