GUIDED SH-WAVES FOR ANALYSIS OF STRATIFIED NANO-MATERIALS

a joint proposal prepared by

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Executive Summary

The proposed research is targeted to address the problems associated with characterizing the properties of nano-layers in multilayered plates commonly used for MEMS and other microelectronic devices. In order to do this in a rapid, reliable, nondestructive fashion, it is necessary to solve the main problem on identification of physical properties and structure of anisotropic nano-layers in multilayered plates composed of layers having different physical properties and structure. For resolving this problem, the joint team is developing a combined theoretical and experimental technique based on propagation of guided SH- and Love waves, and capable of analyzing multilayered plates containing up to 20 nano-layers of different physical properties and structure.

In the course of the proposed research work the following theoretical and experimental problems should be analyzed and solved:

- Propagation of guided SH-waves in a multilayerd plate composed of anisotropic layers with contrast physical properties and satisfying possibly asymmetric boundary conditions, which model real boundary conditions imposed on the outer surfaces.
- Obtaining assessments and bounds of applicability of the continuum theory for analyzing wave propagation in nano-structures, by comparing with the molecular dynamic approaches.
- Developing an adequate experimental technique for excitation, registration, and filtering guided SH-waves propagating in multilyared nano-structures.
- Inverse problem on identification of physical properties and structure of a particular internal layer by analyzing the dispersion relations.

The main objectives of the proposed research flowing out directly from its title are as follows:

- Developing the combined theoretical and experimental non-destructive technique exploiting guided SH-waves for analyzing properties of the internal nano-layers in multilayared plates.
- Developing numerical algorithms capable of analyzing surface SH-waves propagating in stratified anisotropic media containing large number of nano-layers.
- Developing algorithms for solution of the inverse problems on identifying physical properties of an internal particular layer.

While principally oriented to addressing the characterization of microelectronic devices, the proposed research effort also has applications in several different areas of science and technology where nondestructive evaluation of material properties of multiple layers is needed: seismology, acoustical microscopy, composite manufacturing, biomechanics, etc. Of particular importance in this regard is the ability to characterize the properties of very thin films as they are deposited. Functional gradient materials (FGM) are being utilized with increasing frequency in practical applications. Micro-electromechanical systems (MEMS) devices are often built up via multiplayer deposition. The methods under development in this research program are well suited for real-time on-line process control applications; principally through the use of laser based ultrasonic techniques as they are nondestructive, noncontact and minimally invasive.

Methods of analyses:

- Propagation of surface SH-waves in a homogeneous layer with monoclinic elastic anisotropy will be studied using the six-dimensional complex formalism approach, allowing us to obtain both qualitative (structure and existence of the solutions, polarization of the surface waves, etc.), and quantitative (values for the phase and group speed, the dispersion relations, etc.) results.
- Waves in the stratified media will be analyzed by the straightforward method combining the six-dimensional complex formalism for an individual layer, then formulating contact type boundary conditions on the interfaces, and resolving an eigenproblem for the specially constructed matrix (modified Transfer matrix method).
- The inverse problem of identification of the material properties of a single layer in a multilayered plate will be studied with a variety of approaches including iterative methods such as Levenberg-Marquardt, simplex methods, and the use of genetic algorithms.

The successful completion of this research effort will promote a better understanding nature of the surface waves and giving methods for predicting properties and structure of internal layers inaccessible by the direct measurements and lead to a variety of important materials characterization applications.

Project Description

1 Introduction

Growing demands in microelectronics and other areas of modern technology require the development of precise, nondestructive materials characterization techniques. Typically these methods are based on acoustics, heat conduction or electromagnetics (including optics and x-ray propagation). The use of extremely high frequencies in acoustical measurements, permits the analysis of both the fine structure of a material and the presence of microscopic defects. Experimental acoustical analyses of multilayered plates composed by anisotropic layers on an anisotropic substrate has revealed that frequencies of about 1 GHz are capable of analyzing physical properties and structure of the internal layers with the typical thickness 0.1-1 micron.

Generally, the acoustical measurements needed for material structure identification are the velocities and polarization of the propagating waves. These measurements allow us to plot the dispersion relations (velocities vs. frequency). Using an appropriate forward propagation model it is possible to predict the precise nature of these dispersion relationships given an initial estimate of the material properties/geometric features of interest. Then, through the use of one of the iterative algorithms mentioned above, it is possible to perturb these property estimates in a systematic fashion to bring the predicted dispersion curves into good agreement with the experimentally measured quantities. Therefore, in order to exploit the obtained experimental data for the internal layer identification, a suitable wave propagation model must be developed in order to analyze propagation of the guided waves in laminated anisotropic media.

As will be shown further the existing theoretical methods on surface waves are mainly confined to either isotropic layers on an isotropic substrate with a relatively large number of layers (but, generally, not exceeding ten layers). With additional simplifying assumptions on structure of layers and the propagating waves or for materials with fewer layers (generally, 1-3 layers), some degree of material anisotropy may be introduced.

Meanwhile, the needs of the modern microelectronics industry demand a theoretical framework and numerical algorithms efficient enough to analyze plates containing up to 20 layers lying on an anisotropic substrate (typically single crystal silicon). It is not out of place to note here that a similar problem arises in seismology as well. In this case the frequencies are much lower and generally do not exceed 1KHz. Numerous existing theoretical and experimental works in seismological sciences have revealed the lack of a suitable methodology for studying this complex problem.

In this joint research effort, a team of investigators has been assembled to attack this problem both theoretically and experimentally. The main goal is to develop a sound theoretical framework for analysis of the guided acoustic waves in the multilayered anisotropic bodies containing up to ten layers with arbitrary elastic anisotropy.

2 Literature Review

The following three main types of guided waves can propagate in a laminated plate lying on a substrate: Love and Lamb waves which propagate in a plate, and Rayleigh wave propagating on a substrate. The following review of the guided wave literature is not intended to be exhaustive; rather it covers only those papers which authors regarded as essential for the subsequent analysis.

2.1 LOVE AND SH-WAVES

These are waves which can propagate in a layer, or multiple layers in contact with an elastic half-space, where an exponentially attenuating (with depth) wave of the same polarization propagates. Described by A.E.H. Love (1927), these waves were then extensively studied both analytically, see (Dieulesaint and Royer, 1974), (Achenbach, 1975) and experimentally. These waves can play an important role in nondestructive mechanical property characterization.

A single isotropic layer on isotropic half-space with doubly corrugated surfaces (both the interface and free surface) was studied by Elbahrawy (1994), see also (Lobkis and Chimenti, 1997). A theoretical analysis of Love waves propagating in layered isotropic media by reducing the problem to a series of step-continuous ordinary differential equations was suggested by Mal and Knopoff (1968).

Quite often Love waves are registered in the course of seismic activity, see (Mal 1962), (Chastel and Dawson, 1993) and explosions (Penttila, 1960), (Mclaughlin et al., 1992), (Simons, Zielhuis, van der Hilst, 1999). These waves are also used in seismology for identifying the properties of sedimentary basins (Kennett, 1995, 1998), (Zhang Y.-S., and Tanimoto, 1991), (Hisada, Yamamoto, and Tani, 2001). See also recent papers on Love and SH-wave propagation (Kuznetsov, 2004, 2005).

It should be noted, that in Love's original treatise and in most subsequent works, a wave propagating in a layer is assumed to have real wave numbers. This results in neglecting possible wave modes with the exponential variation of the amplitude. However, the latter type of waves arise for some types of anisotropy when the wave length is comparable or smaller than the typical layer thickness.

2.2 LAMB WAVES

These waves were originally proposed by Lamb (1904, 1917) and arise in an isotropic layer with the traction-free boundary surfaces. In contrast to Love waves, Lamb waves, generally are composed by several partial waves having different polarization. Lamb waves are widely used in NDT because of their low attenuation. One of the early theoretical studies of Lamb waves propagating in isotropic layers is due to Victorov (1967), where structure of the dispersion relations was analyzed, and the three fundamental brunches of the wave spectrum were observed. Correlation of Lamb waves with a membrane carrier wave in an isotropic plate was considered by Achenbach (1998).

Presumably, the first derivation of equations for analysis of Lamb waves propagating in a stratified medium containing arbitrary number of *isotropic* layers was proposed by Thomson (1950), who introduced a transfer matrix, which allows us to express the displacements and surface tractions at the bottom of a particular layer in terms of the corresponding parameters at the top of a layer. Later on this method was corrected by Haskell (1953), and at present is known as Thomson-Haskell or "Transfer matrix" method. Various numerical implementations of this method revealed, that it leads to numerical instability in the course of degenerate matrices when layers of large thickness compared to the wavelength are presented, see Lowe (1995). An alternative approach known as "Global matrix" method, for analysis of Lamb waves propagating in *isotropic* laminates, was proposed by Knopoff (1964). In this method a single matrix comprising all of the boundary conditions for all of the layers is constructed. Numerical implementations of this method revealed that it is much more robust in comparison with the Thomson-Haskell method, see Mal (1988).

The study of Lamb waves in anisotropic layers with s specific anisotropy goes back to Lekhnitskii (1949), Newman and Mindlin (1957), and Mindlin (1960). Adler (1990) reduced the problem of Lamb wave propagation in a multilayered structure containing anisotropic layers with specific anisotropy, to purely a algebraical one; see (Adler et al., 1990) and an early paper by Fahmy and Adler (1972). A simplified analytical method for analysis of Lamb waves in a multilayer plate containing anisotropic layers was later proposed by Yang and Kundu (1998).

The following papers are also devoted to the analysis of Lamb waves propagating in anisotropic plates with specific anisotropy (Dayal and Kinra; 1989, 1991), (Liu et al., 1990), (Lin and Keer, 1992). A combination of analytical solutions and numerical procedures for analysis of a thin anisotropic film on an anisotropic substrate with cubic or hexagonal symmetry was used by Mallah, Philippe, and Khater (1999), similar approach was applied by Nakahata et al. (1995). Extrapolation of the corresponding results to layers with the arbitrary anisotropy was undertaken only recently, see theoretical works by Shuvalov (2000) and Kuznetsov (2001).

Lamb waves in the periodically layered anisotropic composites were studied by Ting and Chadwick (1988) by application of the sextic formalism. Obliquely traveling Floquet partial wave solutions for analyzing Lamb waves propagating in a periodically layered composite plate were used by Safaeinili et al. (1995). A method based on the asymptotic expansions for analysis of both Lamb and Rayleigh waves in layered media containing layers with weak anisotropy, was proposed by Rossikhin (1992). A heuristic homogenization technique for analysis of surface waves in layered anisotropic structures containing periodically alternating layers, was proposed by Park (1996), see also (Potel et al., 1999) for experimental verification of the theory of surface waves in multilayered structures with infinite number of periodical layers (in the latter paper the resulting wave turns out to be a Rayleigh wave, while in a particular layer it is a Lamb wave). Lamb waves in a composite plate having the internal structure composed by thin layers oriented transversely to the plate surfaces were considered by Chimenti (1994).

2.3 RAYLEIGH WAVES

In the pioneering work by Lord Rayleigh (1885) a secular equation for the speed of an exponentially decaying with depth surface wave propagating on isotropic half-space was found. Only much later were approximate formulae (Bergmann, 1933), (Victorov, 1967), (Mozhaev, 1991) and analytical solutions (Rahman and Barber, 1995), (Grishin, 2001) obtained for Rayleigh wave on an isotropic half-space.

The Rayleigh method was later extrapolated to anisotropic media by Stoneley (1955), who obtained expressions for the Rayleigh wave speed, provided that wave propagates in the plane of elastic symmetry of a cubic crystal and in a direction of crystallographic axes. Some errors in Stoneley's arguments were, however, introduced by neglecting the possibility oscillating solution. Tthis was eventually corrected by Synge (1956). Subsequently, the solution was extrapolated to the high symmetry directions in hexagonal crystals (Dielesaint and Royer, 1980) and in orthorombic crystals (Royer and Dielesaint, 1985).

A numerical approach based on the three-dimensional complex formalism, was developed by Farnell (1970). He studied both the Rayleigh wave speed and its polarization for a great number of monocrystals mainly of cubic symmetry, and did not discover any "forbidden direction" along which Rayleigh wave could not propagate. It should be mentioned that even though this approach constitutes the most powerful tool for numerical Rayleigh wave analysis, this method can lead to wrong solutions when multiple roots of the characteristic polynomials associated with the Christoffel equation arise.

A kind of six-dimensional formalism for Rayleigh wave analysis was proposed by Stroh (1962). It is based on similarity of solutions for line dislocations in unbounded medium and propagation of Rayleigh waves. This approach was mainly developed by Barnett and Lothe (1973, 1974) and later by Chadwick et al. (1977, 1979). By application of this formalism, theorems of uniqueness and existence for such waves were proved.

A newly developed variant of the six-dimensional formalism (Kuznetsov, 2002a, b) allowed him to obtain analytical solutions for some cubic and hexagonal crystals, when a special kind of degeneracy occurs. See also (Tanuma, 1996) and (Ting, 1997), where the similar situation is studied by applying Stroh's formalism. Comparing these two types of complex formalism, it should be noted that both are equally applicable to analysis of half-spaces or layers with homogeneous boundary conditions. Presumably, inhomogeneous or contact type boundary conditions could be analyzed more easily by a newer variant of the six-dimensional formalism.

2.4 CONCLUDING REMARK ON THE LITERATURE REVIEW

The literature review reveals that the following theoretical problems need to be analyzed and solved in the course of the proposed research effort: (i) constructing solutions for Rayleigh and Lamb waves propagating in (homogeneous) media with arbitrary elastic anisotropy and satisfying the inhomogeneous boundary conditions for surface traction fields; (ii) constructing and analyzing solutions for guided waves in laminated bodies composed by finite number of anisotropic layers.

Along with the main theoretical problems, several technical questions should be also solved including: (i) development of numerical algorithms for resolving matrix differential equations associated with the Christoffel equation, (ii) development of high precision algorithms for root determination for polynomials of the high order (up to 63^d for 10 anisotropic layers on an anisotropic substrate with arbitrary anisotropy); (iii) constructing the solution for the eigenproblem associated with the special non-symmetric matrices arising in the surface wave analysis of multilayered structures.

3 Work in progress

Recent work at the Institute for Problems in Mechanics of Russian Academy of Sciences (IPM) on surface wave analyses for determination of physical properties of layers in multilayered structures has focused on (i) developing a theory of bulk, Rayleigh, Love and Lamb waves propagating in anisotropic media with arbitrary elastic anisotropy, based on the six-dimensional complex formalism with a view to avoid restrictions of known analytical solutions, and (ii) developing adequate theory and numerical algorithms for analysis of the layered structures.

3.1 BASIC NOTATIONS

An outline of the theory of surface waves based on six-dimensional complex formalism, is given for Rayleigh and Lamb waves, similar approach with obvious simplifications and modifications can be applied to analysis of Love waves.

The equation of dynamics for anisotropic hyperelastic media has the form:

$$\operatorname{div} \mathbf{C} \cdot\cdot \nabla \mathbf{u} - \rho \ddot{\mathbf{u}} = 0 \qquad (1)$$

where $\mathbf{u}$ is the displacement, ρ is the density of the medium, and $\mathbf{C}$ is a positive definite four-dimensional tensor of elasticity; i.e.

$$\mathbf{S} \cdot\cdot \mathbf{C} \cdot\cdot \mathbf{S} > 0, \qquad \underset{\mathbf{S}\neq 0,\ \ \mathbf{S}\in \operatorname{sym}(R^3 \otimes R^3)}{\forall \mathbf{S}} \qquad (2)$$

The displacement field for plane surface wave has the following representation:

$$\mathbf{u}(\mathbf{x}) = \mathbf{m}\, e^{i(\gamma\, \mathbf{v}\cdot\mathbf{x} + \mathbf{n}'\cdot\mathbf{x} - ct)} = \mathbf{m}\, e^{-\alpha \mathbf{v}\cdot\mathbf{x}}\ e^{i(\beta \mathbf{v}\cdot\mathbf{x} + \mathbf{n}'\cdot\mathbf{x} - ct)}$$

$$\beta = \operatorname{Re}(\gamma), \quad \alpha = \operatorname{Im}(\gamma) \qquad (3)$$

where $\mathbf{m}$ is a complex amplitude vector, $\mathbf{v}$ is the unit vector normal to the plane of propagation Π_ν, $\mathbf{n}' \subset \Pi_\nu$ is the unit vector defining the direction of propagation of Rayleigh or Lamb wave, and c is the corresponding phase speed. For Rayleigh waves it will be assumed that $\nu \cdot \mathbf{x} > 0$ and that the wave attenuates with depth, so $\alpha > 0$, while β can be arbitrary real. For Lamb waves both parameters α and β are arbitrary.

Along the boundary surfaces, boundary conditions for the zero surface tractions must be given; e.g.

$$\mathbf{t}_\nu \equiv \nu \cdot \mathbf{C} \cdot\cdot \nabla \mathbf{u}\big|_{\Pi_\nu} = 0 \qquad (4)$$

3.2 LIMITING SPEEDS

Substitution of the Eq. (3) into Eq. (1) gives Christoffel's equation for the determination of the exponent γ ; i.e.

$$\begin{aligned}&\det\left[(\gamma\nu+\mathbf{n}')\cdot\mathbf{C}\cdot(\mathbf{n}'+\gamma\nu)-\rho c^2\mathbf{I}\right]\equiv\\ &\equiv\det\left[\gamma^2(\nu\cdot\mathbf{C}\cdot\nu)+\gamma(\nu\cdot\mathbf{C}\cdot\mathbf{n}'+\mathbf{n}'\cdot\mathbf{C}\cdot\nu)+\mathbf{n}'\cdot\mathbf{C}\cdot\mathbf{n}'-\rho c^2\mathbf{I}\right]=0\end{aligned} \tag{5}$$

At the fixed speed c this is a polynomial of degree 6 in γ .

Definition. Limiting speeds which correspond to the unit vectors ν and $\mathbf{n}'$, are defined by:

$$c_i^{\lim} = \inf_{\varphi\in\left[-\frac{\pi}{2};\frac{\pi}{2}\right]}\left(\cos^{-1}(\varphi)\sqrt{\rho^{-1}\lambda_i(\mathbf{w}\cdot\mathbf{C}\cdot\mathbf{w})}\right), \quad i=1,2,3 \tag{6}$$

where λ_i, i=1,2,3 are eigenvalues arranged in descending mode, and **w** is the unit (real) vector belonging to the sagittal plane, and $\mathbf{w}=\cos(\varphi)\mathbf{n}'+\sin(\varphi)\boldsymbol{\nu}$.

It is obvious that if $c < c_1^{\lim}$, then Christoffel's equation has only one pair of complex-conjugate roots, and if $c < c_3^{\lim}$, then there are three pairs of complex- conjugate roots. Since for existence of the Rayleigh wave at least one pair of complex conjugate roots is needed, one concludes the following rule:

Proposition 1 Speed of the Rayleigh wave can not exceed $c_1^{\lim}$.

For Lamb waves limiting speed $c_3^{\lim}$ specifies waves traveling with the subsonic speed.

3.3 PROPERTIES OF CHRISTOFFEL'S EQUATION

Christoffel's equation, written in terms of a complex root, produces an equation for the appropriate (complex) eigenvectors in C^3

$$\begin{aligned}&(\mathbf{G}-\rho c^2\mathbf{I})\cdot\mathbf{m}=0, \qquad \mathbf{G}\equiv\mathbf{A}+i\mathbf{B}\\ &\mathbf{A}\equiv\left[\mathbf{n}'\cdot\mathbf{C}\cdot\mathbf{n}'+(\beta^2-\alpha^2)\nu\cdot\mathbf{C}\cdot\nu+\beta(\mathbf{n}'\cdot\mathbf{C}\cdot\nu+\nu\cdot\mathbf{C}\cdot\mathbf{n}')\right]\\ &\mathbf{B}\equiv\alpha\left[2\beta\nu\cdot\mathbf{C}\cdot\nu+(\nu\cdot\mathbf{C}\cdot\mathbf{n}'+\mathbf{n}'\cdot\mathbf{C}\cdot\nu)\right]\\ &\mathbf{m}'\equiv\mathrm{Re}(\mathbf{m}),\ \ \mathbf{m}''\equiv\mathrm{Im}(\mathbf{m})\end{aligned} \tag{7}$$

Hence, the following additional conclusion directly flows from the analyses of Eq. (7)

Proposition 2. *a*) If $\mathbf{m}', \mathbf{m}'' \notin \ker(\mathbf{A} - \rho c^2\mathbf{I})$, then $\mathbf{m}', \mathbf{m}'' \notin \ker(\mathbf{B})$ and

$$\left[\mathbf{B}^{-1} \circ (\mathbf{A} - \rho c^2 \mathbf{I})\right]^2 = -\mathbf{I} \tag{8}$$

in the real (necessarily two-dimensional) space generated by vectors $\mathbf{m}'$ and $\mathbf{m}''$;

b) If $\mathbf{m}', \mathbf{m}'' \in \ker(\mathbf{A} - \rho c^2\mathbf{I})$, then $\mathbf{m}', \mathbf{m}'' \in \ker(\mathbf{B})$;

c) If $\mathbf{m}' \in \ker(\mathbf{A} - \rho c^2\mathbf{I})$ and $\mathbf{m}'' \notin \ker(\mathbf{A} - \rho c^2\mathbf{I})$, then $\mathbf{m}'' \in \ker \mathbf{B}$ and $\mathbf{m}'' \in \ker \mathbf{B}$ and $\mathbf{m}' \notin \ker \mathbf{B}$ (and vice versa).

It is obvious that Proposition 2 covers all possibilities for components of the eigenvector of matrix **G**.

Corollary 1. Condition of the Proposition 2.a ensures that:

a) Both matrices **B** and $(\mathbf{A} - \rho c^2\mathbf{I})$ are not of fixed sign in the two-dimensional subspace $Z \subset R^3$ generated by the components $\mathbf{m}'$ and $\mathbf{m}''$;

b) $\mathbf{B}(Z) \subset Z$, $(\mathbf{A} - \rho c^2\mathbf{I}) \subset Z$;

c) Unimodal matrix $\mathbf{B}^{-1} \circ (\mathbf{A} - \rho c^2\mathbf{I})$ in any basis in *Z* has the form

$$\mathbf{B}^{-1} \circ (\mathbf{A} - \rho c^2\mathbf{I}) = \begin{pmatrix} \delta & \chi \\ -\frac{1+\delta^2}{\chi} & -\delta \end{pmatrix} \tag{9}$$

where δ and χ are real, and $\chi \neq 0$;

d) Matrices **A** and **B** do not commute with each other.

Corollary 2. Condition of the Proposition 2.c ensures that:

a) Vectors $\mathbf{m}'$ and $\mathbf{m}''$ both are noncollinear;

b) Tensors $\mathbf{A} - \rho c^2\mathbf{I}$ and **B** have following structure

$$\begin{aligned} \mathbf{A} - \rho c^2\mathbf{I} &= 0 \quad \mathbf{m}' \otimes \mathbf{m}' + c_1 \quad \mathbf{v}_1 \otimes \mathbf{v}_1 - c_1 \quad \mathbf{v}_2 \otimes \mathbf{v}_2, \\ \mathbf{B} &= \;\; 0 \quad \mathbf{m}'' \otimes \mathbf{m}'' + c_2 \quad \mathbf{w}_1 \otimes \mathbf{w}_1 - c_2 \quad \mathbf{w}_2 \otimes \mathbf{w}_2 \end{aligned} \tag{10}$$

where c_1, c_2 are non-zero real numbers, vectors $\mathbf{m}', \mathbf{v}_1, \mathbf{v}_2 \in R^3$ are mutually orthogonal, and vectors $\mathbf{m}'', \mathbf{w}_1, \mathbf{w}_2 \in R^3$ are mutually orthogonal also.

Corollary 3. The real part β of the complex root satisfies the inequality

$$-\frac{\lambda_{\max}(\nu \cdot \mathbf{C} \cdot \mathbf{n}' + \mathbf{n}' \cdot \mathbf{C} \cdot \nu)}{2\,\lambda_{\max}(\nu \cdot \mathbf{C} \cdot \nu)} \leq \beta \leq -\frac{\lambda_{\min}(\nu \cdot \mathbf{C} \cdot \mathbf{n}' + \mathbf{n}' \cdot \mathbf{C} \cdot \nu)}{2\,\lambda_{\min}(\nu \cdot \mathbf{C} \cdot \nu)} \tag{11}$$

Proposition 3. For any complex root γ the matrix **G** is not normal.

Proposition 4. Under condition of the proposition 2.b the eigenspace in R^3 generated by vectors $\mathbf{m}'$, $\mathbf{m}''$ is one-dimensional.

Let $W_{\mathbf{G}}$ be eigenspace of matrix $\mathbf{G}$ corresponding to the eigenvalue ρc^2.

Proposition 5. a) $\dim W_{\mathbf{G}} = 1$, provided that both matrices $\mathbf{A}' \equiv \mathbf{A} - \rho c^2 \mathbf{I}$ and $\mathbf{B}$ do not have zero eigenvalues, and relation (8) holds;

b) $\dim W_{\mathbf{G}} = 2$, provided that relation (8) holds, and both matrices $\mathbf{A}' \equiv \mathbf{A} - \rho c^2 \mathbf{I}$ and $\mathbf{B}$ have zero eigenvalue;

c) $\dim W_{\mathbf{G}} = 1$, provided that relation (8) does not hold, and both matrices $\mathbf{A}' \equiv \mathbf{A} - \rho c^2 \mathbf{I}$ and $\mathbf{B}$ have zero eigenvalue.

3.4 BOUNDARY CONDITIONS ON THE OUTER SURFACE

For any value of the parameter $\rho c^2 < c_1^{\lim}$, the surface wave can be composed of $n \le 3$ partial waves:

$$\mathbf{u}(\mathbf{x}) = \sum_{j=1}^{n} C_j \ \mathbf{m}_j \ e^{i(\gamma_j \nu \cdot \mathbf{x} + \mathbf{n}' \cdot \mathbf{x} - ct)} \tag{12}$$

where C_j are complex scalars. In Equation (12) complex roots are considered according to their multiplicity. Substitution of this representation into boundary conditions (4) gives the following matrix equation with respect to C_j:

$$\begin{aligned} &(\nu \cdot \mathbf{C} \cdot \nu) \cdot \left(\sum_{j=1}^{n} \gamma_j C_j \mathbf{m}_j \right) + (\nu \cdot \mathbf{C} \cdot \mathbf{n}') \cdot \left(\sum_{j=1}^{n} C_j \mathbf{m}_j \right) \equiv \\ &\equiv \sum_{j=1}^{n} \left(\gamma_j (\nu \cdot \mathbf{C} \cdot \nu) + (\nu \cdot \mathbf{C} \cdot \mathbf{n}') \right) \cdot \mathbf{m}_j \quad C_j = 0 \end{aligned} \tag{13}$$

Equation (13) can be written in the form $\mathbf{H} \cdot \vec{C} = 0$. Generally, the matrix **H** is not Hermitian, but it is possible to construct Hermitian matrix $\mathbf{H}^* \cdot \mathbf{H}$ which is equivalent to **H** with respect to its rank

$$(\mathbf{H}^* \cdot \mathbf{H})_{ij} = \overline{\mathbf{m}}_i \otimes (\overline{\gamma}_i \mathbf{v} + \mathbf{n}') \otimes \mathbf{v} \cdots \mathbf{C} \cdot \mathbf{C} \cdots \mathbf{v} \otimes (\mathbf{n}' + \gamma_j \mathbf{v}) \otimes \mathbf{m}_j \quad (14)$$

This matrix is more convenient for the computations. Vanishing of the determinant of this matrix ensures the existence of a nontrivial solution for coefficients C_j.

3.5 BOUNDARY CONDITIONS ON THE INTERFACE

At the interface plane Π_{k-1} the following contact type boundary conditions are formulated:

$$\begin{aligned} \mathbf{t}_{k-1} &= -\mathbf{t}_k; \\ \mathbf{u}_{k-1} &= \mathbf{u}_k \end{aligned} \quad (15)$$

where $\mathbf{t}_k$ is the surface traction field for the k-th layer. Substituting the corresponding surface tractions and displacements into Eqs. (15) yields equations containing the unknown coefficients C_j. The desired secular equation will be obtained by equating the corresponding determinant to zero, which ensures existence of non-trivial solutions for a multilayered plate.

Direct analysis shows that for the general case of elastic anisotropy in both layers and the substrate, the order of thus obtained system S of linear equations becomes

$$\operatorname{ord}(S) = 6k + 3 \quad (16)$$

where k is number of layers. The nontrivial solution of the system S exists if and only if $\operatorname{rank}(S) < \operatorname{ord}(S)$.

It should be noted that when both layers and the substrate have a plane of elastic symmetry coinciding with the sagittal plane (the latter is determined by direction of wave propagation $\mathbf{n}$ and the unit normal $\mathbf{v}$ to the plane boundary), the order of the system S can be computed by the following expression

$$\operatorname{ord}(S) = 4k + 2 \quad (17)$$

3.6 CONCLUDING REMARK

A more detailed analysis of Rayleigh and Lamb waves propagating in anisotropic media with arbitrary elastic anisotropy, along with some of solutions for cubic and hexagonal crystals can be found in the recent papers by one of the authors (Kuznetsov, 2001, 2002a, b).

4 Objectives

The proposed research effort has several objectives having significance for both theory and applications:

1. Development of the theory of surface waves (Rayleigh, Lamb, surface SH, and Love waves) propagating in homogeneous media with arbitrary anisotropy, free from inherent limitations in the existing approaches.
2. Development of numerical and analytical methods based on the six-dimensional complex formalism for analyses of speed and polarization of surface waves propagating in arbitrary directions in anisotropic media.
3. Development of the theory of surface waves in laminated anisotropic bodies composed by finite number of different layers lying on an anisotropic substrate.
4. Development of the regularization techniques and inverse numerical algorithms for determination of physical properties of layer(s) principally through the analysis of the dispersion relations of guided waves in multiplayer structures.

Along with the main objectives, the following immediate goals should be mentioned:

1. Contribution to non-destructive evaluating properties of the internal layers in microelectronics, as well as seismology, biomechanics, and acoustical microscopy by analyzing speed and polarization of the surface waves propagating in the stratified media.
2. Contribution to numerical mathematics by developing high precision program packages for the root determination of the polynomials of high order; solving eigenproblems for matrices of the special structure, and developing numerical algorithms for solving the impedance boundary value problems for matrix ODE.

It is believed that the research effort will lead to a better understanding of the problem of surface waves propagation in the stratified media containing multiple anisotropic layers.

5 Scope

5.1 DEVELOPMENTS IN THE THEORY OF SURFACE WAVES

As was pointed out earlier, previous theories of the regarded surface waves propagating in homogeneous anisotropic media ignore the case of inhomogeneous boundary conditions for the surface traction fields (with the only exception of the clamped boundary conditions). The theory which takes into account this circumstances is been developing by one of the teams (IPM) for several years. The following steps should be made to complete the theory:

- Proof of the equality of algebraic multiplicity of eigenvalue ρc^2 to its geometric multiplicity in relation to the Christoffel equation for surface waves; this will result in the complete characterization of spectral properties of the Christoffel equation;
- Analyses of conditions imposed on the elasticity coefficients of cubic and hexagonal crystals and on the inhomogeneous boundary conditions, at which no Rayleigh, Love, surface SH, or Lamb wave can propagate, resulting in revealing the situations at which barriers for the surface waves exist;
- Study of the spectral properties of the equations for surface waves propagating in the stratified media with finite number of anisotropic layers on the substrate with cubic or hexagonal symmetry, resulting in obtaining analytical expressions for the dispersion relations.

5.2 DEVELOPMENTS IN THE THEORY OF INVERSE PROBLEMS FOR IDENTIFICATION OF THE PROPERTIES OF LAYER(S) BY ANALYZING THE DISPERSION RELATIONS

Application of the considered theory needs in solution of the following theoretical problems:

- Analysis of the (multivalued) operator mapping the whole set of admissible values of the parameters describing the process of wave propagation onto the set of possible values of the wave velocities; proof of the compactness of any of the continuous branches of the operator, resulting in proof of the ill-conditionality of the inverse operator for a continuous branch operator.
- Application of the regularization technique based on construction of the Tychonov regularization operator for obtaining numerically stable solutions for the regarded inverse problem; numerical determination of the optimal regularization parameters for constructing the continuous inverse operators .

- In the event that no continuous inverse operator can be obtained, iterative schemes for this operation will be developed. Of particular importance in this phase of the effort will be the potential use of genetic algorithms to avoid problems in the reconstruction process due to the presence of local minima.

5.3 SOFTWARE DEVELOPMENT

Computer codes based on the preceding analyzes will be developed bearing in mind (i) the reliability of the obtained data; (ii) the speed of computing; and (iii) the ease of use. The source program will be developed in FORTRAN (main computations) and in C++ (shell, user interface, graphical visualization). The following program packages utilizing the high precision arithmetic (with mantissas up to 1K digits) will be developed:

- Program package for analysis of the surface waves in homogeneous media with arbitrary elastic anisotropy, based on the developed six-dimensional complex formalism.
- Program package for solution of the multiple contact problems on the interfaces for surface waves traveling in the multilayered media
- Program package for solution of the inverse problem on identifying properties of the layer(s) by applying the regularization techniques.

Special attention will be given to the problem of relocation of the program to different platforms (PC's, RISC work stations, Main frame computers).

5.4 SIMULATION

In order to assess the utility of this approach for the characterization of multiple functional layers on an anisotropic substrate, a series of simulated reconstruction experiments will be conducted. The theoretical dispersion curves for guided wave propagation on a series of samples of varying composition and geometry will be studied. The configurations will be chosen to be representative of microelectronic applications. The substrate under consideration will be single crystal silicon with a [100] orientation. A variety of different layer sequences will be studied. Typical coating layer materials will be isotropic and include polycrystalline silicon, silicon carbide and silicon nitride. A variety of layer thicknesses will be investigated ranging from 100 Angstroms to 1000 Angstroms. Dispersion curves will be generated sequentially for each layer as it is being deposited. The inversion algorithm developed in this program will then be used to reconstruct the elastic moduli and thickness of the multiplayer structure.

5.5 Experimental Verification

The next stage in the development of this technique for practical application to electronic materials characterization is experimental verification. Samples will be created with the same composition and geometry of the simulation. A high power Q-switched Nd-YAG laser will be used to excite the acoustic waves on the sample and a confocal Fabry-Pereot interferometer will be used to sense the resulting acoustic disturbance. The detected waveform information will be used to construct the experimental dispersion curves required for the reconstruction.

The basic physics behind laser generation of ultrasound are well documented and understood. When a target material is exposed to a localized laser pulse, the material in the vicinity will experience a rapid thermal expansion. This serves as a center of dilatation within the material and launches stress waves into the material. Thus we have a noncontact, nondestructive means of launching stress waves in a media in a controlled fashion. The bandwidth for these pulses is quite wide and well suited for characterizing thin films and coatings (Doxbeck et. al. , 2002). It should be noted that, as the intensity of the laser is increased, there is the possibility of surface ablatement. This is of course, a means of generating large amplitude stress waves but is destructive. Here, stress waves are launched as matter is ejected from the surface via momentum transfer, As we seek a nondestructive measure of material properties, we will operate well below the threshold energy for surface ablatement. Depending on the geometry, both bulk waves (longitudinal and shear) and guided waves (Rayleigh, Lamb , Love, Stoneley) can be generated. Since we are dealing with layered media in this research effort, we will concentrate here on Love waves. Laser generation has been used extensively to study guided waves in solids, albeit at somewhat lower frequencies than those required for thin film characterization.

Similarly, there has been a great deal of study regarding noncontact laser sensing of the surface displacements. One of the authors of this proposal (RAK) was involved with some of the original applications of laser detection to ultrasonic wave propagation phenomena (Kline et. al 1978, 1981). In these early investigations, a Michaelson interferometer was used to precisely measure the normal component of surface displacement. In order to address sensitivity fluxuations due to small random, low frequency changes in the operating environment, a path stabilization feature was introduced into the design of the interferometer through the use of a piezoelectrically driven mirror on the reference arm of the interferometer. This approach has been supplanted more recently through the use of a confocal Fabry-Perot design which results in a significantly more stable signal.

Most of the experimental work to date with guided waves has involved plate waves. Plate waves are multi-mode and highly dispersive and have much in common with the Love waves of interest in this study. In most cases, this presents a problem as it difficult to isolate a particular mode of interest in the complex waveforms that are usually found in these experiments. Therefore, a great deal of research effort has been devoted to developing techniques of mode isolation for plate wave applications, both isotropic and anisotropic. These methods include:

- Signal Processing
- Electromagnetic Acoustic Transducers (EMAT's)
- Laser Techniques
- Interdigital Transducers

The most common approach to mode isolation is through the use of advanced signal processing techniques. Spectral refinement using narrow band signals and Fourier processing techniques, for example, can be used to isolate a particular component of interest in a complex waveform as demonstrated by Cawley and Alleyne (1993). Alternatively, one can use specialized generation techniques, to produce a particular mode of interest by tailoring the source to match the desired characteristics of the mode of interest, Here, the goal is to excite a propagating disturbance of a single wavelength While the physical generation mechanism is different, this approach is the basis for EMAT, laser and interdigital generation. For laser based experiments, a diffraction grating is used to produce multiple lines which are spaced according to the wavelength of the plate mode of interest (Addison and McKie, 1995 and Nagata et. al. 1995). In this way a single mode can be readily isolated. This is the approach we will utilize in this study.

Laser based techniques will be used to construct dispersion curves for guided wave propagation in each layer of the electronic device after deposition. These results will then be used to reconstruct the mechanical properties of the newly deposited, unknown layer. This means that we will rely upon the known properties of the substrate as well as the experimentally determined properties in the previously deposited layers in the reconstruction. In this way we will be able to determine all pertinent mechanical properties throughout the structure. These results will be compared with literature values for these parameters. However, there is a considerable spread in the reported data for thin films of many of these materials 9 Maximenko et. al. 2002. This variation is largely attributable to sensitivity to small variations in processing conditions during deposition. Therefore, we will supplement this phase of the investigation with direct stiffness measurements from the vibrational characteristics of cantilever beam samples made with isolated thin film material. This of course means using much lower frequencies than those of the ultrasonic tests. However, these ceramic materials do not appear to exhibit a large frequency dependence in their mechanical response for bulk specimens. It is reasonable to believe that the same would be true for the thin films as well.

5.6 Facilities

Several of the support facilities required for this project are already in place at SDSU. We have a high power Q-switched Nd-YAG laser from Continuum that can be used for ultrasonic excitation. We will need to build the optical system for generating multiple line sources and controlling their spacing. We are currently working closely with the U.S. Navy's Spawar's facility on a related project on modeling the mechanical behavior of MEMS assemblies. We will be able to use some of the specimens developed for the current U. S. Navy project in the research program proposed here. There is one main equipment purchase planned for this program. We will need to purchase a a confocal Fabry-Perot interferometer for precise , high frequency surface displacement measurements. This equipment will be purchased in year 1 of this program.

Sample characterization equipment includes a Buehler precision saw, polishing machine Rotoforce-2, dilatometer from Theta Inc. (for thermal expansion measurements), optical image analysis system, and a cold and hot mounting press (for SEM preparation). Computational facilities include Silicon Graphics computers, each with Stereographic Crystal Eyes, and thirty SUN Sparc Ultras, networked with myrnet running UC Berkeley's NOW network. SDSU is also a member of the national CRAY Supercomputer Consortium with on-campus vBNS network connection. There is also a scanning electron microscope on campus that will be available for use in this program.

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Year 1 Budget

Salaries

R. Kline	Academic Year (3 months at 10%)	$ 3,230
	Summer (1 month at 100%)	$10,770
S. Kuznetsov	(3 months)	$15,000
Postdoctoral RA	(1 year)	$30,000

Fringe Benefits

R. Kline	$ 3,500
S. Kuznetsov	$ 2,000
Postdoctoral RA	$ 6,000

Materials and Supplies

Specimen Fabrication	$ 5,000
Optics for Laser Generation(diffraction grating, optical fibers, etc.)	$ 2,500

Travel

3 Trips between Moscow and San Diego for PI's & RA	$ 7,500

Total Direct Costs	$85,500
Total Indirect Costs	$44,460

Equipment

Confocal Fabry-Perot Interferometer	$ 75,000
Total	$204,460

Year 2 - Budget

Salaries

R. Kline	Academic Year	(3 months at 10%)	$ 3,360
	Summer	(1 month at 100%)	$11,200
S. Kuznetsov		(3 months)	$15,600

Postdoctoral RA (1 year)	$31,200
Fringe Benefits	
R. Kline	$ 3,640
S. Kuznetsov	$ 2,080
Postdoctoral RA	
	$ 6,240
Materials and Supplies	
Miscellaneous	$ 2,500
Travel	
3 Trips between Moscow and San Diego for PI's & RA	$ 7,500
Total Direct Costs	$83,320
Total Indirect Costs	$43,326
Total	$126,646