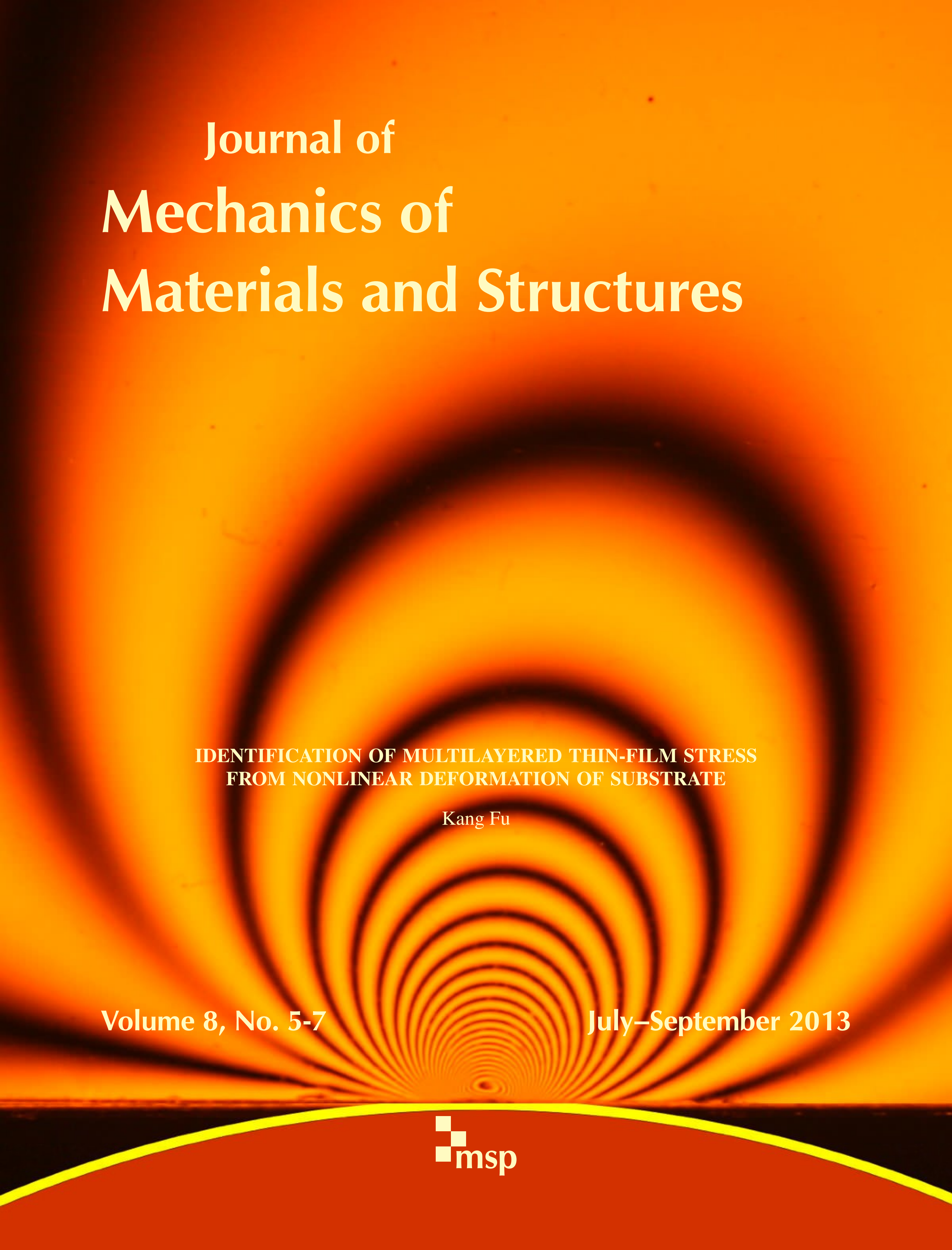
Journal of Mechanics of Materials and Structures



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Volume 8, No. 5-7 July–September 2013

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JOURNAL OF MECHANICS OF MATERIALS AND STRUCTURES
Vol. 8, No. 5-7, 2013
dx.doi.org/10.2140/jomms.2013.8.369

IDENTIFICATION OF MULTILAYERED THIN-FILM STRESS FROM NONLINEAR DEFORMATION OF SUBSTRATE

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Due to the enlargement of wafer size and the increase of product integrity, thin-film stress problems inevitably get into the range of geometric nonlinearity and are found in multilayered thin-film materials. In this work, multilayered thin-film materials are modeled as a large-deflection multilayered composite plate in the framework of geometrically nonlinear plate theory. Based on the principle of virtual work for a thin-film material plate with thin-film stresses of multiple layers as driving forces, a nonlinear plate finite element system for kinematic fields of thin-film materials, which includes in-plane displacements, cross section rotations, and out-of-plane deflection, is established. The least squares method with regularization applied for total or partial kinematic fields obtained by the finite element method solution versus those given by experiments leads to an iterative procedure for identification of the nonlinear multilayered thin-film stresses.

1. Introduction

Thin-film materials are widely used in the microelectronics, opticoelectronics, and microelectromechanical systems industries. An understanding of the mechanical properties of thin-film materials plays an important role in quality control in component fabrication and in reliability assurance. Among all thin-film material mechanical properties, thin-film stress is a key factor which has to be determined. Thin-film stress in fabrication processes may introduce undesirable warping of wafers, peeling of thin films from substrates, and cracking of thin films. Thin-film stress may influence the functional properties of products, for example, the electronic properties of microelectronic circuits and the performance of microelectromechanical systems. Along with the enlargement of wafer diameter and the increase of product integrity, thin-film stress problems inevitably get into the range of geometric nonlinearity and are found in the multilayered thin-film materials.

Thin-film stress is introduced in thin-film materials during the thin-film material development process. The mismatch of the microstructures and the difference in thermoexpansion coefficients of the materials constituting substrates and thin films are the origins of thin-film stress. Thin-film stress is divided by origin into intrinsic and thermal thin-film stresses, which generally coexist. Although intrinsic and thermal thin-film stress can be determined, respectively, from microscopic and macroscopic models, the methods that determine thin-film stress directly from integrated thin-film materials remain the first choice owing to their simplicity in application and the sufficient precision they offer under certain conditions. In this category is the method which uses the measured curvature variation of thin-film material to evaluate thin-film stress, proposed first by Stoney [1909] and developed further in [Brenner and Senderoff 1949;

MSC2000: 74K35, 74G75, 74S05.
Keywords: thin-film stress, thin-film material, inverse problem, numerical method, nonlinearity.

Glang et al. 1965]. This method is valid in the case of small deformation and constant thin-film material thickness, as well as for isotropic and homogeneous thin-film stress distributions. The classic Stoney formula is used in many industrial applications [Flinn 1989; Nix 1989]. Extensions to the cases of multilayered thin-film materials, nonconstant thin-film material thicknesses, nonhomogeneous thin-film stress distributions, and geometric nonlinearity have been made in the last three decades [Harper and Wu 1990; Finot and Suresh 1996; Finot et al. 1997; Freund et al. 1999; Freund 2000; Giannakopoulos et al. 2001; Feng et al. 2006; Huang and Rosakis 2006]. In dealing with thin-film stress problems with geometric nonlinearity, Masters and Salamon [1993] and Salamon and Masters [1995] resorted to a Ritz-type method based on the potential energy minimization principle, where the relations of the thin-film stress to both the deflection and the curvature of thin-film materials are studied. The aforementioned methods are all analytic methods. In these cases, various types of restrictions must be retained in order to guarantee the possibility of obtaining analytic solutions. Less restricted methods are developed in the framework of finite element methods. The calculation of thin-film stress from measured thin-film material deformation based on an inverse solution of thin-film material problems with a finite element model is found in [Engelstad et al. 2005]. An inverse problem technique based on a linear plate finite element method that is used to identify thin-film stress is presented in [Fu 2012]. Many advantages can be found in the two numerical-type methods due to the inherent adaptability of the finite element method.

In this paper, the author's previous work is extended to determine the geometrically nonlinear thin-film stress of multilayered thin-film materials. The mechanical modeling of multilayered thin-film material as a special nonlinear composite plate is given in Section 2, where the principle of virtual work for multilayered thin-film stress in the range of geometric nonlinearity is applied at the end of the section. A nonlinear finite element system is established from the virtual work equation by finite element discretization in Section 3. In Section 4, a nonlinear inverse problem for determining thin-film stress using measured kinematic data of thin-film materials is set up via a least squares formula together with the solution scheme. Examples are provided in Section 5 for illustrating the effectiveness of the proposed approach in the determination of nonlinear multilayered thin-film stress. Section 6 contains conclusions.

In the text, Greek subscripts vary in the range $\{1, 2\}$ and Latin subscripts take values in $\{1, 2, 3\}$. The summation convention applies to each repeated pair of indices in the formulas unless otherwise indicated.

2. Mechanical modeling of nonlinear multilayered thin-film materials

2.1. ***Basic formulations.*** Nonlinear multilayered thin-film material is here modeled as a special composite plate, which consists of a substrate and n thin-film layers of different materials. An infinitesimal portion of the thin-film material is illustrated in Figure 1, where h^s and h_i^f are the thicknesses of the substrate and the i-th thin-film layer for $i = 1, \dots, n$, respectively. For thin films, $h_i^f \ll h^s$. For the thin-film materials considered in this work, the thicknesses of the thin films do not have to be constant and no defaults such as cracks exist in the materials.

Suppose that the total macroscopic deformation of a thin-film material stems only from the nonconformal internal eigenstrains of the thin films and the substrate without the intervention of external loads, and it is the continuity requirement on the total deformation of the thin-film material that will introduce the elastic strains and corresponding stresses in the thin films as well as in the substrate.

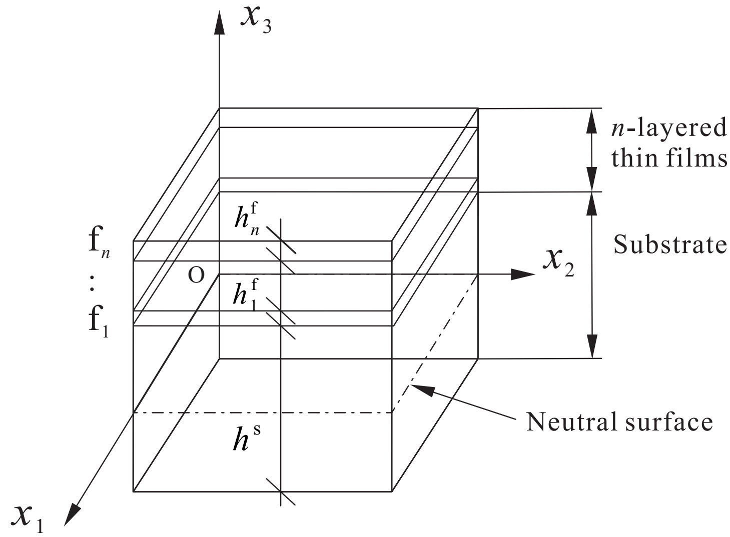

Figure 1. Multilayered thin-film materials.

In modeling the structure of a thin-film material as a nonlinear multilayered thin or moderately thick plate [Reddy 2003; Roccabianca et al. 2010; 2011] under the hypothesis of large deflection [von Kármán 1910; Timoshenko and Woinowsky-Krieger 1959], the primary kinematic fields of the first-order shear deformable plate model used to represent the total deformation of the thin-film material are the in-plane displacements u_α, the out-of-plane displacement u_3, and the plate cross section rotations θ_α, which are all defined on the neutral surface of the plate and are in reference to a configuration that is free of any strain.

In a Cartesian coordinate system, the origin of which is on the neutral surface of the thin-film material plate as shown in Figure 1, the geometrically nonlinear strain-displacement relations in the two longitudinal directions of the thin-film material plate are given by

$$\epsilon_{11} = \partial_1 u_1 + x_3 \partial_1 \theta_2 + (\partial_1 u_3 \partial_1 u_3)/2, \tag{1}$$

$$\epsilon_{22} = \partial_2 u_2 - x_3 \partial_2 \theta_1 + (\partial_2 u_3 \partial_2 u_3)/2, \tag{2}$$

$$2\epsilon_{12} = \partial_2 u_1 + \partial_1 u_2 - x_3 \partial_1 \theta_1 + x_3 \partial_2 \theta_2 + (\partial_1 u_3 \partial_2 u_3 + \partial_2 u_3 \partial_1 u_3)/2, \tag{3}$$

where $\epsilon_{\alpha\beta}$ are the strain components in the two longitudinal directions of the thin-film material plate and x_3 is the coordinate in the normal direction of the plate neutral surface, and, as in the following, $\partial_\alpha(*) = \partial(*)/\partial x_\alpha$. The components of the transversal shear strain are given by

$$\epsilon_{13} = (\partial_1 u_3 - \theta_2)/2, \tag{4}$$

$$\epsilon_{23} = (\partial_2 u_3 - \theta_1)/2. \tag{5}$$

The strain component formulations given by (1)–(5) are applied for the strain components of the substrate, $\epsilon^s_{\alpha\beta}$, or for those of the i-th thin-film layer, $\epsilon^{f_i}_{\alpha\beta}$, $i = 1, \dots, n$, depending on whether the coordinate x_3 is placed in the substrate or in the i-th thin-film layer. The application of the identical geometric relations of (1)–(5) to the substrate and the thin films implicates automatically the continuity of the total deformation of the thin-film materials at the interfaces between all the adjacent thin-film layers as well as at that between the first thin-film layer and the substrate. Since the kinematic fields have a strain-free reference configuration, the total strains given by (1)–(5) consist of elastic strains and eigenstrains.

The deformations of the substrate and thin films given by (1)–(3) are total strains, which consist of eigenstrains, $\epsilon^{*}_{\alpha\beta}$, and elastic strains, $\epsilon^{e}_{\alpha\beta}$, for the substrate as well as for the thin films:

$$\epsilon_{\alpha\beta} = \epsilon^{e}_{\alpha\beta} + \epsilon^{*}_{\alpha\beta}. \tag{6}$$

The eigenstrains of the substrate, $\epsilon^{s*}_{\alpha\beta}$, are usually isotropic thermal strains, while those of the thin films, $\epsilon^{f*}_{\alpha\beta}$, consist of thermal strains and intrinsic strains. In the substrate and the thin films, the elastic strains are developed to compensate the nonconformal eigenstrains in order to ensure the continuity of the total deformation of the thin-film materials.

The stresses in the substrate and thin films are related to their mechanical conjugated elastic strains. For the sake of simplicity of presentation, the constitutive relations for the isotropic and linear elastic materials that constitute the substrate and thin films are discussed in this paper. For substrate materials, the stress components, $\sigma^{s}_{\alpha\beta}$, and the elastic strain components, $\epsilon^{es}_{\alpha\beta}$, are supposed to be related by a constitutive law of the pseudo-three-dimensional stress state given by

$$\sigma^{s}_{\alpha\alpha} = \frac{E^{s}}{1-\nu^{s2}}(\epsilon^{es}_{\alpha\alpha} + \nu^{s}\epsilon^{es}_{\beta\beta}), \tag{7}$$

$$\sigma^{s}_{\alpha\beta} = \frac{E^{s}}{1+\nu^{s}}\epsilon^{es}_{\alpha\beta} \quad \text{for } \alpha \neq \beta, \tag{8}$$

$$\sigma^{s}_{\alpha 3} = \frac{\kappa E^{s}}{1+\nu^{s}}\epsilon^{es}_{\alpha 3}, \tag{9}$$

where E^{s} and ν^{s} are the Young's modulus and Poisson's ratio of the substrate materials, respectively, and κ is the shear force numerical corrector of the plate model. The transversal normal stress component σ_{33} is considered to vanish both in the substrate and the thin films. The transversal shear deformation and the transversal shear stress are considered to be negligible in the thin films, supposing that they are in the region that is sufficiently approximated to the thin-film material plate top or bottom surface. Therefore, the thin-film stress components, $\sigma^{f_i}_{\alpha\beta}$, and the thin-film elastic strain components, $\epsilon^{ef_i}_{\alpha\beta}$, in the i-th thin-film layer are considered to be related by a constitutive law of plane stress state given by

$$\sigma^{f_i}_{\alpha\alpha} = \frac{E^{f_i}}{1-\nu^{f_i 2}}(\epsilon^{ef_i}_{\alpha\alpha} + \nu^{f_i}\epsilon^{ef_i}_{\beta\beta}), \tag{10}$$

$$\sigma^{f_i}_{\alpha\beta} = \frac{E^{f_i}}{1+\nu^{f_i}}\epsilon^{ef_i}_{\alpha\beta} \quad \text{for } \alpha \neq \beta, \tag{11}$$

where E^{f_i} and ν^{f_i} are the Young's modulus and Poisson's ratio of the material of the i-th thin-film layer, respectively.

Similarly to the previous work [Fu 2012], the principle of virtual work for geometrically nonlinear multilayered thin-film materials in its established equilibrium state is formulated as follows:

$$\int_{\Omega^{s}} \sigma^{s}_{kl}(u_\alpha, u_3, \theta_\alpha)\delta\epsilon^{s}_{kl}\, d\Omega^{s} + \sum_{i=1}^{n}\int_{\Omega^{f_i}} \sigma^{f_i}_{\alpha\beta}\delta\epsilon^{f_i}_{\alpha\beta}\, d\Omega^{f_i} = 0, \tag{12}$$

where Ω^s and Ω^{f_i} are the volumes of the substrate and the i-th thin-film layer, respectively. The identification of thin-film stress means that the thin-film stress components of all the thin-film layers $\sigma_{\alpha\beta}^{f_i}$, $i = 1, \ldots, n$, in the second term of the left-hand side of (12) are considered as independent variables, which have to be determined from some of the kinematic fields that are obtained from physical measurements.

2.2. *Identification-oriented formulations.* The use of the relation between the total kinematic fields of the thin-film materials and the thin-film stresses of all the thin-film layers of (12) is not sufficient to identify the thin-film stresses from the total kinematic fields, since total deformation of a thin-film material may correspond to different combinations of multilayered thin-film stresses. Two approaches that can be used to solve this problem are suggested in this subsection.

One approach is based on the use of a series of measured substrate deformations of thin-film material $\Delta\bar{u}^{f_i}$, $i = 1, \ldots, n$, of which the i-th measured deformation is related to the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$, for $i = 1, \ldots, n$, respectively. In practice, there are two occasions in which the substrate deformation of thin-film material $\Delta\bar{u}^{f_i}$ with respect to the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$, for $i = 1, \ldots, n$, can be measured experimentally: One is that when the i-th thin-film layer is deposited on the $(i-1)$-th thin-film layer during a normal layer-by-layer thin-film forming process, which is realized in order from the first thin-film layer to the n-th. This measurement may be carried out at an interval of every two normal deposition operations. Another occasion is that when the i-th thin-film layer is removed from the $(i-1)$-th thin-film layer during a layer-by-layer thin-film sacrificing process, which is realized in order from the n-th thin-film layer to the first. This second process is a type of investigative test with the use of destructive techniques such as chemical etching or mechanical grinding upon fabricated multilayered thin-film material samples. Usually, these operations on the i-th thin-film layer should not change the intrinsic thin-film strains of the lower-ordered layers that are bound in in-processing thin-film materials. As for possible changes of the temperature strains of lower-ordered layer thin films or the substrate, they are easily estimated.

Notice that in the two measurement processes, the measured deformation of the thin-film material $\Delta\bar{u}^{f_i}$ is a deformation induced by adding or removing the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$ on an in-processing thin-film material. At this moment, the substrate deformation of the thin-film material $\Delta\bar{u}^{f_i}$ depends not only on the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$, but also on all the thin-film stresses $\sigma_{\alpha\beta}^{f_p}$, $p = 1, \ldots, i-1$, since the first through $(i-1)$-th layer thin films are still bound on the substrate.

In accordance with these properties of the layer-by-layer deformation measurement processes on an in-processing thin-film material, the principle of virtual work for the in-processing thin-film material under the action both of the substrate stress σ_{kl}^s and thin-film stresses $\sigma_{\alpha\beta}^{f_p}$, $p = 1, \ldots, i$, is formulated as

$$\int_{\Omega^s} \sigma_{kl}^s \Bigl(\sum_{p=1}^{i} \Delta\bar{u}^{f_p}\Bigr) \delta\epsilon_{kl}^s \, d\Omega^s + \sum_{p=1}^{i} \int_{\Omega^{f_p}} \sigma_{\alpha\beta}^{f_p} \delta\epsilon_{\alpha\beta}^{f_p} \, d\Omega^{f_p} = 0, \tag{13}$$

where the summation of $\Delta\bar{u}^{f_p}$ from 1 to i constitutes the total change of the kinematic fields induced by the thin-film stresses of all the thin-film layers $\sigma_{\alpha\beta}^{f_p}$, $p = 1, \ldots, i$. When the deformations of the thin-film material with respect to all the thin-film stresses $\Delta\bar{u}^{f_i}$, $i = 1, \ldots, n$, are in disposition after one of the aforementioned measurement processes has been completely carried out, the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$, $i = 1, \ldots, n$, can be evaluated according to (13) in order from the first thin-film layer to the n-th in a layer-by-layer cumulative way.

In the identification process of the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$, the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$ is evaluated according to (13) from the measured deformations $\Delta\bar{u}^{f_p}$, $p=1,\ldots,i$, and the thin-film stresses $\sigma_{\alpha\beta}^{f_p}$, $p=1,\ldots,i-1$. Meanwhile the thin-film stresses $\sigma_{\alpha\beta}^{f_p}$, $p=1,\ldots,i-1$, also have to be updated so as to take into account the influence on them of the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$. For this purpose, the measured deformations $\Delta\bar{u}^{f_p}$, $p=1,\ldots,i$, and the thin-film stresses $\sigma_{\alpha\beta}^{f_p}$, $p=1,\ldots,i-1$, obtained in the previous layer evaluation are used at the beginning of the process to evaluate a first i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$. Then, the p-th layer thin-film stress $\sigma_{\alpha\beta}^{f_p}$, for $p=1,\ldots,i-1$, is updated according to (6) and (10) and (11) from the p-th layer total strain $\epsilon_{\alpha\beta}^{f_p}$ given by the kinematic fields obtained in the actual layer evaluation, and the p-th layer invariant eigenstrain $\epsilon_{\alpha\beta}^{f_p*}$ obtained in the previous layer evaluations. The process proceeds iteratively until the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$ is finally identified. At this moment, the i-th layer invariant eigenstrain $\epsilon_{\alpha\beta}^{f_i*}$ is once for all evaluated from the i-th layer thin-film stress $\sigma_{\alpha\beta}^{f_i}$ and the actual i-th layer total strain $\epsilon_{\alpha\beta}^{f_i}$ according to (6) and (10) and (11). The final thin-film stresses of all the thin-film layers are identified when this layer-by-layer cumulative process is finished at $i=n$.

Another approach is to identify the thin-film stresses of all the thin-film layers from the total deformation of thin-film materials with the use of (12), which is possible when the continuity condition of deformations between all the adjacent thin-film layers can be formulated with the use of thin-film eigenstrains. When the thin-film layers are bound together, the in-plane strain components must be equal on the interface of the adjacent i-th and $(i+1)$-th thin-film layers owing to the deformation continuity requirement:

$$\epsilon_{\alpha\beta}^{f_i}=\epsilon_{\alpha\beta}^{f_{i+1}}. \tag{14}$$

By substituting (6) into (14), the continuity condition of (14) becomes

$$\epsilon_{\alpha\beta}^{ef_{i+1}}=\epsilon_{\alpha\beta}^{ef_i}-\Delta\epsilon_{\alpha\beta}^{*(i+1,i)}, \tag{15}$$

where $\Delta\epsilon_{\alpha\beta}^{*(i+1,i)}$ is the difference of the eigenstrain components between the i-th and $(i+1)$-th thin-film layers at their interface. By substituting (10) and (11) into (15), the transitional conditions for the thin-film stresses on the interface between the i-th and $(i+1)$-th thin-film layers are found as

$$\sigma_{\alpha\alpha}^{f_{i+1}}=\frac{E^{f_{i+1}}}{[1-(\nu^{f_{i+1}})^2]}\left\{\frac{1}{E^{f_i}}[(1-\nu^{f_i}\nu^{f_{i+1}})\sigma_{\alpha\alpha}^{f_i}-(\nu^{f_i}-\nu^{f_{i+1}})\sigma_{\beta\beta}^{f_i}]-\left(\Delta\epsilon_{\alpha\alpha}^{*(i+1,i)}+\nu^{f_{i+1}}\Delta\epsilon_{\beta\beta}^{*(i+1,i)}\right)\right\}, \tag{16}$$

$$\sigma_{\alpha\beta}^{f_{i+1}}=\frac{E^{f_{i+1}}}{(1+\nu^{f_{i+1}})}\left[\frac{(1+\nu^{f_i})}{E^{f_i}}\sigma_{\alpha\beta}^{f_i}-\Delta\epsilon_{\alpha\beta}^{*(i+1,i)}\right]\quad \text{for } \alpha\neq\beta. \tag{17}$$

With the use of these transitional conditions on the thin-film stresses, the thin-film stresses of all the thin-film layers can be represented by a generic thin-film stress of a chosen principal thin-film layer. After doing this, (12) can be used to determine the generic thin-film stress from the integral deformation of the n-layered thin-film materials. The key in this approach is that all the differences of the eigenstrains between the i-th and $(i+1)$-th thin-film layers $\Delta\epsilon_{\alpha\beta}^{*(i+1,i)}$, $i=1,\ldots,n-1$, must be known, for the acquisition of which one may turn to the solution of other important problems such as the thermal strains, experimental measurements, multiscale modeling and computations, etc., which are left to be the research subjects of other works.

In the present work, the second approach is used partially in the aforementioned layer-by-layer cumulative approach. Notice that once the thin-film stress of a layer is determined in the layer-by-layer cumulative process, it can be used with the previously evaluated and newly updated thin-film stress of the lower-ordered layer to calculate the difference of eigenstrain components between the two layers according to (16) and (17). The eigenstrains as well as their differences between adjacent layers are generally unchanged or may be easily determined during the layer-by-layer cumulative evaluation process, and the layer-by-layer cumulative approach can use these properties to establish a more efficient solution strategy. The advantages of the application of these properties are illustrated in the following.

For an in-processing thin-film material with one thin-film layer at the beginning, both the substrate stress σ^s_{ij} and the first-layer thin-film stress $\sigma^{f_1}_{\alpha\beta}$ are first evaluated as before from $\Delta\bar{u}^{f_1}$. Then, the difference of the eigenstrain components at the interface between the substrate and the first thin-film layer $\Delta\epsilon^{*(1,0)}_{\alpha\beta}$ is determined from (16) and (17), in which the substrate stress $\sigma^s_{\alpha\beta}$ at the one surface of the substrate that is in contact with the first thin-film layer is used as the lower-ordered layer stress.

Following the preceding step, in identifying the second-layer thin-film stress $\sigma^{f_2}_{\alpha\beta}$ and in updating the substrate stress σ^s_{ij} and the first-layer thin-film stress $\sigma^{f_1}_{\alpha\beta}$ from $\Delta\bar{u}^{f_1}$ and $\Delta\bar{u}^{f_2}$, the actual first-layer thin-film stress $\sigma^{f_1}_{\alpha\beta}$ in (13) is represented by the actual substrate stress σ^s_{ij} according to (16) and (17) with the use of the unchanged difference of the eigenstrain components at the interface between the substrate and the first thin-film layer $\Delta\epsilon^{*(1,0)}_{\alpha\beta}$. After the updated substrate stress σ^s_{ij} and the identified second-layer thin-film stress $\sigma^{f_2}_{\alpha\beta}$ are determined from $\Delta\bar{u}^{f_1}$ and $\Delta\bar{u}^{f_2}$ according to (13), the updated first-layer thin-film stress $\sigma^{f_1}_{\alpha\beta}$ is given according to (16) and (17) with the use of the updated substrate stress σ^s_{ij} and the unchanged difference of the eigenstrain components at the interface between the substrate and the first thin-film layer $\Delta\epsilon^{*(1,0)}_{\alpha\beta}$. The difference of the eigenstrain components at the interface between the first and second thin-film layers $\Delta\epsilon^{*(2,1)}_{\alpha\beta}$ is then calculated according to (16) and (17) with the use of the updated first-layer thin-film stress $\sigma^{f_1}_{\alpha\beta}$ and the just-identified second-layer thin-film stress $\sigma^{f_2}_{\alpha\beta}$.

Similarly, in identifying the i-th layer thin-film stress $\sigma^{f_i}_{\alpha\beta}$ and in updating the substrate stress σ^s_{ij} and the thin-film stresses $\sigma^{f_p}_{\alpha\beta}$, $p = 1, \ldots, i-1$, from $\Delta\bar{u}^{f_q}$, $q = 1, \ldots, i$, all the actual thin-film stresses $\sigma^{f_p}_{\alpha\beta}$, $p = 1, \ldots, i-1$, in (13) are represented successively by the actual substrate stress σ^s_{ij} according to (16) and (17), in which the differences of the eigenstrain components at the interfaces between the $(p-1)$-th and p-th thin-film layers $\Delta\epsilon^{*(p,p-1)}_{\alpha\beta}$, $p = 1, \ldots, i-1$, are already known. After the updated substrate stress σ^s_{ij} and the identified i-th layer thin-film stress $\sigma^{f_i}_{\alpha\beta}$ are determined according to (13) from $\Delta\bar{u}^{f_q}$, $q = 1, \ldots, i$, the thin-film stresses $\sigma^{f_p}_{\alpha\beta}$, $p = 1, \ldots, i-1$, are updated with successive uses of (16) and (17) from the updated substrate stress σ^s_{ij} and the unchanged differences of the eigenstrain components at the interfaces between the $(p-1)$-th and p-th thin-film layers $\Delta\epsilon^{*(p,p-1)}_{\alpha\beta}$, $p = 1, \ldots, i-1$. The difference of the eigenstrain components at the interface between the $(i-1)$-th and i-th thin-film layers $\Delta\epsilon^{*(i,i-1)}_{\alpha\beta}$ is then calculated according to (16) and (17) with the use of the updated $(i-1)$-th layer thin-film stress $\sigma^{f_{i-1}}_{\alpha\beta}$ and the just-identified i-th layer thin-film stress $\sigma^{f_i}_{\alpha\beta}$. The thin-film stresses of all the thin-film layers are ultimately identified when this process is finished at $i = n$.

Since the identification process for multilayered thin-film stress is similar to a successive identification process of single layered thin-film stress and the updating of the thin-film stresses of the lower-ordered layers is not in the core of the identification process, the efficiency of the method is largely improved.

3. Finite element discretization

Since the kinematic fields are defined on the plate neutral surface, only two-dimensional quadrilateral or triangular element meshes are needed to mesh the neutral surface of the thin-film material plates.

Thin-film materials may be considered as very thin or moderately thick plates depending on the ratio of thickness to characteristic longitudinal dimensions of the thin-film materials studied. In these cases, the suitable elements for the mechanical model of the multilayered thin-film materials presented in Section 2 are those of transversal shear locking-free plate elements without the appearance of "hourglass" phenomena. Many successful elements for this type of problem can be implemented in the present work with minor modifications. The MITC4 elements [Brezzi et al. 1989; Bucalem and Bathe 1993] used in work [Fu 2012] are here extended to study geometrically nonlinear problems with five kinematic fields. The resulting finite element equation from (12) or (13) can be written as

$$Ku = F\sigma, \tag{18}$$

where K is the global geometrically nonlinear finite element rigidity matrix; u is the column vector matrix containing all nodal degrees of freedom of the mesh; σ is the column vector matrix of multilayered thin-film stresses defined in elements or on nodes, which contains only the unknown thin-film stresses of the thin-film layer actually considered during the identification process; and F is the geometrically nonlinear matrix which transforms the stress column matrix vector σ into an equivalent nodal force column vector matrix of the finite element system, and which contains also the previously identified thin-film stresses of the lower-ordered thin-film layers if the cumulative layer-by-layer method that is presented in Section 2.2 is used. In the identification process of the thin-film stresses, the sensitivity of the kinematic fields to the thin-film stresses is needed in the next section. From (18), the system of the sensitivity is formulated as

$$K\frac{\partial u}{\partial \sigma_{\alpha\beta}^{f_i}} = F\frac{\partial \sigma}{\partial \sigma_{\alpha\beta}^{f_i}}. \tag{19}$$

Equations (18) and (19) are geometrically nonlinear systems dependent on u, which have to be solved by an iterative procedure. In the same iteration, the factorized matrix K can be used for the solution processes both of the kinematic nodal values u and their sensitivity to the thin-film stresses.

4. Identification procedure of geometrically nonlinear multilayered thin-film stress

The determination of the thin-film stresses from the kinematic fields is an inverse problem from the point of view of (18). It is in general impossible to obtain the thin-film stresses σ from the nodal degrees of freedom u with the direct use of (18) since (18) is usually not well-posed mathematically and only a part of the nodal degrees of freedom u can, in fact, be provided by the experimental measurements. In order to overcome these difficulties, a least squares condition is used to establish a feasible solution scheme as

$$L = \min_{\{\sigma\}}[(u-\bar{u})^T(u-\bar{u})], \tag{20}$$

where $\bar{u}$ is a subset of the nodal degrees of freedom u, which are provided by the experimental measurements. In the layer-by-layer cumulative identification process of the thin-film stress of the i-th thin-film layer $\sigma_{\alpha\beta}^{f_i}$ following (13), $\bar{u}$ is the summation of all the measured substrate deformations $\Delta\bar{u}^{f_p}$, $p = 1, \dots, i$. The necessary condition of the minimization leads to an iterative type of equation for the determination of the thin-film stresses given as follows:

$$S_k^T S_k(\sigma_{k+1} - \sigma_k) = S_k^T(u_k - \bar{u}), \tag{21}$$

where the subscript indices k and $k+1$ designate the k-th and $(k+1)$-th steps of the iterations, and $S_k = (\partial u/\partial \sigma)_k$ is the sensitivity of the kinematic fields to the thin-film stresses at the k-th iteration step, which is calculated from (19). Equation (21) is a generalized linear system which may be solved by various techniques, for example, the singular-value-decomposition method, the regularization method, the iterative regularization method, etc. Here the regularization method is used. According to the Tikhonov regularization strategy [Tikhonov and Arsenin 1974], the minimization of (20) leads to

$$(S_k^T S_k + \alpha H^T H)(\sigma_{k+1} - \sigma_k) = S_k^T (u_k - \bar{u}), \tag{22}$$

where H is a regularization matrix, which is derived from regularization functions, and α is a regularization parameter, which may be determined by the L-curve method, the minimum discrepancy method, etc. [Golub et al. 1979; Hansen 1992; Engl et al. 1996]. In the case of ensuring the first-order derivative smoothness of the thin-film stresses, the regularization function may be taken as the L^2-norm of the thin-film stress field:

$$\Phi = \sum_{i=1}^{n} \int_{\Omega^{f_i}} \left(\frac{\partial \sigma_{\alpha\beta}^{f_i}}{\partial x_\alpha} \right) d\Omega^{f_i}, \tag{23}$$

where no summation convention is used. The discretized form of (23) leads to

$$\Phi = \sigma^T H^T H \sigma, \tag{24}$$

where the corresponding regularization matrix H is defined. The regularization matrix H given by (24) is invariant in the iteration process. Other regularization functions can be used depending on the smoothness requirement of the thin-film stress fields.

In the identification process of the thin-film stresses from a set or subset of the degrees of freedom of the measured deformation $\bar{u}$ provided by the experiments, an iterative solution procedure with the use of (18), (19), (21), (22), and (24) is given in following algorithm.

Algorithm. (i) Beginning of the identification process.

(ii) Initialization of the iterations on thin-film layers: $i = 1$ and $\bar{u} = \Delta \bar{u}^{f_i}$.

(iii) Initialization of the identification iterations on $\sigma_{\alpha\beta}^{f_i}$: $k = 0$, $u_k = 0$, and $\sigma_k = 0$.

(iv) Computation of H according to (24).

(v) Update of the thin-film stresses of the lower-ordered layers from $\Delta \bar{u}^{f_i}$.

(vi) Computation of u_k with the use of (18) from σ_k.

(vii) Computation of S_k with the use of (19) from u_k.

(viii) Computation of σ_{k+1} with the use of (21) or (22) from u_k, σ_k, S_k, and H.

(ix) Examination of convergence:
If u_k converges to $\bar{u}$, go to (x); else $k = k+1$, go to (vi).

(x) Output of σ_{k+1} as the identified thin-film stresses of the i-th thin-film layer; go to (xi).

(xi) Examination of the iteration on thin-film layers:
If $i = n$, go to (xii); else $i = i+1$, $\bar{u} = \bar{u} + \Delta \bar{u}^{f_i}$, go to (iii).

(xii) End of the identification process.

5. Numerical examples

In this section, two examples are presented to illustrate the characteristics and effectiveness of the proposed method. In the identification processes of the two examples, the least squares method with regularization is used, while the convergence criterion is set to be of a relative error of 1.0×10^{-4} for deflection fields.

5.1. ***Nonlinear thin-film stress of a two-layered thin-film material strip.*** In this example, a strip of rectangular plan shape of two-layered thin-film material is considered. The substrate material is of silicon (Si) and its original shape is flat. A uniform thin-film layer of tungsten (W) is supposed to be deposited on the substrate. The sizes and material parameters of the thin-film material are given in Table 1.

A Cartesian coordinate system is set up in such a way that the origin is taken at the centroid of the strip geometry; the longitudinal axis of symmetry of the strip, the normal of the longitudinal vertical plan of symmetry, and the upward normal of the neutral surface are taken as the x_1, x_2, and x_3-axes, respectively. Consider that a uniformly distributed thin-film stress exists in the thin film, of which the stress components denoted by σ_{11}^f, σ_{22}^f, and σ_{12}^f are 1111.0 MPa, 0.0 MPa, and 0.0 MPa, respectively.

According to the large deflection theory of thin plates, an analytic solution on the deflection of the free strip along the longitudinal direction in the above-mentioned thin-film stress state is found based on [Zhang et al. 2004] as

$$u_3(x_1) = \frac{h^s}{2\cosh\bigl(L\sqrt{h^f \sigma_{11}^f / D}\bigr)}\bigl[\cosh\bigl(x_1\sqrt{h^f \sigma_{11}^f / D}\bigr) - 1\bigr], \tag{25}$$

where h^s, h^f, L, and D are the substrate thickness, the thin-film thickness, the semilength of the strip, and the bending stiffness of the plate, respectively.

The deflection of the strip under the aforementioned state of stress calculated from (25) is used as the pseudoexperimental data for the identification of the thin-film stress. The entire strip is discretized with the use of a 2×22 mesh of quadrilateral elements of equal size. The values of the deflection u_3 at the element nodal points given by (25) are used as a subset of the nodal degrees of freedom $\bar{u}$, which are used in the inverse calculations of both the present nonlinear numerical approach and the linear numerical approach of [Fu 2012]. The curvature of the strip deformation derived from (25) in the same state of stress is also used for the evaluation of the thin-film stress from Stoney's formula. The results of identified thin-film stresses obtained from three different methods in comparison with the original exact stresses in half of the strip are shown in Figure 2. It is noticed that the results of the present nonlinear numerical approach accord well with the original thin-film stresses, while those given by the linear numerical approach and Stoney's formula manifest important discrepancies with respect to the exact values in the same way.

	Young's modulus (GPa)	Poisson's ratio	Thickness (μm)	Plan sizes (mm^2)
Substrate (Si)	130	0.28	350	100×2
Film (W)	248	0.30	0.9	100×2

Table 1. Sizes and material parameters of a thin-film material strip.

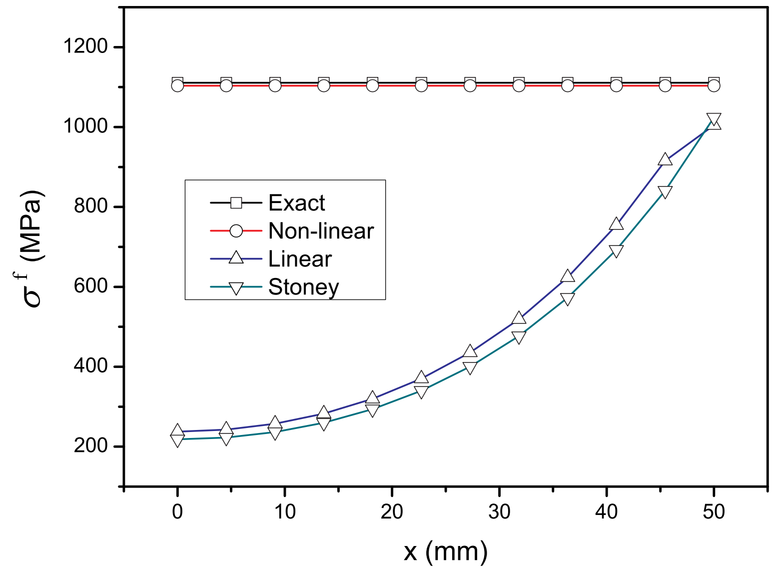

Figure 2. Comparison of the identified thin-film stresses from different methods.

5.2. ***Nonlinear thin-film stress in a three-layered wafer.*** A wafer of three-layered thin-film material is considered in this example. The material parameters and geometrical sizes of the thin-film materials are given in Table 2.

The initial shape of the substrate of silicon is flat, on which the first thin-film layer of nickel and the second thin-film layer of tungsten are supposed to be deposited uniformly. The thin-film material is discretized on its neutral surface with the use of a mesh of 400 four-node quadrilateral elements.

As an example for algorithmic test, the degrees of freedom of experimental measurement $\bar{u}$ in this example are given by solving a direct problem of the thin-film material with the use of (18), of which the uniformly distributed thin-film stress fields of the first and second thin-film layers are prescribed such that $\sigma_{11}^{f_1} = \sigma_{22}^{f_1} = 345.0\,\text{MPa}$, $\sigma_{11}^{f_2} = \sigma_{22}^{f_2} = 1044.7\,\text{MPa}$, and $\sigma_{12}^{f_1} = \sigma_{12}^{f_2} = 0.0\,\text{MPa}$. Here, the thin-film stresses of the two thin-film layers are intentionally related by the transitional conditions of (16) and (17) in supposing that the eigenstrains of the two thin-film layers are equal, which means also that the elastic strains of the two thin-film layers are equal on the interface between the two layers.

The direct solution of the substrate deflection under only the prescribed thin-film stress of the first thin-film layer $\Delta\bar{u}_3^{f_1}$ is shown in Figure 3, and is considered as a deflection field of the substrate configuration change due to the removal of the first thin-film layer from the substrate, and has in addition been adjusted by the action of the thin-film stress of the second layer. The direct solution of the substrate deflection

	Young's modulus (GPa)	Poisson's ratio	Thickness (μm)	Radius (mm)
Substrate (Si)	130	0.28	350	50
Layer 1 (Ni)	130	0.31	0.9	50
Layer 2 (W)	385	0.30	0.9	50

Table 2. Sizes and material parameters of a three-layered wafer.

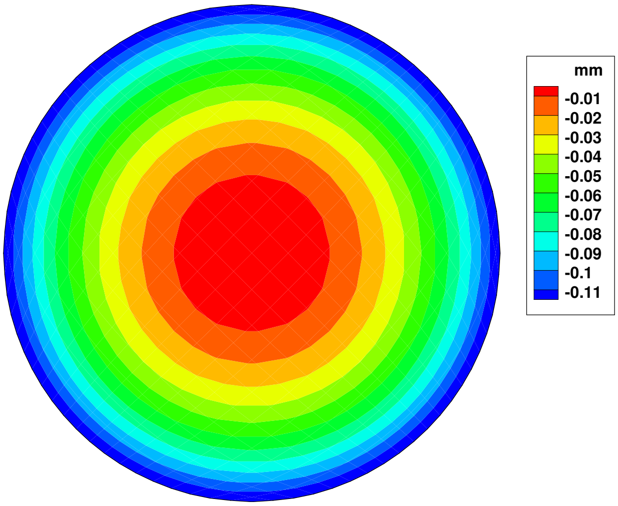

Figure 3. Change of substrate deflection due to the removal of the first thin-film layer.

under the prescribed thin-film stresses of the first and second thin-film layers $\Delta\bar{u}_3 = \Delta\bar{u}_3^{f_1} + \Delta\bar{u}_3^{f_2}$ is given in Figure 4, which is considered as a deflection field of the total substrate configuration change due to the removal of all the two thin-film layers from a fabricated two-layered thin-film material. Since the maximum values of the deflections in Figures 3 and 4 are of the same order as the thin-film material thickness, the deformations of the thin-film material belong to large deflection problems. In this case, the geometrically nonlinear deformation is more sensitive to the loads at the primary deformation stage. As a consequence, the first deflection field $\Delta\bar{u}_3^{f_1}$ given by the first-layer thin-film stress $\sigma_{\alpha\beta}^{f_1}$ is more important than the adding-up deflection field $\Delta\bar{u}_3^{f_2} = \Delta\bar{u}_3 - \Delta\bar{u}_3^{f_1}$ given by the adding-up second-layer thin-film stress $\sigma_{\alpha\beta}^{f_2}$.

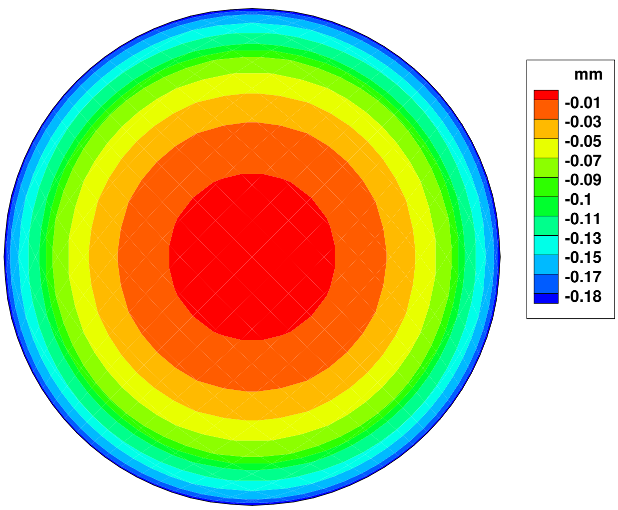

Figure 4. Change of substrate deflection due to the removal of the two thin-film layers.

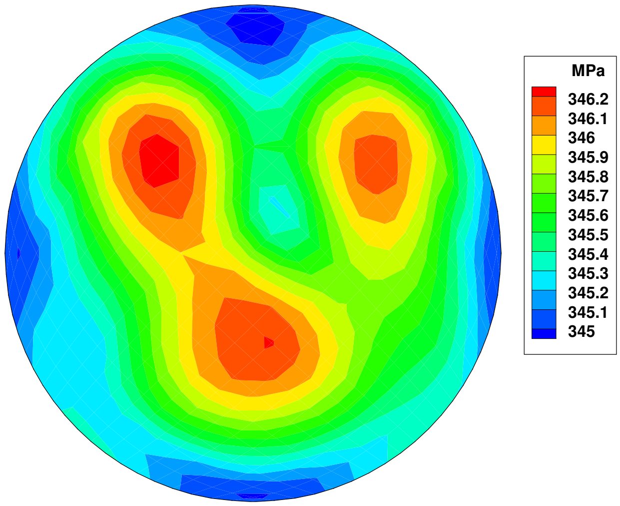

Figure 5. Identified maximum principal thin-film stress of the first thin-film layer.

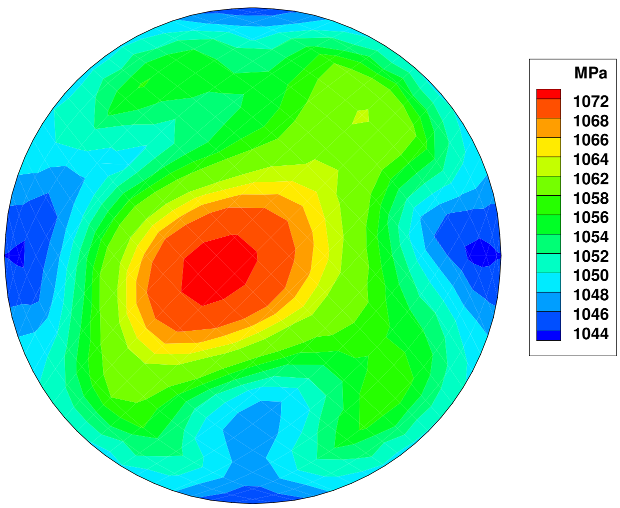

Figure 6. Identified maximum principal thin-film stress of the second thin-film layer.

In following the first approach proposed in Section 2.2, the first-layer thin-film stress $\sigma_{\alpha\beta}^{f_1}$ is first identified with the use of the deflection field $\Delta\bar{u}_3^{f_1}$. Then, the second-layer thin-film stress $\sigma_{\alpha\beta}^{f_2}$ is identified with the use of the total deflection field $\Delta\bar{u}_3$ and the previously identified first-layer thin-film stress $\sigma_{\alpha\beta}^{f_1}$.

The identified maximum principal thin-film stress of the first thin-film layer and that of the second thin-film layer are shown in Figures 5 and 6, respectively. Notice from Figures 5 and 6 that the identified thin-film stresses of the two thin-film layers are in general similar to the prescribed thin-film stresses of the two thin-film layers. The maximum discrepancies on the maximum principal stresses of the first and second thin-film layers with respect to those of the prescribed thin-film stresses of the two thin-film layers are only locally 0.3% and 2.6%, respectively. The existing discrepancies of the values and distributions compared with those of the original fields may be improved by various numerical means such as mesh refinement, regularization parameter optimization, convergence criteria enhancement, etc.

Finally, notice that the second approach can be also applied in this example. With the use of the transitional conditions for the thin-film stresses on the interface between the first and the second thin-film layers, the thin-film stress of a chosen principal layer can be first identified from the total deformation and then the thin-film stress of other layer can be determined according to the transitional conditions from the identified thin-film stress.

6. Conclusions

The identification of thin-film stress in nonlinear multilayered thin-film materials is studied, combining use of mechanical modeling, the finite element method, and the theory of inverse problems. From the method and numerical examples presented, the main findings of the work are summarized as follows.

(1) When the deformation of the thin-film materials is as large as in the range of the large deflection theory of classical plates, the estimation of thin-film stress should turn to the plate models of nonlinear large deflection theories. The important differences between the geometrically nonlinear and linear theories may manifest in this range of thin-film material deformations. It is shown that the thin-film stress determined from the linear models is underestimated for a given nonlinear correlating kinematic field.

(2) In the nonlinear identification process, the change of the configuration of thin-film materials does not linearly depend on the thin-film stress. The layer-by-layer cumulative formulation allows for identifying the thin-film stress of each layer from the cumulative deformation and the corresponding cumulative thin-film stresses.

(3) The transitional conditions for the thin-film stresses at the interfaces between thin-film layers are proposed according to the deformation continuity requirement. In supposing that the eigenstrains as well as their differences between thin-film layers are invariant in the identification process, the stress transitional conditions can be obtained in the layer-by-layer cumulative identification process, and are used as key factors in establishing an efficient solution strategy.

(4) The applied inverse problem method allows for using a subset of the total degrees of freedom to determine the thin-film stresses, which provides great flexibility in choosing appropriate methods or techniques for measuring correlating fields. The method itself is also adaptive to different computations.

(5) With use of the finite element method, the nonhomogeneities of geometrical shapes, material characteristics, and mechanical fields in thin-film materials no longer constitute major hurdles in the modeling and solution of the thin-film stress problems since they can be defined element-by-element over the thin-film materials.

(6) The structural model used in the present work is suitable for both thin and moderately thick thin-film materials. The application of a reliable finite element ensures the validity of the numerical approach in the two cases. The structural model used here can be easily enriched in kinematic fields or in thin-film stress fields whenever needed.

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Received 1 Apr 2013. Revised 22 May 2013. Accepted 3 Jun 2013.

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Journal of Mechanics of Materials and Structures

Volume 8, No. 5-7 July–September 2013

1559-3959(2013)8:5;1-7