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EVALUATION OF THE ELASTIC CONSTANTS OF SiO THIN FILMS FROM SAW PROPAGATION MEASUREMENTS[1]

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The dependence of the velocity of surface acoustic waves propagating in a layered structure on the elastic properties of the layer material has been used to determine the elastic stiffnesses of the isotropic layer material SiO. The applied algorithm for evaluating c_{11} and c_{44} is outlined and the role of Rayleigh-type and Love waves in layer elastic investigations is discussed.

I. INTRODUCTION

The elastic properties of thin solid films show some differences from their bulk counterparts [1]. For example, the mass density of deposited films is slightly lower than that of the corresponding bulk material. The elastic constants are different from those of the bulk material and depend on the chosen film growth conditions. Besides, there are nonstoichiometric films which have no bulk counterparts. In all these cases the elastic properties cannot be predetermined from bulk material parameters.

The purpose of this paper is to present a method for evaluating the elastic constants of a thin solid films deposited onto a substrate with well-known material parameters. This method utilizes the velocity dispersion of surface acoustic waves (SAW) in a layered structure. Some theoretical background, a description of performed experimental measurements and results for this SiO layers on lithium niobate are given.

II. SUMMARY OF WAVE PROPAGATION PROPERTIES OF LAYERED STRUCTURE [2]

Consider the configuration is shown in Fig. 1. The substrate occupies the half space $x_3 > 0$. Its surface is covered by a nonconducting thin films of thickness h

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in intimate contact with the substrate. The direction of the SAW propagation is taken as the x_1 axis. We are seeking surface waves which satisfy the mechanical boundary conditions

$$T_{31}^{(II)} = T_{32}^{(II)} = T_{33}^{(II)} = 0 \text{ at } x_3 = -h \tag{1a}$$

$$T_{3j}^{(I)} = T_{3j}^{(II)}, \; u_j^{(I)} = u_j^{(II)} \text{ at } x_3 = 0 \tag{1b}$$

$$(j = 1, 2, 3)$$

and, if the substrate and/or the layer material is piezoelectric, the electric boundary conditions

$$\varphi^{(II)} = \varphi^{(III)}, \; D_3^{(II)} = D_3^{(III)} \text{ at } x_3 = -h \tag{2a}$$

$$\varphi^{(I)} = \varphi^{(II)}, \; D_3^{(I)} = D_3^{(II)} \text{ at } x_3 = 0 \tag{2b}$$

where T_{ij} are the stresses, u_j are the particle displacements, φ is the electric potential, and D_3 is the normal component of the dielectric displacement. The superscripts I, II, III relate to the media as denoted in Fig. 1. The potential outside of the solid must satisfy Laplace's equation and must vanish for $x_3 \to \infty$.

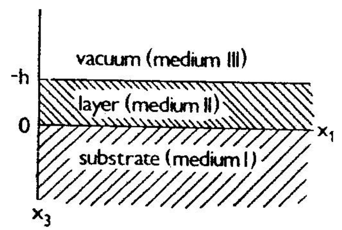

Fig. 1. Coordinate system for surface wave propagation in a layered structure. The propagation vector lies along x_1.

The coupled wave equations

$$\varrho \frac{\partial^2 u_j}{\partial t^2} = c_{ijkl} \frac{\partial^2 u_k}{\partial x_i \partial x_l} + e_{kij} \frac{\partial^2 \varphi}{\partial x_k \partial x_i} \tag{3a}$$

$$\varepsilon_{ik} \frac{\partial^2 \varphi}{\partial x_i \partial x_k} = e_{ikl} \frac{\partial^2 u_k}{\partial x_i \partial x_l} \tag{3b}$$

must be solved for the medium I (substrate) as well as the medium II (layer) where ϱ is the mass density and c_{ijkl}, e_{ijk}, ε_{ij} are the stiffnesses, the piezoelectric constants and the components of permitivity of the considered medium, respectively. The indices run from 1 to 3.

The general solution is assumed to be a linear combination of partial waves each of the form

$$u_j = A_j \exp[-\alpha k x_3] \exp[j(\omega t - k x_1)] \tag{4a}$$

$$\varphi = A_4 \exp[-\alpha k x_3] \exp[j(\omega t - k x_1)]. \tag{4b}$$

A_j are partial wave amplitudes, k is a wave number, α is a decay constant, $\omega = 2\pi f$ and f is the frequency.

Substituting (4) into (3) gives a set of linear homogeneous equations for the amplitudes A_j. This set has a nontrivial solution if the determinant of the coefficients vanishes. Solving the resulting algebraic equation yields in general (piezoelectric anisotropic medium) eight α's each as a function of the unknown phase velocity. In order to ensure that the displacement and potential amplitudes vanish for $x_3 \to \infty$ the real part of α must be positive for the substrate. Thus, because the α's occur in complex pairs with positive and negative real parts, respectively, four partial waves of the substrate and eight partial waves of the layer contribute to the general solution.

$$u_j = B_m A_j^{(m)} \exp[-\alpha^{(m)} k x_3] \exp[j(\omega t - k x_1)] \tag{5a}$$

$$\varphi = B_m A_4^{(m)} \exp[-\alpha^{(m)} k x_3] \exp[j(\omega t - k x_1)] \tag{5b}$$

where B_m are weighting factors of the partial wave amplitudes. The parameter m numbers the really existing decay constants and partial waves and the Einstein summation rule is used. Substituting (5) into (1) and (2) leads to a second set of homogeneous linear equations for the weighting factors B_m. To obtain a nontrivial solution the determinant of coefficients must vanish. The resulting equation can be considered as an implicit equation in the wave propagation velocity $v = \omega/k$. The value of v satisfying that equation can only be found by numerical methods with the help of a computer. The found v then is used to calculate the α's, A's, and B's and, thus, the general solution is known.

In some cases the complexity of computation can be reduced but use of a computer is still necessary. This happens if (a) the sagittal plane (x_1, x_3 plane) is a plane of reflection symmetry for both media, (b) the sagittal plane is perpendicular to a twofold axis of both media, (c) both media are isotropic.

Then the sets of equations separate into lower order sets. Accordingly, two different types of SAW can exist in such layered structures, the Love waves and the Rayleigh-type waves. This holds also for the intermediate case of a layered structure consisting of an anisotropic substrate and an isotropic layer provided that the sagittal plane is a plane of reflection symmetry or is perpendicular to a twofold axis of the substrate. It should be noticed that the main difference between the conditions (a) and (b) consists in the coupling behaviour of electric potential and particle displacements. Condition (a) leads to a coupling of the electric potential to the sagittal plane components of displacement. Condition (b) leads to a coupling of the electric potential to the transverse displacement component. Thereby, the generation of one of the allowed modes can be controlled in experiments.

The Love waves are surface modes polarized perpendicular to the sagittal plane. They exist if the layer shear velocity is lower than a substrate shear velocity in the considered geometry. If they exist there is a family of modes. For each mode the phase velocity at a cutoff value of hk is equal to the mentioned substrate velocity and decrease with increasing hk. At large values of hk it approximates the layer shear velocity. It can be shown by a more detailed analysis that for an isotropic layer the stiffness c_{44} of the layer material is the responsible elastic constant which influences the Love wave velocity. That means, on the other hand, that c_{44} of the layer material should be determinable from velocity measurements and otherwise measured mass density of the isotropic layer.

The Rayleigh-type waves are surface modes polarized in the sagittal plane. They degenerate at a vanish layer thickness to the Rayleigh-type wave of the substrate. There are two different situations: If the shear velocity of the layer material is lower than that of the substrate, there is also a family of modes as in the case of the Love waves. Staring at the Rayleigh-type wave velocity of the substrate the velocity in the layered structure decreases with increasing hk to the layer Rayleigh wave velocity. At a certain value of hk the second mode starts with the substrate shear velocity. It also decreases with increasing hk etc.

If the shear velocity of the layer material is much larger than that of the substrate, there is only mode. Starting at the Rayleigh-type wave velocity of the substrate the velocity in the layered structure increases towards the shear velocity of the substrate (at least for sufficiently large values of hk). Near the point where the two velocities are equal the wave becomes leaky because the penetration of the vertical component of displacement becomes very deep.

A Rayleigh-type wave consists of both a longitudinal and a vertical component of particle displacement. It can be considered as a combination of a longitudinal and a shear wave each of them contributing to the common velocity by the relevant elastic constants c_{11} and c_{44} of the isotropic layer, respectively. Therefore, these constants should be determinable from velocity measurements and the otherwise measured mass density.

III. EXPERIMENT

SiO layers were deposited onto Y-cut lithium niobate samples by the thermal evaporation method described in [3]. SAW were generated by interdigital transducers located at the interface between substrate and layer. The velocity of SAW propagating along the crystalline Z axis was determined by a delay time method yielding the group velocity v_g. The length of the propagating path was 1 cm. Different values of hk were obtained by using samples with different layer thickness h, whereas the wave number was kept constant at $k = 2\pi/48\,\mu m^{-1}$ applying always the same transducer pattern.

The dependence of the measured velocity on hk is shown in Fig. 2. The wave is classified as a Rayleigh-type wave because condition (a) of chapter 2 is satisfied and in case of decoupled modes only that mode shows an increasing velocity with increasing values of hk.

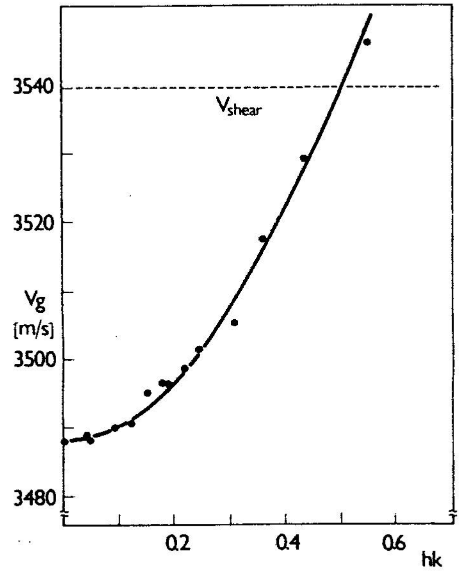

Fig. 2. Dispersion curve for an isotropic SiO layer on a YZ-LiNbO$_3$ substrate.

IV. EVALUATION OF c_{11} AND c_{44} AND DISCUSSION

The evaluation of the elastic constants of SiO was started with the computation of the phase velocity in the SiO_2/YZ-LiNbO$_3$ layered structure because the material parameters of fused quartz are known. Then the density of the layer material was changed to the actual value $\varrho_L = 2 \times 10^3\,kg/m^3$ [4] for SiO and a set of computations was performed with the layer elastic constants changed step by step. The obtained phase velocities were transformed into group velocities to be compared with the measured velocities. The elastic constants giving the best agreement of the calculated with the measured dependence of velocity on hk were found to be

$$c_{11} = 8.27 \times 10^{10}\,\mathrm{N/m^2},\ c_{44} = 3.25 \times 10^{10}\,\mathrm{N/m^2} \text{ and}$$
$$c_{12} = c_{11} - 2c_{44} = 1.77 \times 10^{10}\,\mathrm{N/m^2}.$$

From those the Poisson ratio follows as $\nu = 0.177$. The values should be compared with results obtained by measuring the SAW velocity in the SiO/YX-quartz layered structure and applying the Fernell approximation [3]. The stiffnesses obtained by converting the bulk wave velocities of SiO from [3] and assuming $\nu = 0.177$ are

$$c_{11} = 7.97 \times 10^{10}\,\mathrm{N/m^2},\ c_{44} = 3.13 \times 10^{10}\,\mathrm{N/m^2} \text{ and}$$
$$c_{12} = c_{11} - 2c_{44} = 1.71 \times 10^{10}\,\mathrm{N/m^2}.$$

The difference (about 4 %) seem to be too large with regard to the accuracy of the measured velocity of better than 0.1 %. We suppose that the following facts are mainly responsible for the observed differences:

Firstly, the film growth conditions cannot be kept absolutely constant. For example, small uncontrolled changes of the evaporation rate of SiO cause variations of the layer composition leading to regions of limited thickness with different mass density and different elastic constants. The computation algorithm, on the other hand, presumes a homogeneous layer.

Secondly, the two rows of stiffnesses were obtained from layers grown on different substrate materials leading at least to growth differences in the initial state.

Thirdly, the fitting procedure can give inaccurate values of c_{44} and c_{12}, respectively, because the velocity in the layered structure was found to be only weakly dependent on c_{44}. Therefore, one should look for a substrate configuration where the SiO layer will lead to a love wave in order to determine independently the stiffness c_{44}.

Last not least, it should be remembered that the results for SiO on quartz were obtained by an approximation method.

V. CONCLUSIONS

The elastic constants of thin layers of isotropic materials can be evaluated from a measured SAW velocity dispersion in a layered structure by using a fitting procedure. The stiffnesses c_{11} and c_{44} are simultaneously obtained by using the Rayleigh-type waves as demonstrated in case of SiO layers on lithium niobate. An independent and more accurate determination of c_{44} by the Love waves is recommended.

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ОПРЕДЕЛЕНИЕ УПРУГИХ ПОСТОЯННЫХ ТОНКИХ ПЛЕНОК SiO НА ОСНОВЕ ИЗМЕРЕНИЙ РАСПРОСТРАНЕНИЯ ПОВЕРХНОСТНЫХ АКУСТИЧЕСКЫХ ВОЛН

Для определения постоянных жесткостей изотропного слоя материала SiO использована зависимость скорости распространения поверхностных акустических волн в слоистой структуре на его эластические свойства. Описана схема вычисления коэффициентов c_{11} и c_{44}, а также обсуждается роль волн типа Релея и Лава в исследованиях эластических свойств тонких пленок.