Stresses in a Multilayer Thin Film/Substrate System Subjected to Nonuniform Temperature

X. Feng
Department of Engineering Mechanics,
Tsinghua University,
Beijing, 100084, P.R. China

Y. Huang[1]
e-mail: y-huang@northwestern.edu
Department of Civil/Environmental Engineering
and Department of Mechanical Engineering,
Northwestern University,
Evanston, IL 60208

A. J. Rosakis
Graduate Aeronautical Laboratory,
California Institute of Technology,
Pasadena, CA 91125

Current methodologies used for the inference of thin film stress through curvature measurements are strictly restricted to uniform film stress and system curvature states over the entire system of a single thin film on a substrate. By considering a circular multilayer thin film/substrate system subjected to nonuniform temperature distributions, we derive relations between the stresses in each film and temperature, and between the system curvatures and temperature. These relations featured a "local" part that involves a direct dependence of the stress or curvature components on the temperature at the same point, and a "nonlocal" part, which reflects the effect of temperature of other points on the location of scrutiny. We also derive relations between the film stresses in each film and the system curvatures, which allow for the experimental inference of such stresses from full-field curvature measurements in the presence of arbitrary nonuniformities. These relations also feature a "nonlocal" dependence on curvatures making full-field measurements of curvature a necessity for the correct inference of stress. The interfacial shear tractions between the films and between the film and substrate are proportional to the gradient of the first curvature invariant, and can also be inferred experimentally.
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1 Introduction

Substrates formed of suitable solid-state materials may be used as platforms to support various thin film structures. Integrated electronic circuits, integrated optical devices and optoelectronic circuits, microelectromechanical systems deposited on wafers, three-dimensional electronic circuits, systems-on-a-chip structures, lithographic reticles, and flat panel display systems are examples of such thin film structures integrated on various types of plate substrates. The stress buildup in the thin film is important to the reliability and performance of these devices and systems.

Stoney [1] studied a system composed of a thin film of thickness h_f, deposited on a relatively thick substrate, of thickness h_s, and derived a simple relation between the curvature κ of the system and the stress $\sigma^{(f)}$ of the film as follows:

$$\sigma^{(f)} = \frac{E_s h_s^2 \kappa}{6h_f(1-\nu_s)} \tag{1.1}$$

In the above, the subscripts "f" and "s" denote the thin film and substrate, respectively, and E and ν are the Young's modulus and Poisson's ratio. Equation (1.1) is called the Stoney formula, and it has been extensively used in the literature to infer film stress changes from experimental measurement of system curvature changes [2].

Stoney's formula was based on a number of assumptions:

(i) Both the film thickness h_f and the substrate thickness h_s are uniform and $h_f \ll h_s \ll R$, where R represents the characteristic length in the lateral direction (e.g., system radius R shown in Fig. 1);
(ii) The strains and rotations of the plate system are infinitesimal;
(iii) Both the film and substrate are homogeneous, isotropic, and linearly elastic;
(iv) The film stress states are in-plane isotropic or equibiaxial (two equal stress components in any two, mutually orthogonal in-plane directions) while the out-of-plane direct stress and all shear stresses vanish;
(v) The system's curvature components are equibiaxial (two equal direct curvatures) while the twist curvature vanishes in all directions; and
(vi) All surviving stress and curvature components are spatially constant over the plate system's surface, a situation that is often violated in practice.

Despite the explicitly stated assumptions of spatial stress and curvature uniformity, the Stoney formula is often, arbitrarily, applied to cases of practical interest where these assumptions are violated. This is typically done by applying Stoney's formula pointwise, and thus extracting a local value of stress from a local measurement of the curvature of the system. This approach of inferring film stress clearly violates the uniformity assumptions of the analysis and, as such, its accuracy as an approximation is expected to deteriorate as the levels of curvature nonuniformity become more severe.

Following the initial formulation by Stoney, a number of extensions have been derived to relax some assumptions. Such extensions of the initial formulation include relaxation of the assumption of equibiaxiality as well as the assumption of small deformations/deflections. A biaxial form of Stoney formula (with different direct stress values and nonzero in-plane shear stress) was derived by relaxing the assumption (v) of curvature equibiaxiality [2]. Related analyses treating discontinuous films in the form of bare periodic lines [3] or composite films with periodic line structures (e.g., bare or encapsulated periodic lines) have also been derived [4–6]. These latter analyses have removed the assumptions (iv) and (v) of equibiaxiality and have allowed the

[1]Corresponding author.
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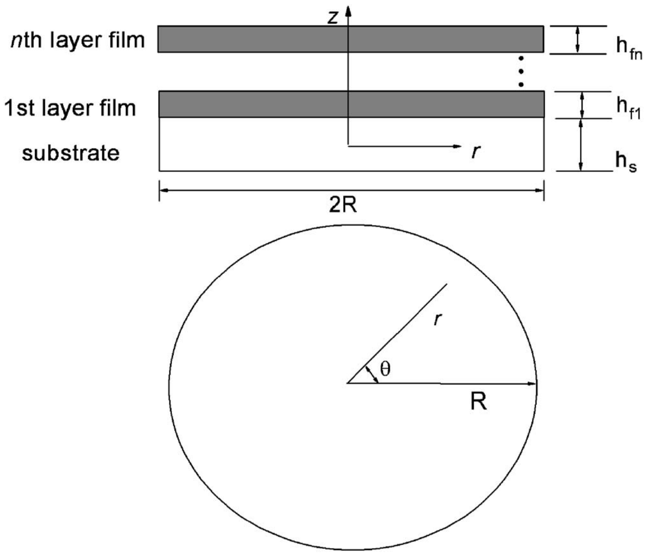

Fig. 1 A schematic diagram of a multilayer thin film/substrate system, showing the cylindrical coordinates (r,θ,z)

existence of three independent curvature and stress components in the form of two, nonequal, direct components and one shear or twist component. However, the uniformity assumption (vi) of all of these quantities over the entire plate system was retained. In addition to the above, single, multiple, and graded films and substrates have been treated in various "large" deformation analyses [7–10]. These analyses have removed both the restrictions of an equibiaxial curvature state as well as the assumption (ii) of infinitesimal deformations. They have allowed for the prediction of kinematically nonlinear behavior and bifurcations in curvature states that have also been observed experimentally [11,12]. These bifurcations are transformations from an initially equibiaxial to a subsequently biaxial curvature state that may be induced by an increase in film stress beyond a critical level. This critical level is intimately related to the system aspect ratio, i.e., the ratio of in-plane to thickness dimension and the elastic stiffness. These analyses also retain the assumption (vi) of spatial curvature and stress uniformity across the system. However, they allow for deformations to evolve from an initially spherical shape to an energetically favored shape (e.g., ellipsoidal, cylindrical, or saddle shapes) that features three different, still spatially constant, curvature components [6,11].

The above-discussed extensions of Stoney's methodology have not relaxed the most restrictive of Stoney's original assumption (vi) of spatial uniformity that does not allow film stress and system curvature components to vary in the thin film/substrate system. This crucial assumption is often violated in practice, since film stresses and the associated system curvatures are nonuniformly distributed. Recently, Huang et al. [13] and Huang and Rosakis [14] relaxed the assumption (vi) (and also (iv) and (v)) to study the thin film/substrate system subjected to nonuniform, axisymmetric misfit strain (in thin film) and temperature change (in both thin film and substrate), respectively, while Huang and Rosakis [15] and Ngo et al. [16] studied the thin film/substrate system subject to arbitrarily nonuniform (e.g., nonaxisymmetric) misfit strain and temperature. The most important result is that *the film stresses depend nonlocally on the system curvatures*; i.e., they depend on curvatures of the entire system. The relations between film stresses and system curvatures are established for arbitrarily nonuniform misfit strain and temperature change, and such relations degenerate to Stoney's formula for uniform, equibiaxial stresses and curvatures.

Feng et al. [17] relaxed part of the assumption (i) to study the thin film and substrate of different radii. Ngo et al. [18] completely relax the assumption (i) to study arbitrarily nonuniform thickness of the thin film. They derived an analytical relation between the film stresses and system curvatures that allows for the accurate experimental inference of film stress from full-field curvature measurements once the film thickness distribution is known. Brown et al. [19] used two independent types of X-ray microdiffraction to measure both substrate slope and film stress across the diameter of an axisymmetric thin film/substrate specimen composed of a Si substrate on which a smaller circular *W* film island was deposited. The substrate slopes, measured by polychromatic (white beam) X-ray microdiffraction, were used to calculate curvature fields and to, thus, infer the film stress distribution using both the "local" Stoney formula and the new, nonlocal relation. The variable film thickness, which was independently measured, was also an input to the new relation. These were then compared with the film stress measured independently through monochromatic X-ray diffraction in the sample to validate the new analytical relation [18].

Many thin film/substrate systems involve multiple layers of thin films. The main purpose of this paper is to extend the above analyses by Huang, Rosakis, and co-workers to a system composed of multilayer thin films on a substrate subjected to nonuniform temperature distribution. We will relate stresses in each film and system curvatures to the temperature distribution, and ultimately derive a relation between the stresses in each film and system curvatures that would allow for the accurate experimental inference of film stresses from full-field and real-time curvature measurements.

2 Axisymmetric Temperature Distribution

We first consider a system of multilayer thin films deposited on a substrate subjected to axisymmetric temperature distribution $T(r)$, where r is the radial coordinate (Fig. 1). The thin films and substrate are circular in the lateral direction and have a radius R. The deformation is axisymmetric and is therefore independent of the polar angle θ, where (r,θ,z) are cylindrical coordinates with the origin at the center of the substrate (Fig. 1).

2.1 Governing Equations. Let $h_{f_i}(i=1,\ldots,n)$ denote the thickness of the ith thin film (Fig. 1). The total film thickness $h_f=\sum_{i=1}^{n} h_{f_i}$ of all n thin films is much less than the substrate thickness h_s, and both are much less than R; i.e., $h_f \ll h_s \ll R$. The Young's modulus, Poisson's ratio, and coefficient of thermal expansion of the ith film and substrate are denoted by E_{f_i}, ν_{f_i}, α_{f_i}, E_s, ν_s, and α_s, respectively.

The substrate is modeled as a plate since it can be subjected to bending and $h_s \ll R$. The thin films are modeled as membranes that have no bending rigidities due to their small thickness $h_{f_i} \ll h_s$. Therefore, they all have the same in-plane displacement $u_f(r)$ in the radial direction. The strains are $\varepsilon_{rr}=du_f/dr$ and $\varepsilon_{\theta\theta}=u_f/r$. The stresses in the ith thin film can be obtained from the linear thermo-elastic constitutive model as

$$\sigma_{rr}^{(i)}=\frac{E_{f_i}}{1-\nu_{f_i}^2}\left[\frac{du_f}{dr}+\nu_{f_i}\frac{u_f}{r}-(1+\nu_{f_i})\alpha_{f_i}T\right]$$

$$\sigma_{\theta\theta}^{(i)}=\frac{E_{f_i}}{1-\nu_{f_i}^2}\left[\nu_{f_i}\frac{du_f}{dr}+\frac{u_f}{r}-(1+\nu_{f_i})\alpha_{f_i}T\right] \tag{2.1}$$

The membrane forces in the ith thin film are

$$N_r^{(f_i)}=h_{f_i}\sigma_{rr}^{(i)} \quad N_\theta^{(f_i)}=h_{f_i}\sigma_{\theta\theta}^{(i)} \tag{2.2}$$

For a nonuniform temperature distribution $T=T(r)$, the shear stress tractions at the film/substrate and film/film interfaces do not vanish, and are denoted by $\tau^{(i)}(r)(i=1,\ldots,n)$ as shown in Fig. 2. The normal stress tractions σ_{zz} still vanish because thin films have

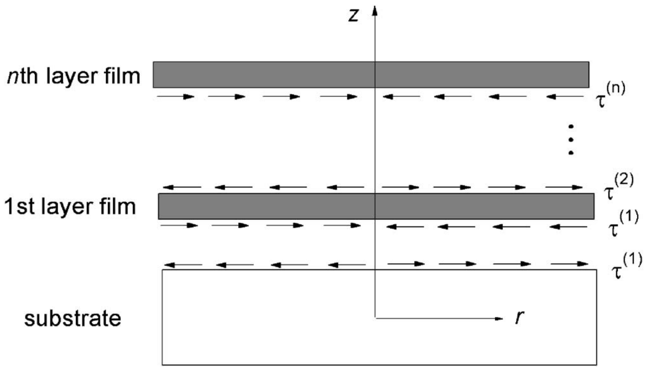

Fig. 2 A schematic diagram of the nonuniform shear traction distribution at the film/film and film/substrate interfaces

no bending rigidities. The equilibrium equations for thin films, accounting for the effect of interface shear stress tractions, become

$$\begin{cases} \dfrac{dN_r^{(f_1)}}{dr} + \dfrac{N_r^{(f_1)} - N_\theta^{(f_1)}}{r} - (\tau^{(1)} - \tau^{(2)}) = 0 \\ \dfrac{dN_r^{(f_2)}}{dr} + \dfrac{N_r^{(f_2)} - N_\theta^{(f_2)}}{r} - (\tau^{(2)} - \tau^{(3)}) = 0 \\ \vdots \\ \dfrac{dN_r^{(f_n)}}{dr} + \dfrac{N_r^{(f_n)} - N_\theta^{(f_n)}}{r} - \tau^{(n)} = 0 \end{cases} \tag{2.3}$$

Substitution of Eqs. (2.1)–(2.3) and the summation of its left-hand side yield

$$\sum_{i=1}^{n} \frac{E_{f_i} h_{f_i}}{1 - \upsilon_{f_i}^2} \left(\frac{d^2 u_f}{dr^2} + \frac{1}{r}\frac{du_f}{dr} - \frac{u_f}{r^2} \right) = \tau^{(1)} + \sum_{i=1}^{n} \frac{E_{f_i} h_{f_i} \alpha_{f_i}}{1 - \upsilon_{f_i}} \frac{dT}{dr} \tag{2.4}$$

Let u_s denote the displacement in the radial (r) direction at the neutral axis ($z=0$) of the substrate, and w the displacement in the normal (z) direction. The forces and bending moments in the substrate are obtained from the linear thermo-elastic constitutive model as

$$N_r^{(s)} = \frac{E_s h_s}{1 - \nu_s^2} \left[\frac{du_s}{dr} + \nu_s \frac{u_s}{r} - (1 + \nu_s)\alpha_s T \right]$$

$$N_\theta^{(s)} = \frac{E_s h_s}{1 - \nu_s^2} \left[\nu_s \frac{du_s}{dr} + \frac{u_s}{r} - (1 + \nu_s)\alpha_s T \right] \tag{2.5}$$

$$M_r = \frac{E_s h_s^3}{12(1 - \nu_s^2)} \left(\frac{d^2 w}{dr^2} + \frac{\nu_s}{r}\frac{dw}{dr} \right)$$

$$M_\theta = \frac{E_s h_s^3}{12(1 - \nu_s^2)} \left(\nu_s \frac{d^2 w}{dr^2} + \frac{1}{r}\frac{dw}{dr} \right) \tag{2.6}$$

The shear stress $\tau^{(1)}$ at the film/substrate interface is equivalent to the distributed axial force $\tau^{(1)}(r)$ and bending moment $(h_s/2)\tau^{(1)}(r)$ applied at the neutral axis ($z=0$) of the substrate. The in-plane force equilibrium equation of the substrate then becomes

$$\frac{dN_r^{(s)}}{dr} + \frac{N_r^{(s)} - N_\theta^{(s)}}{r} + \tau^{(1)} = 0 \tag{2.7}$$

The out-of-plane force and moment equilibrium equations are given by

$$\frac{dM_r}{dr} + \frac{M_r - M_\theta}{r} + Q - \frac{h_s}{2}\tau^{(1)} = 0 \tag{2.8}$$

$$\frac{dQ}{dr} + \frac{Q}{r} = 0 \tag{2.9}$$

where Q is the shear force normal to the neutral axis. Substitution of Eq. (2.5) into Eq. (2.7) yields

$$\frac{d^2 u_s}{dr^2} + \frac{1}{r}\frac{du_s}{dr} - \frac{u_s}{r^2} = (1 + \nu_s)\alpha_s \frac{dT}{dr} - \frac{1 - \nu_s^2}{E_s h_s}\tau^{(1)} \tag{2.10}$$

Elimination of Q from Eqs. (2.8) and (2.9), in conjunction with Eq. (2.6), gives

$$\frac{d^3 w}{dr^3} + \frac{1}{r}\frac{d^2 w}{dr^2} - \frac{1}{r^2}\frac{dw}{dr} = \frac{6(1 - \nu_s^2)}{E_s h_s^2}\tau^{(1)} \tag{2.11}$$

The continuity of displacement across the film/substrate interface requires

$$u_f = u_s - \frac{h_s}{2}\frac{dw}{dr} \tag{2.12}$$

Equations (2.4) and (2.10)–(2.12) constitute four ordinary differential equations for u_f, u_s, w, and $\tau^{(1)}$.

We can eliminate u_f, u_s, and$w$ from these four equations to obtain the shear stress at the film/substrate interface in terms of temperature as

$$\tau^{(1)} = \frac{\displaystyle\sum_{i=1}^{n} \frac{E_{f_i} h_{f_i}}{1 - \nu_{f_i}^2}[(1 + \nu_s)\alpha_s - (1 + \nu_{f_i})\alpha_{f_i}]}{\displaystyle 1 + \sum_{i=1}^{n} 4\frac{E_{f_i} h_{f_i}}{1 - \nu_{f_i}^2}\frac{1 - \nu_s^2}{E_s h_s}} \frac{dT}{dr} \tag{2.13}$$

which is a remarkable result that holds regardless of boundary conditions at the edge $r=R$. Therefore, the interface shear stress is proportional to the gradient of temperature. For uniform temperature T=constant, the interface shear stress vanishes; i.e., $\tau^{(1)}=0$.

Substitution of the above solution for shear stress $\tau^{(1)}$ into Eqs. (2.11) and (2.10) yields ordinary differential equations for displacements w and u_s in the substrate. Their solutions, at the limit $h_f \ll h_s$ are

$$\frac{dw}{dr} = 6\frac{1 - \nu_s^2}{E_s h_s^2} \sum_{i=1}^{n} \frac{E_{f_i} h_{f_i}}{1 - \nu_{f_i}^2}[(1 + \nu_s)\alpha_s - (1 + \nu_{f_i})\alpha_{f_i}] \frac{1}{r}\int_0^r \eta T(\eta) d\eta + \frac{B_1}{2} r \tag{2.14}$$

$$u_s = (1 + \nu_s)\alpha_s \frac{1}{r}\int_0^r \eta T(\eta) d\eta + \frac{B_2}{2} r \tag{2.15}$$

where B_1 and B_2 are constants to be determined by boundary conditions. The displacement in the thin films is then obtained from Eq. (2.12) as

$$u_f = (1 + \nu_s)\alpha_s \frac{1}{r}\int_0^r \eta T(\eta) d\eta + \left(\frac{B_2}{2} - \frac{h_s B_1}{4} \right) r \tag{2.16}$$

The first boundary condition at the free edge $r=R$ requires that the net force vanish

$$\sum_{i=1}^{n} N_r^{(f_i)} + N_r^{(s)} = 0 \quad \text{at } r = R \tag{2.17}$$

which gives

$$B_2 = (1-\nu_s)\alpha_s \bar{T} \tag{2.18}$$

for $h_f \ll h_s$, where $\bar{T}=(2/R^2)\int_0^R \eta T(\eta)d\eta = \iint T dA/\pi R^2$ is the average temperature over the entire system. The second boundary condition at the free edge $r=R$ is vanishing of net moment, i.e.,

$$M_r - \frac{h_s}{2}\sum_{i=1}^{n} N_r^{(f_i)} = 0 \quad \text{at } r=R \tag{2.19}$$

which gives

$$B_1 = 6\frac{1-\nu_s^2}{E_s h_s^2}\sum_{i=1}^{n}\frac{E_{f_i}h_{f_i}}{1-\nu_{f_i}^2}\left[\frac{(1+v_{f_i})(1-v_s)}{1+v_s}(\alpha_s-\alpha_{f_i})-(v_s-\nu_{f_i})\alpha_s\right]\bar{T} \tag{2.20}$$

2.2 Stresses in Multilayer Thin Films and System Curvatures. The system curvatures are related to the out-of-plane displacement w by $\kappa_{rr}=d^2w/dr^2$ and $\kappa_{\theta\theta}=dw/rdr$. Their sum is given by

$$\kappa_{rr}+\kappa_{\theta\theta} = 12\frac{1-\nu_s}{E_s h_s^2}\left[A_\alpha \bar{T} + \frac{1+\nu_s}{2}A_{\nu\alpha}(T-\bar{T})\right] \tag{2.21}$$

where $\bar{T}$ is the average temperature in the thin film/substrate system, and

$$A_\alpha \equiv \sum_{i=1}^{n}\frac{E_{f_i}h_{f_i}}{1-v_{f_i}}(\alpha_s-\alpha_{f_i})$$

$$A_{\nu\alpha} \equiv \sum_{i=1}^{n}\frac{E_{f_i}h_{f_i}}{1-v_{f_i}^2}[(1+\nu_s)\alpha_s-(1+\nu_{f_i})\alpha_{f_i}] \tag{2.22}$$

The first term on the right-hand side corresponds to the (constant) average temperature $\bar{T}$, while the second term gives the deviation $T-\bar{T}$ from the constant temperature.

The difference between two system curvatures is

$$\kappa_{rr}-\kappa_{\theta\theta} = 6\frac{1-\nu_s^2}{E_s h_s^2}A_{\nu\alpha}\left[T-\frac{2}{r^2}\int_0^r \eta T(\eta)d\eta\right] \tag{2.23}$$

As compared to the system curvatures for a single thin film [14], Eqs. (2.21) and (2.23) can be obtained by replacing the single film properties by the sum of multilayer film properties in Eq. (2.22).

The stresses in the ith thin film can be obtained from the in-plane displacement u_f as

$$\sigma_{rr}^{(f_i)}+\sigma_{\theta\theta}^{(f_i)} = \frac{E_{f_i}}{1-\nu_{f_i}}\{2(\alpha_s-\alpha_{f_i})\bar{T}+[(1+\nu_s)\alpha_s-2\alpha_{f_i}](T-\bar{T})\} \tag{2.24}$$

$$\sigma_{rr}^{(f_i)}-\sigma_{\theta\theta}^{(f_i)} = \frac{E_{f_i}}{1+\nu_{f_i}}(1+\nu_s)\alpha_s\left[T-\frac{2}{r^2}\int_0^r \eta T(\eta)d\eta\right] \tag{2.25}$$

They are identical to Huang and Rosakis [14] for a single thin film if the Young's modulus, Poisson's ratio, and coefficient of thermal expansion are substituted by E_i, v_i, and α_i of the ith thin film, respectively. The shear stresses along the film/film or film/substrate interface can be obtained from the equilibrium equation (2.3). Specifically, the shear stress of ith thin film is given by

$$\tau^{(i)} = \sum_{j=i}^{n}\frac{E_{f_j}h_{f_j}}{1-v_{f_j}^2}[(1+v_s)\alpha_s-(1+v_{f_j})\alpha_{f_j}]\frac{dT}{dr} \tag{2.26}$$

where the summation is from the ith thin film to the last (nth).

3 Extension of Stoney Formula for a Multilayer Thin Film/Substrate System Subjected to Axisymmetric Temperature Distribution

We extend the Stoney formula for a multilayer thin film/substrate system by eliminating the nonuniform axisymmetric temperature in order to establish a direct relation between the stresses in the ith thin film and system curvatures. Both $\kappa_{rr}-\kappa_{\theta\theta}$ in Eq. (2.23) and $\sigma_{rr}^{(f_i)}-\sigma_{\theta\theta}^{(f_i)}$ in Eq. (2.25) are proportional to $T-(2/r^2)\int_0^r \eta T(\eta)d\eta$, and therefore can be directly related by

$$\sigma_{rr}^{(f_i)}-\sigma_{\theta\theta}^{(f_i)} = \frac{E_s h_s^2 \alpha_s}{6(1-v_s)}\frac{E_{f_i}}{1+v_{f_i}}\frac{\kappa_{rr}-\kappa_{\theta\theta}}{A_{\nu\alpha}} \tag{3.1}$$

where $A_{\nu\alpha}$ is given in Eq. (2.22). We define the average system curvature $\overline{\kappa_{rr}+\kappa_{\theta\theta}}$ as

$$\overline{\kappa_{rr}+\kappa_{\theta\theta}} = \frac{1}{\pi R^2}\int\int_A (\kappa_{rr}+\kappa_{\theta\theta})\eta d\eta d\theta = \frac{2}{R^2}\int_0^R \eta(\kappa_{rr}+\kappa_{\theta\theta})d\eta \tag{3.2}$$

which can be related to the average temperature $\bar{T}$ by averaging both sides of Eq. (2.21), i.e.,

$$\overline{\kappa_{rr}+\kappa_{\theta\theta}} = 12\frac{1-\nu_s}{E_s h_s^2}A_\alpha \bar{T} \tag{3.3}$$

where A_α is given in Eq. (2.22). The deviation from the average curvature $\kappa_{rr}+\kappa_{\theta\theta}-\overline{\kappa_{rr}+\kappa_{\theta\theta}}$ can be related to the deviation from the average temperature $T-\bar{T}$ from Eq. (2.21) as

$$\kappa_{rr}+\kappa_{\theta\theta}-\overline{\kappa_{rr}+\kappa_{\theta\theta}} = 6\frac{1-\nu_s^2}{E_s h_s^2}A_{\nu\alpha}(T-\bar{T}) \tag{3.4}$$

Elimination of temperature deviation $T-\bar{T}$ and average temperature $\bar{T}$ from Eqs. (3.3), (3.4), and (2.24) gives the sum of stresses in the ith thin film in terms of curvature as

$$\sigma_{rr}^{(f_i)}+\sigma_{\theta\theta}^{(f_i)} = \frac{E_s h_s^2}{6(1-\nu_s)}\frac{E_{f_i}}{1-v_{f_i}}\left[\frac{\alpha_s-\alpha_{f_i}}{A_\alpha}\overline{\kappa_{rr}+\kappa_{\theta\theta}} + \frac{(1+v_s)\alpha_s-2\alpha_{f_i}}{(1+v_s)A_{\nu\alpha}}(\kappa_{rr}+\kappa_{\theta\theta}-\overline{\kappa_{rr}+\kappa_{\theta\theta}})\right] \tag{3.5}$$

Equations (3.1) and (3.5) provide direct relations between stresses in each thin film and system curvatures. Stresses at a point in each thin film depend not only on curvatures at the same point (local dependence), but also on the average curvature in the entire substrate (nonlocal dependence).

The interface stress $\tau^{(i)}$ can also be directly related to system curvatures via

$$\tau^{(i)} = \frac{E_s h_s^2}{6(1-v_s^2)}\frac{\sum_{k=i}^{n}\frac{E_{f_k}h_{f_k}}{1-v_{f_k}^2}[(1+v_s)\alpha_s-(1+v_{f_k})\alpha_{f_k}]}{A_{\nu\alpha}}\frac{d(\kappa_{rr}+\kappa_{\theta\theta})}{dr} \tag{3.6}$$

This provides a remarkably simple way to estimate the interface shear stress from radial gradients of the two nonzero system curvatures.

4 Arbitrary Temperature Distribution

Similar to Huang and Rosakis [15] for a single thin film on a substrate, we expand the arbitrary nonuniform temperature distribution $T(r,\theta)$ to the Fourier series:

$$T(r,\theta)=\sum_{m=0}^{\infty}T_c^{(m)}(r)\cos m\theta+\sum_{m=0}^{\infty}T_s^{(m)}(r)\sin m\theta \tag{4.1}$$

where

$$T_c^{(0)}(r)=\frac{1}{2\pi}\int_0^{2\pi}T(r,\theta)d\theta$$

$$T_c^{(m)}(r)=\frac{1}{\pi}\int_0^{2\pi}T(r,\theta)\cos m\theta d\theta$$

and

$$T_s^{(m)}(r)=\frac{1}{\pi}\int_0^{2\pi}T(r,\theta)\sin m\theta d\theta \quad (m\geq 1)$$

The analysis is similar to Huang and Rosakis [15], except it is now for multilayer thin films on a substrate.

The system curvatures are

$$\kappa_{rr}=\frac{\partial^2 w}{\partial r^2}\quad \kappa_{\theta\theta}=\frac{1}{r}\frac{\partial w}{\partial r}+\frac{1}{r^2}\frac{\partial^2 w}{\partial \theta^2}\quad \kappa_{r\theta}=\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial w}{\partial \theta}\right)$$

The sum of system curvatures is related to the temperature by

$$\kappa_{rr}+\kappa_{\theta\theta}=12\frac{1-\nu_s}{E_sh_s^2}\Bigg\{A_\alpha\bar{T}+\frac{1+\nu_s}{2}A_{\nu\alpha}(T-\bar{T})+(1+\nu_s)\left(\frac{4}{3+\nu_s}A_\alpha-A_{\nu\alpha}\right)\sum_{m=1}^{\infty}(m+1)\frac{r^m}{R^{2m+2}}\left[\cos m\theta\int_0^R\eta^{m+1}T_c^{(m)}(\eta)d\eta+\sin m\theta\int_0^R\eta^{m+1}T_s^{(m)}(\eta)d\eta\right]\Bigg\} \tag{4.2}$$

where $\bar{T}=(2/R^2)\int_0^R\eta T_c^{(0)}(\eta)d\eta=(1/\pi R^2)\int\int_A T(\eta,\varphi)dA$ is the average temperature over the entire area A of the thin film, $dA=\eta d\eta d\varphi$, and A_α and $A_{\nu\alpha}$ are given in Eq. (2.22).

The difference between two curvatures, i.e., $\kappa_{rr}-\kappa_{\theta\theta}$, and the twist $\kappa_{r\theta}$ are given by

$$\kappa_{rr}-\kappa_{\theta\theta}=6\frac{1-\nu_s^2}{E_sh_s^2}A_{\nu\alpha}\Bigg[T-\frac{2}{r^2}\int_0^r\eta T_c^{(0)}d\eta-\sum_{m=1}^{\infty}\frac{m+1}{r^{m+2}}\left(\cos m\theta\int_0^r\eta^{m+1}T_c^{(m)}d\eta+\sin m\theta\int_0^r\eta^{m+1}T_s^{(m)}d\eta\right)-\sum_{m=1}^{\infty}(m-1)r^{m-2}\left(\cos m\theta\int_r^R\eta^{1-m}T_c^{(m)}d\eta+\sin m\theta\int_r^R\eta^{1-m}T_s^{(m)}d\eta\right)\Bigg]+6\frac{1-\nu_s^2}{E_sh_s^2}\left(\frac{4}{3+\nu_s}A_\alpha-A_{\nu\alpha}\right)\sum_{m=1}^{\infty}\frac{m+1}{R^{m+2}}\left[m\left(\frac{r}{R}\right)^m-(m-1)\left(\frac{r}{R}\right)^{m-2}\right]\left(\cos m\theta\int_0^R\eta^{m+1}T_c^{(m)}d\eta+\sin m\theta\int_0^R\eta^{m+1}T_s^{(m)}d\eta\right) \tag{4.3}$$

$$\kappa_{r\theta}=3\frac{1-\nu_s^2}{E_sh_s^2}A_{\nu\alpha}\Bigg[-\sum_{m=1}^{\infty}\frac{m+1}{r^{m+2}}\left(\sin m\theta\int_0^r\eta^{m+1}T_c^{(m)}d\eta-\cos m\theta\int_0^r\eta^{m+1}T_s^{(m)}d\eta\right)+\sum_{m=1}^{\infty}(m-1)r^{m-2}\left(\sin m\theta\int_r^R\eta^{1-m}T_c^{(m)}d\eta-\cos m\theta\int_r^R\eta^{1-m}T_s^{(m)}d\eta\right)\Bigg]-3\frac{1-\nu_s^2}{E_sh_s^2}\left(\frac{4}{3+\nu_s}A_\alpha-A_{\nu\alpha}\right)\sum_{m=1}^{\infty}\frac{m+1}{R^{m+2}}\left[m\left(\frac{r}{R}\right)^m-(m-1)\left(\frac{r}{R}\right)^{m-2}\right]\left(\sin m\theta\int_0^R\eta^{m+1}T_c^{(m)}d\eta-\cos m\theta\int_0^R\eta^{m+1}T_s^{(m)}d\eta\right) \tag{4.4}$$

As compared to the system curvatures for a single thin film [15], Eqs. (4.2)–(4.4) can be obtained by replacing the film properties by the sum of multilayer film properties in Eqs. (2.22).

The sum of stresses $\sigma_{rr}^{(f_i)}+\sigma_{\theta\theta}^{(f_i)}$ in the ith thin film is related to the temperature by

$$\sigma_{rr}^{(f_i)}+\sigma_{\theta\theta}^{(f_i)}=\frac{E_{f_i}}{1-\nu_{f_i}}\Bigg\{2(\alpha_s-\alpha_{f_i})\bar{T}+[(1+\nu_s)\alpha_s-2\alpha_{f_i}](T-\bar{T})+2(1-\nu_s)\alpha_s\sum_{m=1}^{\infty}\frac{m+1}{R^{2m+2}}r^m\left(\cos m\theta\int_0^R\eta^{m+1}T_c^{(m)}d\eta+\sin m\theta\int_0^R\eta^{m+1}T_s^{(m)}d\eta\right)\Bigg\} \tag{4.5}$$

The difference between stresses, ie., $\sigma_{rr}^{(f_i)}-\sigma_{\theta\theta}^{(f_i)}$, and shear stress $\sigma_{r\theta}^{(f_i)}$ are given by

$$\sigma_{rr}^{(f_i)}-\sigma_{\theta\theta}^{(f_i)}=\frac{E_{f_i}}{1+\nu_{f_i}}(1+\nu_s)\alpha_s\Bigg\{T-\frac{2}{r^2}\int_0^r\eta T_c^{(0)}d\eta-\sum_{m=1}^{\infty}\frac{m+1}{r^{m+2}}\left(\cos m\theta\int_0^r\eta^{m+1}T_c^{(m)}d\eta+\sin m\theta\int_0^r\eta^{m+1}T_s^{(m)}d\eta\right)-\sum_{m=1}^{\infty}(m-1)r^{m-2}\left(\cos m\theta\int_r^R\eta^{1-m}T_c^{(m)}d\eta+\sin m\theta\int_r^R\eta^{1-m}T_s^{(m)}d\eta\right)-\sum_{m=1}^{\infty}\frac{m+1}{R^{m+2}}\left[m\left(\frac{r}{R}\right)^m-(m-1)\left(\frac{r}{R}\right)^{m-2}\right]\times\left(\cos m\theta\int_0^R\eta^{m+1}T_c^{(m)}d\eta+\sin m\theta\int_0^R\eta^{m+1}T_s^{(m)}d\eta\right)\Bigg\} \tag{4.6}$$

$$\sigma_{r\theta}^{(f_i)}=\frac{E_{f_i}}{2(1+\nu_{f_i})}(1+\nu_s)\alpha_s\left\{-\sum_{m=1}^{\infty}\frac{m+1}{r^{m+2}}\left(\sin m\theta\int_0^r\eta^{m+1}T_c^{(m)}d\eta-\cos m\theta\int_0^r\eta^{m+1}T_s^{(m)}d\eta\right)+\sum_{m=1}^{\infty}(m-1)r^{m-2}\left(\sin m\theta\int_r^R\eta^{1-m}T_c^{(m)}d\eta\right.\right.$$
$$\left.\left.-\cos m\theta\int_r^R\eta^{1-m}T_s^{(m)}d\eta\right)+\sum_{m=1}^{\infty}\frac{m+1}{R^{m+2}}\left[m\left(\frac{r}{R}\right)^m-(m-1)\left(\frac{r}{R}\right)^{m-2}\right]\left(\sin m\theta\int_0^R\eta^{m+1}T_c^{(m)}d\eta-\cos m\theta\int_0^R\eta^{m+1}T_s^{(m)}d\eta\right)\right\} \quad (4.7)$$

Equations (4.5)–(4.7) are identical to Huang and Rosakis [15] for a single thin film if the Young's modulus, Poisson's ratio, and coefficient of thermal expansion are substituted by E_i, ν_i, and α_i of the ith thin film, respectively.

The shear stresses $\tau_r^{(i)}$ and $\tau_\theta^{(i)}$ at the film/film and film/substrate interfaces are related to the temperature by

$$\tau_r^{(i)}=\sum_{j=i}^{n}\frac{E_{f_j}h_{f_j}}{1-\nu_{f_j}^2}[(1+\nu_s)\alpha_s-(1+\nu_{f_j})\alpha_{f_j}]\frac{\partial T}{\partial r}+2\left\{\sum_{j=i}^{n}\frac{E_{f_j}h_{f_j}}{1-\nu_{f_j}}(\alpha_s-\alpha_{f_j})-\sum_{j=i}^{n}\frac{E_{f_j}h_{f_j}}{1-\nu_{f_j}^2}[(1+\nu_s)\alpha_s-(1+\nu_{f_j})\alpha_{f_j}]\right\}\sum_{m=1}^{\infty}m(m$$
$$+1)\frac{r^{m-1}}{R^{2m+2}}\left(\cos m\theta\int_0^R\eta^{m+1}T_c^{(m)}d\eta+\sin m\theta\int_0^R\eta^{m+1}T_s^{(m)}d\eta\right) \quad (4.8)$$

$$\tau_\theta^{(i)}=\sum_{j=i}^{n}\frac{E_{f_j}h_{f_j}}{1-\nu_{f_j}^2}[(1+\nu_s)\alpha_s-(1+\nu_{f_j})\alpha_{f_j}]\frac{1}{r}\frac{\partial T}{\partial\theta}-2\left\{\sum_{j=i}^{n}\frac{E_{f_j}h_{f_j}}{1-\nu_{f_j}}(\alpha_s-\alpha_{f_j})-\sum_{j=i}^{n}\frac{E_{f_j}h_{f_j}}{1-\nu_{f_j}^2}[(1+\nu_s)\alpha_s-(1+\nu_{f_j})\alpha_{f_j}]\right\}\sum_{m=1}^{\infty}m(m$$
$$+1)\frac{r^{m-1}}{R^{2m+2}}\left(\sin m\theta\int_0^R\eta^{m+1}T_c^{(m)}d\eta-\cos m\theta\int_0^R\eta^{m+1}T_s^{(m)}d\eta\right) \quad (4.9)$$

where the summation is from the ith thin film to the last (nth).

5 Extension of Stoney Formula for a Multilayer Thin Film/Substrate System Subjected to Arbitrary Temperature Distribution

We extend the Stoney formula for a multilayer thin film/substrate system by establishing the direct relation between the stresses in each thin film and system curvatures. Similar to Huang and Rosakis [15] for a single thin film, we first define the coefficients C_m and S_m, related to the system curvatures by

$$C_m=\frac{1}{\pi R^2}\int\int_A(\kappa_{rr}+\kappa_{\theta\theta})\left(\frac{\eta}{R}\right)^m\cos m\varphi dA$$

$$S_m=\frac{1}{\pi R^2}\int\int_A(\kappa_{rr}+\kappa_{\theta\theta})\left(\frac{\eta}{R}\right)^m\sin m\varphi dA \quad (5.1)$$

where the integration is over the entire area A of the thin film, and $dA=\eta d\eta d\varphi$. Elimination of temperature gives the stresses in each thin film in terms of system curvatures by

$$\sigma_{rr}^{(f_i)}-\sigma_{\theta\theta}^{(f_i)}=\frac{E_sh_s^2}{6(1-\nu_s)}\frac{E_{f_i}}{1+\nu_{f_i}}\frac{\alpha_s}{A_{\nu\alpha}}\left\{\kappa_{rr}-\kappa_{\theta\theta}-\sum_{m=1}^{\infty}(m+1)\times\left[m\left(\frac{r}{R}\right)^m-(m-1)\left(\frac{r}{R}\right)^{m-2}\right]\times(C_m\cos m\theta+S_m\sin m\theta)\right\} \quad (5.2)$$

$$\sigma_{r\theta}^{(f_i)}=\frac{E_sh_s^2}{6(1-\nu_s)}\frac{E_{f_i}}{1+\nu_{f_i}}\frac{\alpha_s}{A_{\nu\alpha}}\left\{\kappa_{r\theta}+\frac{1}{2}\sum_{m=1}^{\infty}(m+1)\left[m\left(\frac{r}{R}\right)^m-(m-1)\left(\frac{r}{R}\right)^{m-2}\right](C_m\sin m\theta-S_m\cos m\theta)\right\} \quad (5.3)$$

$$\sigma_{rr}^{(f_i)}+\sigma_{\theta\theta}^{(f_i)}=\frac{E_sh_s^2}{6(1-\nu_s)}\frac{E_{f_i}}{1-\nu_{f_i}}\left\{\frac{\alpha_s-\alpha_{f_i}}{A_\alpha}\overline{\kappa_{rr}+\kappa_{\theta\theta}}+\frac{(1+\upsilon_s)\alpha_s-2\alpha_{f_i}}{(1+\upsilon_s)A_{\nu\alpha}}(\kappa_{rr}+\kappa_{\theta\theta}-\overline{\kappa_{rr}+\kappa_{\theta\theta}})+\left[\frac{3+\nu_s}{1+\upsilon_s}\frac{\alpha_s-\alpha_{f_i}}{A_\alpha}-2\frac{(1+\nu_s)\alpha_s-2\alpha_{f_i}}{(1+\upsilon_s)A_{\nu\alpha}}\right]\times\sum_{m=1}^{\infty}(m+1)\left(\frac{r}{R}\right)^m(C_m\cos m\theta+S_m\sin m\theta)\right\} \quad (5.4)$$

where $\overline{\kappa_{rr}+\kappa_{\theta\theta}}=C_0=(1/\pi R^2)\int\int_A(\kappa_{rr}+\kappa_{\theta\theta})dA$ is the average curvature over entire area A of the thin film, and A_α and $A_{\nu\alpha}$ are given in Eq. (2.22). Equations (5.2)–(5.4) provide direct relations between individual film stresses and system curvatures. It is important to note that stresses at a point in each thin film depend not only on curvatures at the same point (local dependence), but also on the curvatures in the entire substrate (nonlocal dependence) via the coefficients C_m and S_m.

The shear stresses $\tau_r^{(i)}$ and $\tau_\theta^{(i)}$ at the film/film and film/substrate interfaces can also be directly related to system curvatures via

$$\tau_r^{(i)}=\frac{E_sh_s^2}{6(1-\nu_s^2)}\left(\frac{\sum_{k=i}^{n}\frac{E_{f_k}h_{f_k}}{1-\upsilon_{f_k}^2}[(1+\upsilon_s)\alpha_s-(1+\upsilon_{f_k})\alpha_{f_k}]}{A_{\nu\alpha}}\frac{\partial}{\partial r}(\kappa_{rr}+\kappa_{\theta\theta})-\frac{1}{2R}\left\{\frac{4\sum_{k=i}^{n}\frac{E_{f_k}h_{f_k}}{1-\upsilon_{f_k}^2}[(1+\upsilon_s)\alpha_s-(1+\upsilon_{f_k})\alpha_{f_k}]}{A_{\nu\alpha}}-\frac{(3+\nu_s)\sum_{k=i}^{n}\frac{E_{f_k}h_{f_k}}{1-\upsilon_{f_k}}(\alpha_s-\alpha_{f_k})}{A_\alpha}\right\}\right.$$

$$\times \sum_{m=1}^{\infty} m(m+1)(C_m \cos m\theta + S_m \sin m\theta)\left(\frac{r}{R}\right)^{m-1}\Bigg), \tag{5.5}$$

$$\tau_\theta^{(i)} = \frac{E_s h_s^2}{6(1-\nu_s^2)}\left(\frac{\sum_{k=i}^{n} \frac{E_{f_k} h_{f_k}}{1-\upsilon_{f_k}^2}[(1+\upsilon_s)\alpha_s - (1+\upsilon_{f_k})\alpha_{f_k}]}{A_{\nu\alpha}} \frac{1}{r}\frac{\partial}{\partial\theta}(\kappa_{rr} + \kappa_{\theta\theta}) + \frac{1}{2R}\left\{\frac{4\sum_{k=i}^{n} \frac{E_{f_k} h_{f_k}}{1-\upsilon_{f_k}^2}[(1+\upsilon_s)\alpha_s - (1+\upsilon_{f_k})\alpha_{f_k}]}{A_{\nu\alpha}} - \frac{(3+\nu_s)\sum_{k=i}^{n} \frac{E_{f_k} h_{f_k}}{1-\upsilon_{f_k}}(\alpha_s - \alpha_{f_k})}{A_\alpha}\right\}\right.$$

$$\left.\times \sum_{m=1}^{\infty} m(m+1)(C_m \sin m\theta - S_m \cos m\theta)\left(\frac{r}{R}\right)^{m-1}\right) \tag{5.6}$$

This provides a way to determine the interface shear stresses from the system curvatures. It also displays a nonlocal dependence via the coefficients C_m and S_m.

6 Concluding Remarks

The analytical solution is obtained for a multilayer thin film/substrate system subjected to arbitrary temperature distribution. The stresses in each thin film and system curvatures are obtained in terms of the temperature. The direct relation between the stresses in each thin film and system curvatures is also obtained. The dependence of the film stresses on curvatures is not generally "local," i.e., the stress components at a point on the film will depend on both the local value of the curvature components (at the same point) and on the value of curvatures of all other points (nonlocal dependence).

The presence of nonlocal contributions in such relations also has implications regarding the nature of diagnostic methods needed to perform wafer-level film stress measurements. Notably, the existence of nonlocal terms necessitates the use of full-field methods capable of measuring curvature components over the entire surface of the plate system (or wafer). Furthermore, measurement of all independent components of the curvature field is necessary. This is because the stress state at a point depends on curvature contributions from the entire plate surface.

The nonuniform temperature distribution also results in shear stresses along the film/film and film/substrate interfaces. The relation between the shear stresses and system curvatures provides an effective method to estimate the shear stresses. Since film delamination is a commonly encountered form of failure during wafer manufacturing, the ability to estimate the level and distribution of such stresses from wafer-level metrology might prove to be invaluable in enhancing the reliability of such systems.

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