



RESEARCH ARTICLE

ELASTIC CONSTANTS AND STRESS-STRAIN IN THIN FILMS: APPLICATION IN FIBBER-TEXTURED GOLD FILM BY X-RAY DIFFRACTION

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ABSTRACT

The purpose of the present article is to make a model using analytical equations, based on elasticity theory of continuous media for small deformations, with the aim of completely characterizing the material in their mechanical properties as well as the principal stresses-strains of thin films. The approach differs from the standard literature which usually brings crystal symmetries or is directly concerned with crystalline materials. It is entirely possible to define and to analyse anisotropy in elastic media from first principles in thin films. Therefore, the constitutive relation between strain and stress will be considered orthotropic, obeying the generalized Hooke's law. A new equation for the stress of the film-substrate system is proposed based on Newton's laws and energy conservation. As an application, it uses the technique and data developed by Faurie *et al* (2005) in fiber-textured gold film deposited onto Kapton substrate by combining synchrotron X-Ray diffraction in situ tensile testing. As the gold thin film and substrate are considered transversely isotropic, therefore, is firstly required a texture analysis with the purpose of determining the possible Euler angles (Ψ) and (Φ) for each crystallographic direction that can be used in the model equations. With the data, it is possible to make graphics, $\epsilon(\text{strain}) \times F$, for every force applied to the sample. Comparing the experimental graphs with the theoretical equations it was possible obtained their mechanical properties and the principal stresses-strains of the anisotropic gold thin film. The results are compared with the results of Faurie *et al* (2005).

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INTRODUCTION

Given the fast growth and new challenges of nanotechnology, metallic and non-metallic thin films have a great technological application, for example, metallic films are typically employed as coatings and interconnections in microelectronic, solar cells, optical waveguides, photolithographic masks, solid state devices, among many others (Avilés *et al.*, 2009). Thus, the studies of the physical properties of thin films have caught the attention of the scientific community nowadays. The study of mechanical properties such as Young's modulus, shear modulus and Poisson's ratio are important in materials science (Devarakonda, 2011). Measurements of the elastic constants of thin films have been problematic and usually require sophisticated equipment or destructive techniques (Chen, 2007) being a challenging research topic (Bonderover, 2004). A variety of techniques have been used to measure elastic constants of thin films. Basically, the techniques can be classified into two groups: destructive and non-destructive. The destructive techniques damage or modify the sample film properties being tested. The most common techniques are the tensile tests, technical detection and resonance ultrasound spectroscopy. Non-destructive techniques involve measurements that do not alter the properties of the films, the substrate curvature technique with the X-ray diffraction technique. The X-ray diffraction technique uses the phenomenon of diffraction in the incidence of a wave upon the sample by means of an elastic

scattering. It is a high precision technique, being one of the best choices and tools for measuring the elastic constants of thin films (Chang, 2009). However, the measurement of the elastic constants in thin films by XRD cannot be determined directly. It is necessary to measure some property of the material (such as deformation) (Maniet *et al.*, 2005). We will make use of the technique and data developed by Faure *et al* (2005) in gold thin films deposited onto Kapton substrate, which was studied by using in situ tensile tester in a four-circle goniometer, on a synchrotron beam line (LURE, France) (Faurie *et al.*, 2005), as well as the model proposed by Santos in his PhD thesis (Santos, 2010). A new equation for the stress of the film-substrate system will be deduced. This technique consists of measuring the deformation suffered by the material under uniaxial tension to be applied "in situ". However, first of all, it is important to begin with an anisotropy analysis through the pole figures (measure of the intensity of diffraction planes on the basis of the angles Euler (Ψ) and (Φ)) with the purpose of determining the possible (Ψ) angles for each crystallographic direction that can be used in the model equations. Once the angles of the crystallographic directions are chosen, it is possible to find out the deformation for each force applied to the sample. The determination of the elastic constants as well as the stress-strain in thin films are obtained by using the elasticity theory of continuous media for small deformations. The constitutive relation between strain and stress is considered linear, using the generalized Hooke's law with orthotropic anisotropy. The equation for the stresses of film-substrate system is proposed based on Newton's laws and energy conservation. Our results are compared with the results of Faurie *et al* (2005). This work is organized as follows: In section 2 we review linear elasticity theory and the constitutive relation between stress and strain for orthotropic materials. In section 3 we present our proposal. In section 4 we give an application in fiber-textured gold film. In section 5 we present our results and discussion and in section 6 we present our conclusions.

THEORETICAL BACKGROUND

General Remakes: In the development of a macroscopic phenomenological theory, the use of constitutive relations has a key role. They allow us to characterize the state of macroscopic physical systems experimentally. A constitutive relation is a relationship between two physical quantities that is specific to a material. Constitutive relations are particular to each material and are used to classify different materials according to their behaviour. The mechanical behaviour, relate tension with a parameter of the body's movement, usually the deformation or deformation rate. There are many other types of constitutive equations such as (I) those that relate stress with deformation and temperature, (II) those that relate stress with electric or magnetic fields, (III) Ohm's law, (IV) the law governing the friction force, etc (Santos, 2010). According to Helbig (1994) "Historically the study of anisotropic elastic materials has been synonymous with the study of crystals", and according to L. Bos (2004) "This historical association does not stem from any sort of conceptual necessity. On the contrary, it is entirely possible to define and to analyse anisotropy in elastic media from first principles without any mention of crystals or of crystal symmetry. Pedagogically this makes it clear that the notion of anisotropy rests solely on the equations of elasticity and does not involve any additional assumptions to the effect that an elastic medium can be modelled as a piecewise collection of crystals, which it cannot. This approach differs from the standard literature which typically invokes crystal symmetries as a starting point for the analysis of anisotropy, or it is directly concerned with crystalline materials". Thus, we will begin the studies using the constitutive relation given by the generalized Hooke's law. For any given orthogonal transformations of three-dimensional space, the type of symmetry is triclinic, monoclinic, orthotropic, tetragonal, transverse isotropy and isotropy (Bos *et al.*, 2004). In this work we assume orthotropic material.

Linear elasticity theory: Linear elasticity is a theory used to study the behaviour of material bodies that are deformed when submitted to external actions (forces caused by the contact with other bodies, gravitational force acting on mass, etc.) then returned to their original form when the external action is removed, with no permanent change in the material volume. Within certain limits that depend on the material and temperature, the applied stress is roughly proportional to the strain. In general, the deformation of a solid involves the combination of a volume change and a change in the sample's form. Thus, for a given state of deformation, it is necessary to determine the contributions of changes in volume and shape. The volume change is caused by variation of the principal stresses and shape change of the sample is caused by tangential stresses. In the model, small deformation of the tangential stresses is neglected and the principal stresses are considered, represented on laboratory coordinate system by (Kohnke, 1989):

$$\varepsilon_{\Phi\Psi} = \varepsilon_{xx} \cos^2 \Phi \sin^2 \Psi + \varepsilon_{yy} \sin^2 \Phi \sin^2 \Psi + \varepsilon_{zz} \cos^2 \Psi \quad (1)$$

Where Ψ and Φ are Euler angles.

A more general linear relation between strain and stress is the generalized Hooke's law establishing the proportionality between stress and strain magnitudes, represented in tensor form by (Lempriere, 1968).

$$\sigma_{ij} = \Lambda_{ijkl} \varepsilon_{kl} \quad (2)$$

Here σ_{ij} , Λ_{ijkl} , and ε_{kl} represent the stress tensor, the elasticity tensor and the strain tensor, respectively. The stress, σ_{ij} , is a second-order tensor and it is represented by a square matrix, where the principal diagonal, σ_{ii} are called principal stress and the non-diagonal components are called shear stress. The strains, ε_{kl} , are a second-order symmetric tensor. The elasticity tensor, Λ_{ijkl} , is a fourth-order tensor and contains $3^4 = 81$ elements. Due to the symmetry tensor properties we can reduce the number of elastic constants to only 21. They are called triclinic due to the fact that they have no planes of symmetry.

When the material allows symmetry operations (rotations, reflections or inversions) in its structure, the number of material constants is also reduced (Klug, 1974).

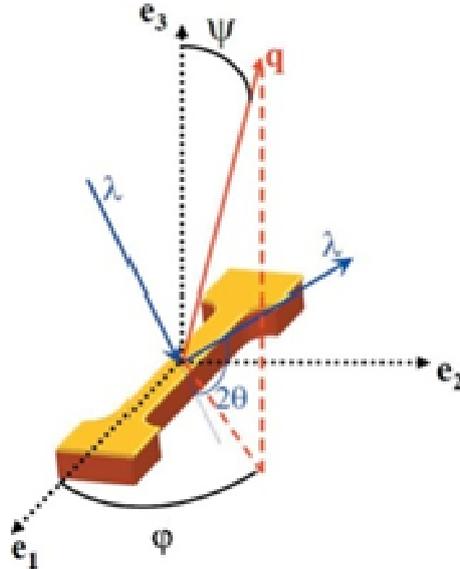


Figure1. The uniaxial tensile stress applied to the film-substrate system is along ε_1 axis. The direction of the scattering vector q is defined by the in-plane azimuthal angle Φ from ε_1 and the polar angle Ψ from the sample normal direction ε_3 . λ is the wavelength of the X-rays (Faurie, 2005)

Orthotropic materials have three planes/axes of symmetry. The elastic behaviour of an orthotropic material is characterized by nine independent constants. In phenomenological terms they are referred to as three longitudinal moduli of elasticity or Young's moduli (E_x , E_y and E_z), which describe the tendency of an object to deform along an axis when opposing forces are applied along that axis, three transverse moduli of elasticity or shear moduli (G_{xy} , G_{yz} and G_{xz}) which describe an object's tendency to shear, (the deformation of a shape at a constant volume) when acted on by opposite forces; and three Poisson coefficients (ν_{xy} , ν_{xz} and ν_{yz}) which describe the ratio of transverse contraction strain to longitudinal extension strain in the direction of the stretching force (Shames, 1964). Given the measurement of all the engineering constants of an orthotropic material along the principal directions using the compliance matrix, the elastic behaviour of an orthotropic material is represented as follows, in Voigt notation (Klug, 1974)

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{pmatrix} = \begin{pmatrix} \frac{1}{E_x} & -\frac{\nu_{yx}}{E_x} & -\frac{\nu_{zx}}{E_x} & 0 & 0 & 0 \\ -\frac{\nu_{xy}}{E_x} & \frac{1}{E_y} & -\frac{\nu_{zy}}{E_y} & 0 & 0 & 0 \\ -\frac{\nu_{xz}}{E_x} & -\frac{\nu_{yz}}{E_y} & \frac{1}{E_z} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2G_{yz}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2G_{xz}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2G_{xy}} \end{pmatrix} \cdot \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \tau_{yz} \\ \tau_{xz} \\ \tau_{xy} \end{pmatrix} \quad (3)$$

Can obtain the following relations from the principal axis:

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \end{pmatrix} = \begin{pmatrix} \frac{1}{E_x} & -\frac{\nu_{yx}}{E_x} & -\frac{\nu_{zx}}{E_x} \\ -\frac{\nu_{xy}}{E_x} & \frac{1}{E_y} & -\frac{\nu_{zy}}{E_y} \\ -\frac{\nu_{xz}}{E_x} & -\frac{\nu_{yz}}{E_y} & \frac{1}{E_z} \end{pmatrix} \cdot \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \end{pmatrix} \quad (4)$$

As the matrix that characterizes the material is symmetric, then we have the following relations:

$$\frac{\nu_{yx}}{E_y} = \frac{\nu_{xy}}{E_x}, \frac{\nu_{zx}}{E_z} = \frac{\nu_{xz}}{E_x}, \frac{\nu_{yz}}{E_y} = \frac{\nu_{zy}}{E_z}; \quad (5)$$

To calculate the state equation of principal triaxial stress, we use the relations (4), taking into account the principal directions. Then:

$$\frac{\sigma_{xx}}{E_x} - \frac{\nu_{yx}}{E_y} \sigma_{yy} - \frac{\nu_{zx}}{E_z} \sigma_{zz} = \varepsilon_{xx} \quad (6)$$

$$-\frac{\nu_{xy}}{E_x}\sigma_{xx} + \frac{\sigma_{yy}}{E_y} - \frac{\nu_{zy}}{E_z}\sigma_{zz} = \varepsilon_{yy} \quad (7)$$

$$-\frac{\nu_{xz}}{E_x}\sigma_{xx} - \frac{\nu_{yz}}{E_y}\sigma_{yy} + \frac{\sigma_{zz}}{E_z} = \varepsilon_{zz} \quad (8)$$

In cases where the shear modules are not found in the equations, since they are in the principal axis, we have the following relations (Kohnke, 1989):

$$G_{xy} = \frac{E_x E_y}{E_x + E_y + 2\nu_{xy} E_x} \quad (9)$$

$$G_{yz} = \frac{E_y E_z}{E_y + E_z + 2\nu_{yz} E_y} \quad (10)$$

$$G_{xz} = \frac{E_x E_z}{E_x + E_z + 2\nu_{xz} E_x} \quad (11)$$

OUR PROPOSAL

Relation between stresses and elastic constants with orthotropic symmetry: Note that from the equations (6), (7) and (8) we could make algebraic operations in order to obtain relations between stresses and the elastic constants. Assuming that the force applied to the thin film is at the x direction, we can divide the equation (7) by (6) and we obtain:

$$\frac{\sigma_{zz}}{\sigma_{yy}} = \frac{(1 - \nu_{xy}\nu_{yx})}{(\nu_{yz} + \nu_{xz}\nu_{yx})} \quad (12)$$

Proceeding analogously, combining equations (8) and (6), and (8) and (7), we get, respectively,

$$\frac{E_z}{E_y} = \frac{\nu_{xy}(1 - \nu_{xy}\nu_{yx})}{(\nu_{yz}^2\nu_{xy} + \nu_{xz}^2\nu_{yx} + 2\nu_{yz}\nu_{xz}\nu_{xy}\nu_{yx})} \quad (13)$$

$$\frac{E_z}{E_x} = \frac{\nu_{yx}(1 - \nu_{xy}\nu_{yx})}{(\nu_{yz}^2\nu_{xy} + \nu_{xz}^2\nu_{yx} + 2\nu_{yz}\nu_{xz}\nu_{xy}\nu_{yx})} \quad (14)$$

In equation (4) we can calculate the determinant of the matrix A associated with the material. Thus, together with the symmetry relation (5) implies:

$$\det A = \frac{\nu_{xy}(1 - \nu_{xy}\nu_{yx})E_y - (\nu_{yz}^2\nu_{xy} + \nu_{xz}^2\nu_{yx} + 2\nu_{yz}\nu_{xz}\nu_{xy}\nu_{yx})E_z}{\nu_{yx}E_x E_y E_x E_z} \quad (15)$$

Using the relation (13) we obtain that:

$$\det A = 0 \quad (16)$$

Where A is material matrix. It's indicating that the matrix is not invertible, therefore it can proposal a new equation. The equation below is "ad hoc" and obeys the equations (6), (7) and (8).

$$\frac{\sigma_{xx}}{\sigma_{yy}} = \frac{(1 - \nu_{xy}\nu_{yx})}{(\nu_{yz} - \nu_{xz}\nu_{yx})} \quad (17)$$

Using equations (12) and (17) in equations (6), (7) and (8), we obtain:

$$\sigma_{xx} = \frac{(\nu_{yz} + \nu_{xz}\nu_{yx})(1 - \nu_{xy}\nu_{yx})\varepsilon_{xx}E_x}{(\nu_{yz} + \nu_{xz}\nu_{yx})(1 - \nu_{xy}\nu_{yx}) - (\nu_{yz} - \nu_{xz}\nu_{yx})(\nu_{xz} + \nu_{xy}\nu_{yz})} \quad (18)$$

$$\sigma_{yy} = \frac{(\nu_{yz} + \nu_{xz}\nu_{yx})(\nu_{yz} - \nu_{xz}\nu_{yx})\varepsilon_{yy}E_y}{(\nu_{yz} + \nu_{xz}\nu_{yx})(\nu_{yz} - \nu_{xz}\nu_{yx}) - (1 - \nu_{xy}\nu_{yx})[\nu_{yx}(\nu_{yz} + \nu_{xz}\nu_{yx}) + \nu_{yz}(\nu_{yz} - \nu_{xz}\nu_{yx})]} \quad (19)$$

$$\sigma_{zz} = \frac{(1 - \nu_{xy}\nu_{yx})(\nu_{yz} - \nu_{xz}\nu_{yx})E_z\varepsilon_{zz}}{(1 - \nu_{xy}\nu_{yx})(\nu_{yz} - \nu_{xz}\nu_{yx}) - (\nu_{yz} + \nu_{xz}\nu_{yx})[\nu_{zx}(1 - \nu_{xy}\nu_{yx}) + \nu_{zy}(\nu_{yz} - \nu_{xz}\nu_{yx})]} \quad (20)$$

The strain and stress tensors are always related to the principal axes. Substituting relations (6), (7) and (8) in equation (1), we obtain the following result:

$$\begin{aligned} \varepsilon_{\Phi, \Psi} = \sin^2 \psi \left\{ \frac{\sigma_{xx}}{E_x} [(1 + \nu_{xy}) \cos^2 \Phi + (\nu_{xz} - \nu_{xy})] + \frac{\sigma_{yy}}{E_y} [(1 + \nu_{yx}) \sin^2 \Phi + (\nu_{yz} - \nu_{yx})] \right. \\ \left. - \frac{\sigma_{zz}}{E_z} (1 + \nu_{zy} \sin^2 \Phi + \nu_{zx} \cos^2 \Phi) \right\} - \left(\frac{\nu_{xz}\sigma_{xx}}{E_x} + \frac{\nu_{yz}\sigma_{yy}}{E_y} - \frac{\sigma_{zz}}{E_z} \right) \end{aligned} \quad (21)$$

Where, ν_{xy} , ν_{yx} , ν_{xz} , ν_{zx} , ν_{yz} and ν_{zy} are the Poisson coefficients, E_x , E_y and E_z are Young's moduli and σ_{xx} , σ_{yy} , σ_{zz} are the principal stresses at the directions x, y and z, respectively. Equation above is the key relation used in the model proposed for the principal triaxial stress state (Santos, 2010).

In what follows we will find a new equation that relates the elastic constants of the thin film with the force applied to the film-substrate system.

An equation for the film-substrate system: In this section we consider a new equation for the stresses of film-substrate system which is proposed based on Newton's laws and energy conservation. We assume the interface between the two-lamina composite (the film and the substrate) which is subjected to an uniaxial tension load along with the direction e_1 , (Fig 1.) to be perfect (Faurie, 2005).

We will assume that, due to the "Poisson's effect" the strain on the z-direction exist and it is not neglectable. Thus, every state of strain and stress are present on the thin film: three principal strains and three principal stresses.

$$\varepsilon_{xx}^f = \varepsilon_{xx}^s \quad (22)$$

$$\varepsilon_{yy}^f = \varepsilon_{yy}^s \quad (23)$$

Using the equation (12) we can relate the ε_{zz} deformations in the ε_{xx} and ε_{yy} directions, as follows:

$$\varepsilon_{zz}^f = \frac{\nu_{yz}^f}{\nu_{yx}^f} \varepsilon_{xx}^f - \left(\frac{\sigma_{yy}^f}{\sigma_{zz}^f} \right)^f \left(\frac{\varepsilon_{xx}^f + \nu_{yx}^f \varepsilon_{yy}^f}{\nu_{yx}^f} \right) \quad (24)$$

Assuming that the substrate is an orthotropic material, we have:

$$\varepsilon_{zz}^s = \frac{\nu_{yz}^s}{\nu_{yx}^s} \varepsilon_{xx}^s - \left(\frac{\sigma_{yy}^s}{\sigma_{zz}^s} \right)^s \left(\frac{\varepsilon_{xx}^s + \nu_{yx}^s \varepsilon_{yy}^s}{\nu_{yx}^s} \right) \quad (25)$$

We can divide the equation (22) by (23), we get:

$$\nu_{xy}^f = \nu_{xy}^s \tag{26}$$

$$\nu_{yx}^f = \nu_{yx}^s \tag{27}$$

If the interface between the two laminas is assumed to be perfect, that is, the resultant load, F_{app} , along the longitudinal direction supported by the specimen film-substrate system is the sum of the loads supported by the film and the substrate. The forces acting upon the film along the directions x, y and z, we have:

$$F_{app} = F_x^f + F_x^s \tag{28}$$

$$F_y = F_y^f + F_y^s = 0 \tag{29}$$

$$F_z = F_z^f + F_z^s = 0 \tag{30}$$

In terms of stresses:

$$\sigma_{app} = g_f \sigma_{xx}^f + g_s \sigma_{xx}^s \tag{31}$$

$$\sigma_{yy} = g_f \sigma_{yy}^f + g_s \sigma_{yy}^s = 0 \tag{32}$$

$$\sigma_{zz} = g_f \sigma_{zz}^f + g_s \sigma_{zz}^s = 0 \tag{33}$$

Where g_f and g_s are the fractional thicknesses of the thin film and the substrate, respectively.

With the equations (32) and (33), we get:

$$\left(\frac{\sigma_{yy}}{\sigma_{zz}} \right)^f = \left(\frac{\sigma_{yy}}{\sigma_{zz}} \right)^s \tag{34}$$

Thus the equation (25) yields:

$$\epsilon_{zz}^s = \frac{\nu_{yz}^f}{\nu_{yx}^f} \epsilon_{xx}^f - \left(\frac{\sigma_{yy}}{\sigma_{zz}} \right)^f \left(\frac{\epsilon_{xx}^f + \nu_{yx}^f \epsilon_{yy}^f}{\nu_{yx}^f} \right) = \epsilon_{zz}^f \tag{35}$$

As a result of the above, we can deduce that:

$$\nu_{yz}^f = \nu_{yz}^s \tag{36}$$

The work done by the stresses during the process of deformation is stored in the form of elastic potential energy (Shames, 1964).

$$dw = \int \sigma d\epsilon dv \tag{37}$$

For a material with linear behavior, the specific strain energy is represented as follows:

$$U_0 = \frac{dw}{dv} = \frac{\sigma \epsilon}{2} \tag{38}$$

In the case of thin films, and considering linear elastic behavior, the specific strain energy is given by:

$$U_0 = \frac{1}{2} \sigma_{xx}^f \epsilon_{xx}^f + \frac{1}{2} \sigma_{xx}^s \epsilon_{xx}^s + \frac{1}{2} \sigma_{yy}^f \epsilon_{yy}^f + \frac{1}{2} \sigma_{yy}^s \epsilon_{yy}^s + \frac{1}{2} \sigma_{zz}^f \epsilon_{zz}^f + \frac{1}{2} \sigma_{zz}^s \epsilon_{zz}^s \tag{39}$$

Where f and s indices are related to the film and the substrate, respectively.

Using equations (22), (23) and (35) and then (32),(33) and (34) in the equation above, we have:

$$U_0 = \frac{1}{2g_s} \sigma_{xx}^f (g_s - g_f) \varepsilon_{xx}^f + \frac{1}{2g_s} \sigma_{app} \varepsilon_{xx}^f + \frac{1}{2g_s \nu_{yx}^f} \sigma_{yy}^f (g_f - g_s) \varepsilon_{xx}^f + \frac{1}{2g_s \nu_{yx}^f} \sigma_{zz}^f \nu_{yz}^f (g_s - g_f) \varepsilon_{xx}^f \quad (40)$$

This equation relates the specific strain energy for the thin film with respect to stress and strain in the film. Let us suppress the index f since all terms are related to the film.

According to Drucker's postulate, (Mase,1970), the work done by the external agent during the deformation process is stored in the form of elastic potential energy, meaning that.

$$W_{ext} = W_{all} \quad (41)$$

$$U_0 = \frac{W_{all}}{V} = 2\sigma_{app} \cdot \varepsilon_{all} \quad (42)$$

The total strain on the film-substrate system is:

$$\varepsilon_{all} = \varepsilon_{all}^f + \varepsilon_{all}^s \quad (43)$$

Where ε_{all} is the sum of the total deformation module of the film and substrate and depends on the geometry. Manipulating (40), (42) and (43) algebraically we obtained:

$$\sigma_{app} = \left\{ \frac{(g_f - g_s) (-\nu_{yx} \sigma_{xx} + \sigma_{yy} - \nu_{yz} \sigma_{zz})}{\nu_{yx} [4g_s (\varepsilon_{all}^f + \varepsilon_{all}^s) - \varepsilon_{xx}]} \right\} \varepsilon_{xx}^f \quad (44)$$

This equation expresses the stresses to the thin film due to the stresses applied on the film-substrate system for orthotropic materials.

Using equation (7) and the properties of symmetry (5) we obtain:

$$E_y = \left\{ \frac{[4g_s (\varepsilon_{all}^f + \varepsilon_{all}^s) - \varepsilon_{xx}]}{(g_f - g_s) \varepsilon_{xx}} \right\} \frac{\sigma_{app} \nu_{yx}}{\varepsilon_{yy}} \quad (45)$$

This equation relates the Young's modulus of the film in the y direction to the stresses applied to the film-substrate system for orthotropic material. Let us now make an application of the obtained equations.

Set of equations with transverse isotropic symmetry

Note that a material with transversely isotropic anisotropy has five constants that characterize its elastic tensor. Assuming an xy plane of symmetry, the elastic constants are E_x , E_z , G_{xy} , ν_{xy} and ν_{xz} . Equations (6), (7) and (8), for transversely isotropic symmetry, ($\nu_{xy} = \nu_{yx}$), become:

$$\frac{\sigma_{xx}}{E_x} - \frac{\nu_{xy}}{E_x} \sigma_{yy} - \frac{\nu_{xz}}{E_x} \sigma_{zz} = \varepsilon_{xx} \quad (46)$$

$$-\frac{\nu_{xy}}{E_x} \sigma_{xx} + \frac{\sigma_{yy}}{E_x} - \frac{\nu_{xz}}{E_x} \sigma_{zz} = \varepsilon_{yy} \quad (47)$$

$$-\frac{\nu_{xz}}{E_x} \sigma_{xx} - \frac{\nu_{xz}}{E_x} \sigma_{yy} + \frac{1}{E_z} \sigma_{zz} = \varepsilon_{zz} \quad (48)$$

With these results we can calculate the coefficients of the Poisson, assuming that the force applied to the thin film is the x direction.

$$v_{xy} = -\frac{\varepsilon_{yy}}{\varepsilon_{xx}}; v_{xz} = -\frac{\varepsilon_{zz}}{\varepsilon_{xx}} \quad (49)$$

Using the assumption that the material is transversely isotropic, equations (12), (13), (17), (18), (19) and (20) then reduce to the following ones:

$$\frac{\sigma_{zz}}{\sigma_{yy}} = \frac{(1 - v_{xy})}{v_{xz}} \quad (50)$$

$$\frac{\sigma_{xx}}{\sigma_{yy}} = \frac{(1 + v_{xy})}{v_{xz}} \quad (51)$$

$$\frac{E_z}{E_x} = \frac{(1 - v_{xy})}{2v_{xz}^2} \quad (52)$$

$$\sigma_{xx} = \frac{(1 + v_{xy})}{(1 + v_{xy} - v_{xz})} \varepsilon_{xx} E_x \quad (53)$$

$$\sigma_{yy} = -\frac{v_{xz}}{v_{xy}(1 + v_{xy} - v_{xz})} \varepsilon_{yy} E_x \quad (54)$$

$$\sigma_{zz} = -\frac{(1 - v_{xy})}{v_{xz}(1 + v_{xy} - v_{xz})} \varepsilon_{zz} E_x \quad (55)$$

Subtracting the relations (53) and (54), we have:

$$(\sigma_{xx} - \sigma_{yy}) = \frac{E_x}{(1 + v_{xy})} (\varepsilon_{xx} - \varepsilon_{yy}) \quad (56)$$

Using the maximum shear theory condition (Nisbett, 2009):

$$(\sigma_{xx} - \sigma_{yy}) = 2G_{xy}(\varepsilon_{xx} - \varepsilon_{yy}) \quad (57)$$

Comparing the equations (56) and (57), we obtained:

$$G_{xy} = \frac{E_x}{2(1 + v_{xy})} \quad (58)$$

Where G_{xy} is the shear modulus in the xy plane.

For the conditions transversely isotropic the equation (21) becomes:

$$\varepsilon_{\Phi, \Psi} = \sin^2 \psi \left\{ \frac{\sigma_{xx}}{E_x} [(1 + v_{xy}) \cos^2 \Phi + (v_{zz} - v_{xy})] + \frac{\sigma_{yy}}{E_x} [(1 + v_{xy}) \sin^2 \Phi + (v_{zz} - v_{xy})] - \frac{\sigma_{zz}}{E_z} (1 + v_{zz} \sin^2 \Phi + v_{zz} \cos^2 \Phi) \right\} - \left(\frac{v_{xz} \sigma_{xx}}{E_x} + \frac{v_{xz} \sigma_{yy}}{E_x} - \frac{\sigma_{zz}}{E_z} \right) \quad (59)$$

And the equation (45) becomes:

$$E = \left\{ \frac{[4g_s (\varepsilon_{all}^f + \varepsilon_{all}^s) - \varepsilon_{xx}]}{(g_s - g_f) \varepsilon_{xx}} \right\} \frac{\sigma_{app}}{\varepsilon_{xx}} \quad (60)$$

This equation relates the Young's modulus of a transversely isotropic film with the stresses applied to the film-substrate system.

DATA APPLICATION ON TRANSVERSELY ISOTROPIC EQUATIONS

Fiber-textured thin gold film: We consider the data of Faurie et al. (2005), which establishes the elastic constants of a fiber-textured thin gold film with transversely isotropic symmetry by combining synchrotron X-ray diffraction and in situ tensile testing.

Gold thin films have been deposited by physical-vapor deposition. The substrate was a 127.5- μm-thick polyimide dog-bone substrate; the in-plane sample dimensions were 14 X 6 mm². A surfaceprofilometer system to be 700 ±10 nm [7]. Once the experimental values are plotted (Ψ= 0°, Φ= 0°) and (Ψ= 0° Φ= 90°), as shown in figure 2, we obtain the following empirical equations:

$$\epsilon_{0,0} = -1,1.10^{-4}F \tag{61}$$

$$\epsilon_{90,0} = -1,1.10^{-4}F \tag{62}$$

Where F is the applied force.

Then, using equation (59), for (Ψ= 0°, Φ= 0°) and (Ψ= 0°, Φ= 90°), we obtain the following theoretical equation:

$$\epsilon_{0,0} = - \left[\frac{v_{xz}}{E} + \left(\frac{\sigma_{yy}}{\sigma_{xx}} \right) \frac{v_{xz}}{E} - \left(\frac{\sigma_{zz}}{\sigma_{xx}} \right) \frac{1}{E_z} \right] \frac{F}{B} \tag{63}$$

$$\epsilon_{90,0} = - \left[\frac{v_{xz}}{E} + \left(\frac{\sigma_{yy}}{\sigma_{xx}} \right) \frac{v_{xz}}{E} - \left(\frac{\sigma_{zz}}{\sigma_{xx}} \right) \frac{1}{E_z} \right] \frac{F}{B} \tag{64}$$

Where F = Bσ_{xx} and B is constant.

Doing the same procedure, now the values (Ψ= 75,04°; Φ = 0°), (Ψ= 75,04°; Φ= 90°) and (Ψ= 54,74°; Φ= 0°), (Ψ= 54,74°; Φ= 90°), which are shown in Figure 3 and 4 respectively, we obtain the equations:

$$\epsilon_{0^\circ ; 75,04^\circ} = 2,2.10^{-4}F \tag{65}$$

$$\epsilon_{90^\circ ; 75,04^\circ} = -1,2.10^{-4}F \tag{66}$$

$$\epsilon_{0^\circ ; 54,74^\circ} = 1,6.10^{-4}F \tag{67}$$

$$\epsilon_{90^\circ ; 54,74^\circ} = -1,5.10^{-4}F \tag{68}$$

We obtain from the equation (59) the following theoretical equations:

$$\epsilon_{0^\circ ; \Psi} = \left\{ \left[\frac{(1 + v_{xz})}{E} + \left(\frac{\sigma_{yy}}{\sigma_{xx}} \right) \frac{(v_{xz} - v_{xy})}{E} - \left(\frac{\sigma_{zz}}{\sigma_{xx}} \right) \frac{(1 + v_{xz})}{E_z} \right] \text{sen}^2 \psi - \left[\frac{v_{xz}}{E} \left(1 + \frac{\sigma_{yy}}{\sigma_{xx}} \right) - \frac{1}{E_z} \left(\frac{\sigma_{zz}}{\sigma_{xx}} \right) \right] \right\} \frac{F}{B} \tag{69}$$

$$\epsilon_{90^\circ ; \Psi} = \left\{ \left[\frac{(v_{xz} - v_{xy})}{E} + \left(\frac{\sigma_{yy}}{\sigma_{xx}} \right) \frac{(1 + v_{xz})}{E} - \left(\frac{\sigma_{zz}}{\sigma_{xx}} \right) \frac{(1 + v_{xz})}{E_z} \right] \text{sen}^2 \psi - \left[\frac{v_{xz}}{E} \left(1 + \frac{\sigma_{yy}}{\sigma_{xx}} \right) + \frac{v_{xz}\sigma_{yy}}{E} - \frac{1}{E_z} \left(\frac{\sigma_{zz}}{\sigma_{xx}} \right) \right] \right\} \frac{F}{B} \tag{70}$$

Based on the obtained relations, we got the following results, for F= 6,6 N, shown in the table 1:

Table 1. Result of the average values of the deformations for Ψ angles, Ψ = 0; Ψ = 54,74° and Ψ =75,04°; applying on film, F=6,6 N.

$\epsilon_{xx} (.10^{-4})(\phi = 0^\circ)$	$\epsilon_{yy} (.10^{-4})(\phi = 90^\circ)$	$\epsilon_{zz} (.10^{-4})(\phi = 0^\circ \text{ and } 90^\circ)$	Ψ
19,21	-11,84	-	54,74°
16,02	-7,47	-	75,04°
-	-	-7,39	0°
17,62	-9,66	-7,39	Average

With this procedure we obtained ε_{xx}, ε_{yy} and ε_{zz} for all force and calculate v_{xy} and v_{xz} using equation (49) shown in table II.

Based on the obtained relations,(50-55), we have the following results shown in Table III and IV.

The other table:

Table 2. The table lists the strain in the film for each applied force

$F(N)$	$\epsilon_{xx} (.10^{-4})$	$\epsilon_{yy} (.10^{-4})$	$\epsilon_{zz} (.10^{-4})$
6,6	17,62	-9,66	-7,39
5,6	14,94	-8,21	-6,27
3,6	9,61	-5,27	-4,03
2,2	5,87	-3,22	-2,46
1,1	2,94	-1,61	-1,23

Table 3. Table to compare the stresses obtained from the equations proposed and stresses obtained by Faurie (2005)

$\sigma_{xx}(2005)(MPa)$	$\sigma_{yy}(2005)(MPa)$	$F(N)$	$\sigma_{xx}(MPa)$	$\sigma_{yy}(MPa)$	$\sigma_{zz}(MPa)$
135	37	6,6	156	42	45
115	31,4	5,6	132	35,8	38,4
73,7	20,2	3,6	85	23	24,7
45	12,3	2,2	52	14	15
22,5	6	1,1	26	7	7,5

Table 4. Table to compare the elastic constants obtained from the proposed equations and the elastic constants obtained by faurie (2005)

	$E(GPa)$	$E_x(GPa)$	$E_z(GPa)$	$G_{xy}(GPa)$	ν	ν_{xy}	ν_{xz}
Faurie (2005)	75,7	-	-	-	0,52	-	-
Today	-	64,6	82,7	20,9	-	0,55	0,42

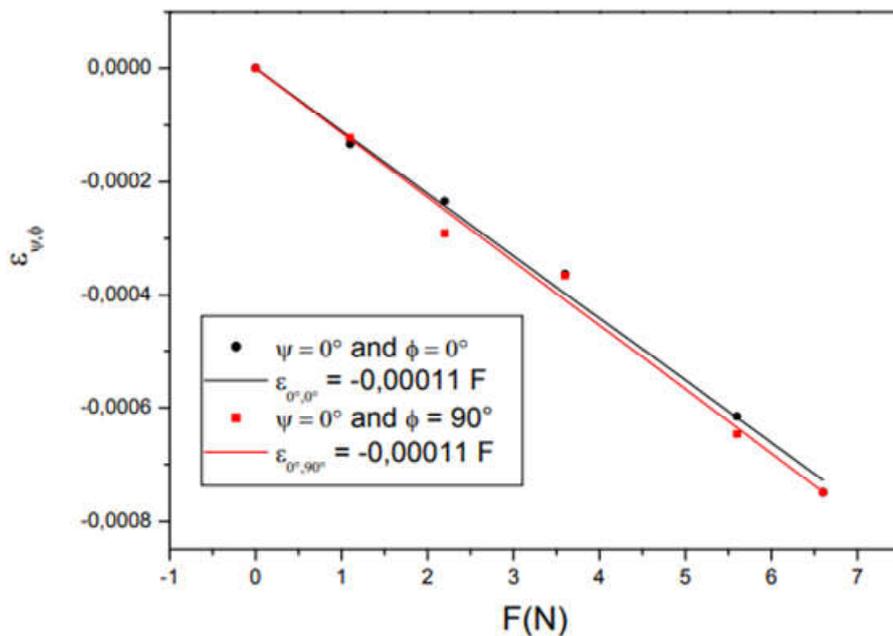


Figure 2. Graph of strain versus force applied to the film for $\Psi=0^\circ$. The black dots represent $\phi=0^\circ$ and the red dots represent $\phi=90^\circ$

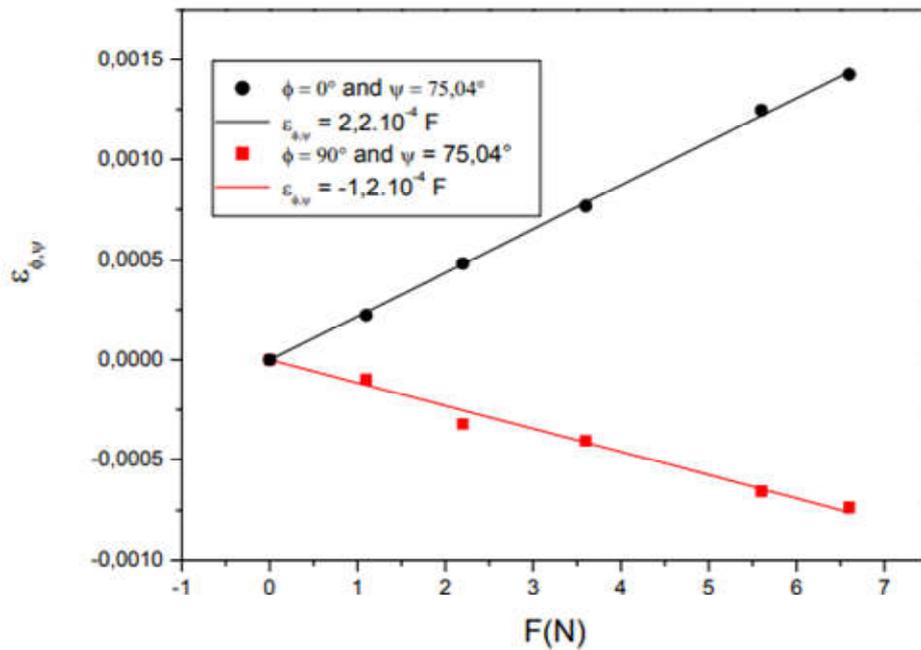


Figure 3. Graph of strain versus force applied to the film for $\Psi = 75,04^\circ$. The black dots represent $\phi = 0^\circ$ and the red dots represent $\phi = 90^\circ$

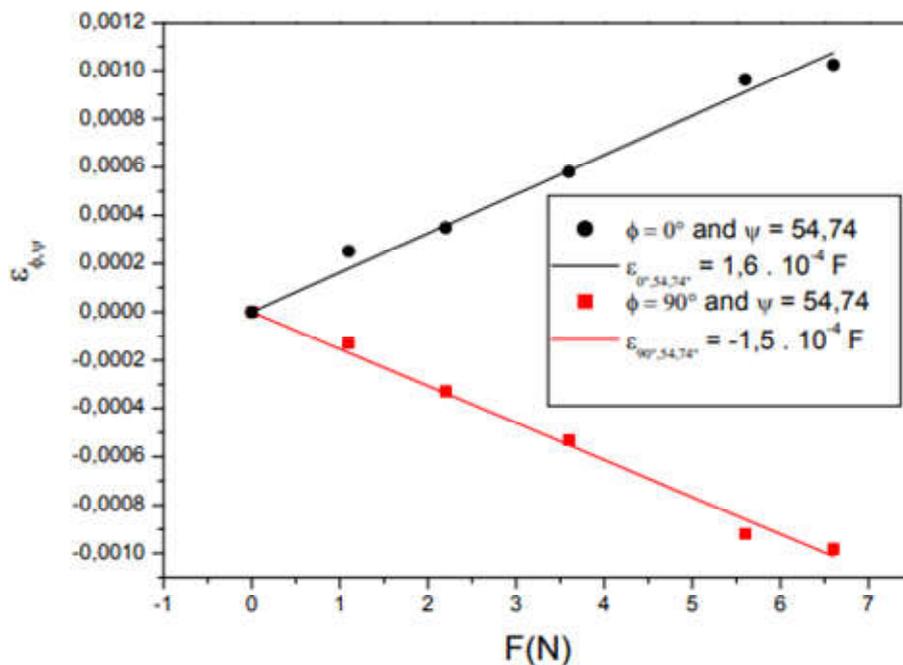


Figure 4. Graph of strain versus force applied to the film for $\Psi = 54,74^\circ$. The black dots represent $\phi = 0$ and the red dots represent $\phi = 90^\circ$

RESULTS AND DISCUSSION

In calculating the determinant of the matrix that characterizes the material, the result is zero, indicating that the matrix is not invertible. In this calculation the symmetry properties of the matrix of the material, equation (5), were considered. In Table II, the values of the strains on the z-direction are not neglectable. The thin film was analyzed in three dimensions and once we take into account the result of the equation (21), we realize how important the sigma σ_{zz} is for its deformation. The tensions obtained are all positive, the sign of σ_{zz} on (21) equation is the inverse of σ_{xx} and σ_{yy} directions. We note that, in this case, the stress is the contraction. Equation (17) was obtained "ad hoc", obeys the equations (6), (7) and (8), and the comparison of the results obtained from the stresses in the film with the results obtained by Faurie (2005), as seen in table III, is consistent with the values for each of the applied forces. Looking at equations (44) and (45) we see that these equation relates the applied stress and the dimensions of the film-substrate system in the stress on the film. Being possible to calculate the Young's modulus of film. Looking the deduction of equation (58). The equation (58) is in agreement with the literature. In table IV, we obtain the five elastic constants, thus completely characterizing the transversely isotropic material.

CONCLUSION

In this work based on elasticity theory of continuous media for small deformations, it was possible to obtain a set of equations which are able to completely characterize a thin film on orthotropic symmetry in their mechanical properties. It was also possible to determine the principal stresses and strains applied to the thin film. When this set of equations was applied to a film-substrate system considered transversely isotropic, the results were consistent with respect to experimental studies of Faurie *et al* (2005) in what concerns elastic constants.

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