Extension of Stoney's Formula to Arbitrary Temperature Distributions in Thin Film/Substrate Systems

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Current methodologies used for the inference of thin film stress through curvature measurements are strictly restricted to stress and curvature states that are assumed to remain uniform over the entire film/substrate system. By considering a circular thin film/substrate system subject to nonuniform and nonaxisymmetric temperature distributions, we derive relations between the film stresses and temperature, and between the plate system's curvatures and the 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 that reflects the effect of temperature of other points on the location of scrutiny. Most notably, we also derive relations between the polar components of the film stress and those of 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. Finally, it is shown that the interfacial shear tractions between the film and the substrate are related to the gradients of the first curvature invariant and can also be inferred experimentally. [DOI: 10.1115/1.2744035]

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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 above-described thin film structures on substrates are often made from a multiplicity of fabrication and processing steps (e.g., sequential film deposition, thermal anneal, and etch steps) and often experience stresses caused by each of these steps. Examples of known phenomena and processes that build up stresses in thin films include, but are not limited to, lattice mismatch, chemical reaction, doping by, e.g., diffusion or implantation, rapid deposition by evaporation or sputtering, and of course thermal treatment (e.g., various thermal anneal steps). The film stress build-up associated with each of these steps often produces undesirable damage (e.g., cracking, interface delamination) that may be detrimental to the manufacturing process because of its cumulative effect on process "yield" [1]. Known problems associated with thermal excursions, in particular, include stress-induced film cracking and film/substrate delamination resulting during uncontrolled wafer cooling that follows the many anneal steps.

The intimate relation between stress-induced failures and process yield loss makes the identification of the origins of stress build-up, the accurate measurement and analysis of stresses, and the acquisition of information on the spatial distribution of stresses a crucial step in designing and controlling processing steps and in ultimately improving reliability and manufacturing yield.

Stress changes in thin films following discrete process steps or occurring during thermal excursions may be calculated in principle from changes in the film/substrate systems curvatures or "bow" based on analytical correlations between such quantities. Early attempts to provide such correlations are well documented [2]. Various formulations have been developed for this purpose and most of these are essentially extensions of Stoney's approximate plate analysis [3].

Stoney used a plate system composed of a stress bearing 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:

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

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, respectively. 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 derived for an isotropic "thin" solid film of uniform thickness deposited on a much "thicker" plate substrate based on a number of assumptions. Stoney's assumptions include the following: (1) 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); (2) the strains and rotations of the plate system are infinitesimal; (3) both the film and substrate are homogeneous, isotropic, and linearly elastic; (4) the film stress states are in-plane isotropic or equibiaxial (two equal stress components in

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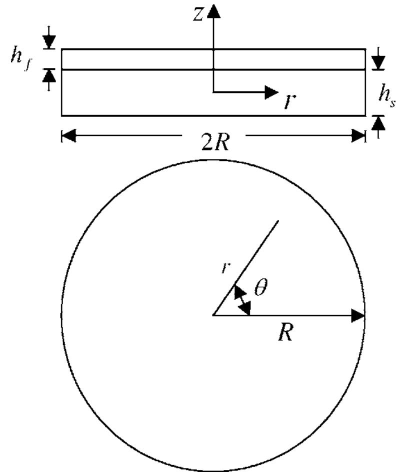

Fig. 1 A schematic diagram of the thin film/substrate system, showing the cylindrical coordinates (r,θ,z)

any two, mutually orthogonal in-plane directions) while the out-of-plane direct stress and all shear stresses vanish; (5) the system's curvature components are equibiaxial (two equal direct curvatures) while the twist curvature vanishes in all directions; and (6) all surviving stress and curvature components are spatially constant over the plate system's surface, a situation which is often violated in practice.

The assumption of equibiaxial ($\kappa_{xx}=\kappa_{yy}=\kappa,\ \kappa_{xy}=\kappa_{yx}=0$) and spatially constant curvature (κ independent of position) is equivalent to assuming that the plate system would deform spherically under the action of the film stress. If this assumption were to be true, a rigorous application of Stoney's formula would indeed furnish a single film stress value. This value represents the common magnitude of each of the two direct stresses in any two, mutually orthogonal directions (i.e., $\sigma_{xx}=\sigma_{yy}=\sigma^{(f)},\ \sigma_{xy}=\sigma_{yx}=0,\ \sigma^{(f)}$ independent of position). This is the uniform stress for the entire film and it is derived from the measurement of a single uniform curvature value that fully characterizes the system provided the deformation is indeed spherical.

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, various researchers have derived a number of extensions to relax some of the other assumptions (other than the assumption of uniformity) made by Stoney's analysis. 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, appropriate for anisotropic film stresses, including different stress values at two different directions and nonzero, in-plane shear stresses, was derived by relaxing the assumption of curvature equibiaxiality [2]. Related analyses treating discontinuous films in the form of bare periodic lines [4] or composite films with periodic line structures (e.g., bare or encapsulated periodic lines) have also been derived [5–7]. These latter analyses have also removed the assumption of equibiaxiality and have allowed the 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 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 [8–11]. These analyses have removed both the restrictions of an equibiaxial curvature state as well as the assumption of infinitesimal deformations. They have allowed for the prediction of kinematically nonlinear behavior and bifurcations in curvature states. 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 systems aspect ratio, i.e., the ratio of in-plane to thickness dimension and the elastic stiffness. These analyses also retain the assumption 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) which features three different, still spatially constant, curvature components [12].

None of the above-discussed extensions of Stoney's methodology has relaxed the most restrictive of Stoney's original assumption of spatial uniformity, which does not allow either film stress or curvature components to vary across the plate surface. This crucial assumption is often violated in practice since film stresses and the associated system curvatures are nonuniformly distributed over the plate area. Huang and Rosakis [13] and Huang et al. [14] have recently made progress to remove the two restrictive assumptions of the Stoney analysis relating to spatial uniformity and equibiaxiality. They have studied the cases of thin film/substrate systems subject to nonuniform but axisymmetric temperature distribution $T(r)$ and misfit strain $\varepsilon_m(r)$, respectively. Their results show that the relations between film stresses and substrate curvatures feature not only a "local" part that involves a direct dependence of stresses on curvatures at the same point, but also a "nonlocal" part which reflects the effect of curvatures at other points on the location of scrutiny. The "nonlocal" effect comes into play in the axisymmetric analysis via the average curvature in the thin film.

The main purpose of the present paper is to remove the two restrictive assumptions of the Stoney analysis relating to spatial uniformity and equibiaxiality for the general case of a thin film/substrate system subject to arbitrary temperature distribution $T(r,\theta)$ whose presence will create a nonaxisymmetric stress and curvature field as well as arbitrarily large stress and curvature gradients. Such a nonuniform temperature field may arise in the processing or application of the thin film/substrate system. Our goal is to relate film stresses and system curvatures to the temperature distribution and to ultimately derive a relation between the film stresses and the system curvatures for general nonaxisymmetric temperature distributions. Such a relation would allow for the accurate experimental inference of film stress from full-field and real-time curvature measurements that may occur during or after thermal processing. The full-field curvature measurements (e.g., [15]), together with the present study, provide the stress field in the film.

2 Governing Equations

A thin film deposited on a substrate is subject to arbitrary temperature distribution $T(r,\theta)$, where r and θ are the polar coordinates (Fig. 1). The thin film and substrate are circular in the lateral direction and have a radius R.

The thin-film thickness h_f 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 film and substrate are denoted by E_f, ν_f, α_f, 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 film is modeled as a membrane which cannot be subject to bending due to its small thickness $h_f \ll h_s$.

Let $u_r^{(f)}$ and $u_\theta^{(f)}$ denote the displacements in the radial (r) and circumferential (θ) directions. The strains in the thin film are

$$\varepsilon_{rr} = \frac{\partial u_r^{(f)}}{\partial r}, \quad \varepsilon_{\theta\theta} = \frac{u_r^{(f)}}{r} + \frac{1}{r}\frac{\partial u_\theta^{(f)}}{\partial \theta}$$

and

$$\gamma_{r\theta} = \frac{1}{r}\frac{\partial u_r^{(f)}}{\partial \theta} + \frac{\partial u_\theta^{(f)}}{\partial r} - \frac{u_\theta^{(f)}}{r}$$

The stresses in the thin film can be obtained from the linear thermo-elastic constitutive model as

$$\sigma_{rr} = \frac{E_f}{1-\nu_f^2}\left[\frac{\partial u_r^{(f)}}{\partial r} + \nu_f\left(\frac{u_r^{(f)}}{r} + \frac{1}{r}\frac{\partial u_\theta^{(f)}}{\partial \theta}\right) - (1+\nu_f)\alpha_f T\right]$$

$$\sigma_{\theta\theta} = \frac{E_f}{1-\nu_f^2}\left[\nu_f \frac{\partial u_r^{(f)}}{\partial r} + \frac{u_r^{(f)}}{r} + \frac{1}{r}\frac{\partial u_\theta^{(f)}}{\partial \theta} - (1+\nu_f)\alpha_f T\right] \tag{2.1}$$

$$\sigma_{r\theta} = \frac{E_f}{2(1+\nu_f)}\left(\frac{1}{r}\frac{\partial u_r^{(f)}}{\partial \theta} + \frac{\partial u_\theta^{(f)}}{\partial r} - \frac{u_\theta^{(f)}}{r}\right)$$

The membrane forces in the thin film are

$$N_r^{(f)} = h_f \sigma_{rr} \quad N_\theta^{(f)} = h_f \sigma_{\theta\theta} \quad N_{r\theta}^{(f)} = h_f \sigma_{r\theta} \tag{2.2}$$

It is recalled that, for uniform temperature distribution T =constant, the normal and shear stresses across the thin film/substrate interface vanish except near the free edge $r=R$; i.e., $\sigma_{zz}=\sigma_{rz}=\sigma_{r\theta}=0$ at $z=h_s/2$ and $r<R$. For nonuniform temperature distribution $T=T(r,\theta)$, the shear stress σ_{rz} and $\sigma_{\theta z}$ at the interface may not vanish anymore, and are denoted by τ_r and τ_θ, respectively. It is important to note that the normal stress traction σ_{zz} still vanishes (except near the free edge $r=R$) because the thin film cannot be subject to bending. The equilibrium equations for the thin film, accounting for the effect of interface shear stresses τ_r and τ_θ, become

$$\frac{\partial N_r^{(f)}}{\partial r} + \frac{N_r^{(f)} - N_\theta^{(f)}}{r} + \frac{1}{r}\frac{\partial N_{r\theta}^{(f)}}{\partial \theta} - \tau_r = 0$$

$$\frac{\partial N_{r\theta}^{(f)}}{\partial r} + \frac{2}{r}N_{r\theta}^{(f)} + \frac{1}{r}\frac{\partial N_\theta^{(f)}}{\partial \theta} - \tau_\theta = 0 \tag{2.3}$$

The substitution of Eqs. (2.1)–(2.3) yields the following governing equations for $u_r^{(f)}$, $u_\theta^{(f)}$, τ_r and τ_θ

$$\frac{\partial^2 u_r^{(f)}}{\partial r^2} + \frac{1}{r}\frac{\partial u_r^{(f)}}{\partial r} - \frac{u_r^{(f)}}{r^2} + \frac{1-\nu_f}{2}\frac{1}{r^2}\frac{\partial^2 u_r^{(f)}}{\partial \theta^2} + \frac{1+\nu_f}{2}\frac{1}{r}\frac{\partial^2 u_\theta^{(f)}}{\partial r\,\partial \theta} - \frac{3-\nu_f}{2}\frac{1}{r^2}\frac{\partial u_\theta^{(f)}}{\partial \theta} = \frac{1-\nu_f^2}{E_f h_f}\tau_r + (1+\nu_f)\alpha_f \frac{\partial T}{\partial r}$$

$$\frac{1+\nu_f}{2}\frac{1}{r}\frac{\partial^2 u_r^{(f)}}{\partial r\,\partial \theta} + \frac{3-\nu_f}{2}\frac{1}{r^2}\frac{\partial u_r^{(f)}}{\partial \theta} + \frac{1-\nu_f}{2}\left(\frac{\partial^2 u_\theta^{(f)}}{\partial r^2} + \frac{1}{r}\frac{\partial u_\theta^{(f)}}{\partial r} - \frac{u_\theta^{(f)}}{r^2}\right) + \frac{1}{r^2}\frac{\partial^2 u_\theta^{(f)}}{\partial \theta^2} = \frac{1-\nu_f^2}{E_f h_f}\tau_\theta + (1+\nu_f)\alpha_f \frac{1}{r}\frac{\partial T}{\partial \theta} \tag{2.4}$$

Let $u_r^{(s)}$ and $u_\theta^{(s)}$ denote the displacements in the radial (r) and circumferential (θ) directions, respectively, at the neutral axis (z =0) of the substrate, and w the displacement in the normal (z) direction. It is important to consider w since the substrate can be subject to bending and is modeled as a plate. The strains in the substrate are given by

$$\varepsilon_{rr} = \frac{\partial u_r^{(s)}}{\partial r} - z\frac{\partial^2 w}{\partial r^2}$$

$$\varepsilon_{\theta\theta} = \frac{u_r^{(s)}}{r} + \frac{1}{r}\frac{\partial u_\theta^{(s)}}{\partial \theta} - z\left(\frac{1}{r}\frac{\partial w}{\partial r} + \frac{1}{r^2}\frac{\partial^2 w}{\partial \theta^2}\right) \tag{2.5}$$

$$\gamma_{r\theta} = \frac{1}{r}\frac{\partial u_r^{(s)}}{\partial \theta} + \frac{\partial u_\theta^{(s)}}{\partial r} - \frac{u_\theta^{(s)}}{r} - 2z\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial w}{\partial \theta}\right)$$

The stresses in the substrate can then be obtained from the linear thermo-elastic constitutive model as

$$\sigma_{rr} = \frac{E_s}{1-\nu_s^2}\left\{\frac{\partial u_r^{(s)}}{\partial r} + \nu_s\left(\frac{u_r^{(s)}}{r} + \frac{1}{r}\frac{\partial u_\theta^{(s)}}{\partial \theta}\right) - z\left[\frac{\partial^2 w}{\partial r^2} + \nu_s\left(\frac{1}{r}\frac{\partial w}{\partial r} + \frac{1}{r^2}\frac{\partial^2 w}{\partial \theta^2}\right)\right] - (1+\nu_s)\alpha_s T\right\}$$

$$\sigma_{\theta\theta} = \frac{E_s}{1-\nu_s^2}\left[\nu_s\frac{\partial u_r^{(s)}}{\partial r} + \frac{u_r^{(s)}}{r} + \frac{1}{r}\frac{\partial u_\theta^{(s)}}{\partial \theta} - z\left(\nu_s\frac{\partial^2 w}{\partial r^2} + \frac{1}{r}\frac{\partial w}{\partial r} + \frac{1}{r^2}\frac{\partial^2 w}{\partial \theta^2}\right) - (1+\nu_s)\alpha_s T\right] \tag{2.6}$$

$$\sigma_{r\theta} = \frac{E_s}{2(1+\nu_s)}\left[\frac{1}{r}\frac{\partial u_r^{(s)}}{\partial \theta} + \frac{\partial u_\theta^{(s)}}{\partial r} - \frac{u_\theta^{(s)}}{r} - 2z\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial w}{\partial \theta}\right)\right]$$

The forces and bending moments in the substrate are

$$N_r^{(s)} = \int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} \sigma_{rr}dz = \frac{E_s h_s}{1-\nu_s^2}\left[\frac{\partial u_r^{(s)}}{\partial r} + \nu_s\left(\frac{u_r^{(s)}}{r} + \frac{1}{r}\frac{\partial u_\theta^{(s)}}{\partial \theta}\right) - (1+\nu_s)\alpha_s T\right]$$

$$N_\theta^{(s)} = \int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} \sigma_{\theta\theta}dz = \frac{E_s h_s}{1-\nu_s^2}\left[\nu_s\frac{\partial u_r^{(s)}}{\partial r} + \frac{u_r^{(s)}}{r} + \frac{1}{r}\frac{\partial u_\theta^{(s)}}{\partial \theta} - (1+\nu_s)\alpha_s T\right] \tag{2.7}$$

$$N_{r\theta}^{(s)} = \int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} \sigma_{r\theta}dz = \frac{E_s h_s}{2(1+\nu_s)}\left(\frac{1}{r}\frac{\partial u_r^{(s)}}{\partial \theta} + \frac{\partial u_\theta^{(s)}}{\partial r} - \frac{u_\theta^{(s)}}{r}\right)$$

$$M_r = -\int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} z\sigma_{rr}dz = \frac{E_s h_s^3}{12(1-\nu_s^2)}\left[\frac{\partial^2 w}{\partial r^2} + \nu_s\left(\frac{1}{r}\frac{\partial w}{\partial r} + \frac{1}{r^2}\frac{\partial^2 w}{\partial \theta^2}\right)\right]$$

$$M_\theta = -\int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} z\sigma_{\theta\theta}dz = \frac{E_s h_s^3}{12(1-\nu_s^2)}\left(\nu_s\frac{\partial^2 w}{\partial r^2} + \frac{1}{r}\frac{\partial w}{\partial r} + \frac{1}{r^2}\frac{\partial^2 w}{\partial \theta^2}\right) \tag{2.8}$$

$$M_{r\theta} = -\int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} z\sigma_{r\theta}dz = \frac{E_s h_s^3}{12(1+\nu_s)}\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial w}{\partial \theta}\right)$$

The shear stresses τ_r and τ_θ at the thin film/substrate interface are equivalent to the distributed forces τ_r in the radial direction and τ_θ in the circumferential direction, and bending moments $(h_s/2)\tau_r$ and $(h_s/2)\tau_\theta$ applied at the neutral axis ($z=0$) of the substrate. The in-plane force equilibrium equations of the substrate then become

$$\frac{\partial N_r^{(s)}}{\partial r} + \frac{N_r^{(s)} - N_\theta^{(s)}}{r} + \frac{1}{r}\frac{\partial N_{r\theta}^{(s)}}{\partial \theta} + \tau_r = 0$$

$$\frac{\partial N_{r\theta}^{(s)}}{\partial r} + \frac{2}{r}N_{r\theta}^{(s)} + \frac{1}{r}\frac{\partial N_{\theta\theta}^{(s)}}{\partial \theta} + \tau_\theta = 0 \tag{2.9}$$

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

$$\begin{aligned}\frac{\partial M_r}{\partial r} + \frac{M_r - M_\theta}{r} + \frac{1}{r}\frac{\partial M_{r\theta}}{\partial \theta} + Q_r - \frac{h_s}{2}\tau_r = 0\\ \frac{\partial M_{r\theta}}{\partial r} + \frac{2}{r}M_{r\theta} + \frac{1}{r}\frac{\partial M_\theta}{\partial \theta} + Q_\theta - \frac{h_s}{2}\tau_\theta = 0\end{aligned} \tag{2.10}$$

$$\frac{\partial Q_r}{\partial r} + \frac{Q_r}{r} + \frac{1}{r}\frac{\partial Q_\theta}{\partial \theta} = 0 \tag{2.11}$$

where Q_r and Q_θ are the shear forces normal to the neutral axis. The substitution of Eq. (2.7) into Eq. (2.9) yields the following governing equations for $u_r^{(s)}$, $u_\theta^{(s)}$, and τ:

$$\begin{aligned}&\frac{\partial^2 u_r^{(s)}}{\partial r^2} + \frac{1}{r}\frac{\partial u_r^{(s)}}{\partial r} - \frac{u_r^{(s)}}{r^2} + \frac{1-\nu_s}{2}\frac{1}{r^2}\frac{\partial^2 u_r^{(s)}}{\partial \theta^2} + \frac{1+\nu_s}{2}\frac{1}{r}\frac{\partial^2 u_\theta^{(s)}}{\partial r\,\partial \theta}\\ &\quad - \frac{3-\nu_s}{2}\frac{1}{r^2}\frac{\partial u_\theta^{(s)}}{\partial \theta} = -\frac{1-\nu_s^2}{E_s h_s}\tau_r + (1+\nu_s)\alpha_s\frac{\partial T}{\partial r}\\ &\frac{1+\nu_s}{2}\frac{1}{r}\frac{\partial^2 u_r^{(s)}}{\partial r\,\partial \theta} + \frac{3-\nu_s}{2}\frac{1}{r^2}\frac{\partial u_r^{(s)}}{\partial \theta} + \frac{1-\nu_s}{2}\left(\frac{\partial^2 u_\theta^{(s)}}{\partial r^2} + \frac{1}{r}\frac{\partial u_\theta^{(s)}}{\partial r} - \frac{u_\theta^{(s)}}{r^2}\right)\\ &\quad + \frac{1}{r^2}\frac{\partial^2 u_\theta^{(s)}}{\partial \theta^2} = -\frac{1-\nu_s^2}{E_s h_s}\tau_\theta + (1+\nu_s)\alpha_s\frac{1}{r}\frac{\partial T}{\partial \theta}\end{aligned} \tag{2.12}$$

Elimination of Q_r and Q_θ from Eqs. (2.10) and (2.11), in conjunction with Eq. (2.8), gives the following governing equation for w (and τ)

$$\nabla^2(\nabla^2 w) = \frac{6(1-\nu_s^2)}{E_s h_s^2}\left(\frac{\partial \tau_r}{\partial r} + \frac{\tau_r}{r} + \frac{1}{r}\frac{\partial \tau_\theta}{\partial \theta}\right) \tag{2.13}$$

where

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}$$

The continuity of displacements across the thin film/substrate interface requires

$$u_r^{(f)} = u_r^{(s)} - \frac{h_s}{2}\frac{\partial w}{\partial r}, \quad u_\theta^{(f)} = u_\theta^{(s)} - \frac{h_s}{2}\frac{1}{r}\frac{\partial w}{\partial \theta} \tag{2.14}$$

Equations (2.4) and (2.12)–(2.14) constitute seven ordinary differential equations for seven variables, namely $u_r^{(f)}$, $u_\theta^{(f)}$, $u_r^{(s)}$, $u_\theta^{(s)}$, w, τ_r, and τ_θ. We discuss below how to decouple these seven equations under the limit $h_f/h_s \ll 1$ such that we can solve $u_r^{(s)}$, $u_\theta^{(s)}$ first, then $u_r^{(f)}$ and $u_\theta^{(f)}$, followed by τ_r and τ_θ, and finally w.

(i) Elimination of τ_r and τ_θ from force equilibrium equations (2.4) for the thin film and (2.12) for the substrate yields two equations for $u_r^{(f)}$, $u_\theta^{(f)}$, $u_r^{(s)}$, and $u_\theta^{(s)}$. For $h_f/h_s \ll 1$, $u_r^{(f)}$ and $u_\theta^{(f)}$ disappear in these two equations, which become the following governing equations for $u_r^{(s)}$ and $u_\theta^{(s)}$ only:

$$\begin{aligned}&\frac{\partial^2 u_r^{(s)}}{\partial r^2} + \frac{1}{r}\frac{\partial u_r^{(s)}}{\partial r} - \frac{u_r^{(s)}}{r^2} + \frac{1-\nu_s}{2}\frac{1}{r^2}\frac{\partial^2 u_r^{(s)}}{\partial \theta^2} + \frac{1+\nu_s}{2}\frac{1}{r}\frac{\partial^2 u_\theta^{(s)}}{\partial r\,\partial \theta}\\ &\quad - \frac{3-\nu_s}{2}\frac{1}{r^2}\frac{\partial u_\theta^{(s)}}{\partial \theta} = (1+\nu_s)\alpha_s\frac{\partial T}{\partial r} + O\left(\frac{h_f}{h_s}\right)\\ &\frac{1+\nu_s}{2}\frac{1}{r}\frac{\partial^2 u_r^{(s)}}{\partial r\,\partial \theta} + \frac{3-\nu_s}{2}\frac{1}{r^2}\frac{\partial u_r^{(s)}}{\partial \theta} + \frac{1-\nu_s}{2}\left(\frac{\partial^2 u_\theta^{(s)}}{\partial r^2} + \frac{1}{r}\frac{\partial u_\theta^{(s)}}{\partial r} - \frac{u_\theta^{(s)}}{r^2}\right)\\ &\quad + \frac{1}{r^2}\frac{\partial^2 u_\theta^{(s)}}{\partial \theta^2} = (1+\nu_s)\alpha_s\frac{1}{r}\frac{\partial T}{\partial \theta} + O\left(\frac{h_f}{h_s}\right)\end{aligned} \tag{2.15}$$

(ii) Elimination of $u_r^{(f)}$ and $u_\theta^{(f)}$ from the continuity condition (2.14) and equilibrium equation (2.4) for the thin film gives τ_r and τ_θ in terms of $u_r^{(s)}$ and w. Their substitution into the moment equilibrium equation (2.13) yields the governing equation for the normal displacement w, from which it can be shown that w is on the order of h_f/h_s, i.e.,

$$w = O\left(\frac{h_f}{h_s}\right) \tag{2.16}$$

Equation (2.16) and the continuity condition (2.14) then give the displacements $u_r^{(f)}$ and $u_\theta^{(f)}$ in the thin film as

$$u_r^{(f)} = u_r^{(s)} + O\left(\frac{h_f}{h_s}\right), \quad u_\theta^{(f)} = u_\theta^{(s)} + O\left(\frac{h_f}{h_s}\right) \tag{2.17}$$

(iii) The equilibrium equation (2.4) for the thin film gives the interface shear stresses in terms of $u_r^{(s)}$ and $u_\theta^{(s)}$ as

$$\begin{aligned}\tau_r &= \frac{E_f h_f}{1-\nu_f^2}\left\{\frac{\nu_s-\nu_f}{2}\left(\frac{1}{r^2}\frac{\partial^2 u_r^{(s)}}{\partial \theta^2} - \frac{1}{r}\frac{\partial^2 u_\theta^{(s)}}{\partial r\,\partial \theta} - \frac{1}{r^2}\frac{\partial u_\theta^{(s)}}{\partial \theta}\right) + [(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f]\frac{\partial T}{\partial r} + O\left(\frac{h_f}{h_s}\right)\right\}\\ \tau_\theta &= \frac{E_f h_f}{1-\nu_f^2}\left\{\frac{\nu_s-\nu_f}{2}\left(-\frac{1}{r}\frac{\partial^2 u_r^{(s)}}{\partial r\,\partial \theta} + \frac{1}{r^2}\frac{\partial u_r^{(s)}}{\partial \theta} + \frac{\partial^2 u_\theta^{(s)}}{\partial r^2} + \frac{1}{r}\frac{\partial u_\theta^{(s)}}{\partial r} - \frac{u_\theta^{(s)}}{r^2}\right) + [(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f]\frac{1}{r}\frac{\partial T}{\partial \theta} + O\left(\frac{h_f}{h_s}\right)\right\}\end{aligned} \tag{2.18}$$

where Eq. (2.15) has been used.

(iv) The displacement w is determined from the moment equilibrium equation (2.13) by eliminating τ_r and τ_θ using Eq. (2.18). It can be verified that the resulting w is indeed on the order of h_f/h_s as suggested in Eq. (2.16).

We expand the arbitrary nonuniform temperature distribution $T(r,\theta)$ to the Fourier series,

$$T(r,\theta) = \sum_{n=0}^{\infty} T_c^{(n)}(r)\cos n\theta + \sum_{n=0}^{\infty} T_s^{(n)}(r)\sin n\theta \tag{2.19}$$

where

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

and

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

Without losing generality, we focus on the $\cos n\theta$ term here. The corresponding displacements and interface shear stresses can be expressed as

$$\begin{aligned}u_r^{(s)} = u_r^{(sn)}(r)\cos n\theta, \quad u_\theta^{(s)} = u_\theta^{(sn)}(r)\sin n\theta, \quad w = w^{(n)}(r)\cos n\theta\\ \tau_r = \tau_r^{(n)}(r)\cos n\theta, \quad \tau_\theta = \tau_\theta^{(n)}(r)\sin n\theta\end{aligned} \tag{2.20}$$

Equation (2.15) then gives two ordinary differential equations for $u_r^{(sn)}$ and $u_\theta^{(sn)}$, which have the general solution

$$
\begin{Bmatrix} u_r^{(sn)} \\ u_\theta^{(sn)} \end{Bmatrix} = \begin{Bmatrix} 1-\nu_s - \dfrac{1+\nu_s}{2}n \\ \dfrac{1+\nu_s}{2}n+2 \end{Bmatrix} \left[A_0 r^{n+1} + \frac{\alpha_s}{4(n+1)} \frac{1+\nu_s}{1-\nu_s} r T_c^{(n)} \right]
$$
$$
+ \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} \frac{\alpha_s}{4(n+1)} \frac{1+\nu_s}{1-\nu_s} \left\{ -\left[1-\nu_s - \frac{n}{2}(1+\nu_s) \right] r T_c^{(n)} + 2(1-\nu_s)(n+1) \frac{1}{r^{n+1}} \int_0^r \eta^{1+n} T_c^{(n)}(\eta) d\eta \right\}
$$
$$
- \begin{Bmatrix} 1-\nu_s + \dfrac{1+\nu_s}{2}n \\ \dfrac{1+\nu_s}{2}n-2 \end{Bmatrix} \frac{\alpha_s}{4(n-1)} \frac{1+\nu_s}{1-\nu_s} r T_c^{(n)} + \begin{Bmatrix} -1 \\ 1 \end{Bmatrix} D_0 r^{n-1} - \begin{Bmatrix} -1 \\ 1 \end{Bmatrix} \frac{\alpha_s}{4(n-1)} \frac{1+\nu_s}{1-\nu_s}
$$
$$
\times \begin{Bmatrix} \left[1-\nu_s + \dfrac{n}{2}(1+\nu_s) \right] r T_c^{(n)} \\ -2(1-\nu_s)(n-1) r^{n-1} \displaystyle\int_r^R \eta^{1-n} T_c^{(n)}(\eta) d\eta \end{Bmatrix} + O\left(\frac{h_f}{h_s} \right) \tag{2.21}
$$

where we have used the condition that the displacements are finite at the center $r=0$, and A_0 and D_0 are constants to be determined.

The interface shear stresses are obtained from Eq. (2.18) as

$$
\tau_r^{(n)} = \frac{E_f h_f}{1-\nu_f^2} \left\{ [(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f] \frac{dT_c^{(n)}}{dr} - 2(\nu_s - \nu_f) n(n+1) A_0 r^{n-1} + O\left(\frac{h_f}{h_s} \right) \right\}
$$
$$
\tau_\theta^{(n)} = \frac{E_f h_f}{1-\nu_f^2} \left\{ -[(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f] \frac{n}{r} T_c^{(n)} + 2(\nu_s - \nu_f) n(n+1) A_0 r^{n-1} + O\left(\frac{h_f}{h_s} \right) \right\} \tag{2.22}
$$

The normal displacement w is determined from Eq. (2.13) as

$$
w^{(n)} = A_1 r^{n+2} + B_1 r^n - \frac{3}{n} \frac{1-\nu_s^2}{E_s h_s^2} \frac{E_f h_f}{1-\nu_f^2} [(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f] \times \left[r^n \int_r^R \eta^{1-n} T_c^{(n)}(\eta) d\eta + r^{-n} \int_0^r \eta^{n+1} T_c^{(n)}(\eta) d\eta \right] + O\left(\frac{h_f^2}{h_s^2} \right) \tag{2.23}
$$

where we have used the condition that the displacement w is finite at the center $r=0$, and A_1 and B_1 are constants to be determined.

3 Boundary Conditions

The first two boundary conditions at the free edge $r=R$ require that the net forces vanish:

$$
N_r^{(f)} + N_r^{(s)} = 0 \quad \text{and} \quad N_{r\theta}^{(f)} + N_{r\theta}^{(s)} = 0 \quad \text{at } r=R \tag{3.1}
$$

which give A_0 and D_0 as

$$
A_0 = \frac{\alpha_s}{R^{2n+2}} \int_0^R \eta^{n+1} T_c^{(n)}(\eta) d\eta + O\left(\frac{h_f}{h_s} \right)
$$
$$
D_0 = -\frac{n+1}{2R^{2n}} (1+\nu_s)\alpha_s \int_0^R \eta^{n+1} T_c^{(n)}(\eta) d\eta + O\left(\frac{h_f}{h_s} \right) \tag{3.2}
$$

under the limit $h_f/h_s \ll 1$. The other two boundary conditions at the free edge $r=R$ are the vanishing of net moments, i.e.,

$$
M_r - \frac{h_s}{2} N_r^{(f)} = 0 \text{ and } Q_r - \frac{1}{r} \frac{\partial}{\partial \theta} \left(M_{r\theta} - \frac{h_s}{2} N_{r\theta}^{(f)} \right) = 0 \text{ at } r=R \tag{3.3}
$$

which give A_1 and B_1 as

$$
A_1 = 3 \frac{E_f h_f}{1-\nu_f^2} \frac{1-\nu_s^2}{E_s h_s^2} \left[(1+\nu_f) \frac{1-\nu_s}{3+\nu_s} (\alpha_s - \alpha_f) - (\nu_s - \nu_f)\alpha_s \right] \frac{1}{R^{2n+2}} \int_0^R \eta^{n+1} T_c^{(n)}(\eta) d\eta + O\left(\frac{h_f^2}{h_s^2} \right)
$$
$$
B_1 = -\frac{n+1}{n} R^2 A_1 + O\left(\frac{h_f^2}{h_s^2} \right) \tag{3.4}
$$

It is important to point out that the boundary conditions can also be established from the variational principle (e.g., [11]). The total potential energy in the thin film/substrate system with the free edge at $r=R$ is

$$
\Pi = \int_0^R r dr \int_0^{2\pi} d\theta \int_{-\frac{h_s}{2}}^{\frac{h_s}{2}+h_f} U dz \tag{3.5}
$$

where U is the strain energy density which gives $\partial U/\partial \varepsilon_{rr} = \sigma_{rr}$, $\partial U/\partial \varepsilon_{\theta\theta} = \sigma_{\theta\theta}$, and $\partial U/\partial \gamma_{r\theta} = \sigma_{r\theta}$. For constitutive relations in Eqs. (2.1) and (2.6), we obtain

$$
U = \frac{E}{2(1-\nu^2)} \left[\varepsilon_{rr}^2 + \varepsilon_{\theta\theta}^2 + 2\nu \varepsilon_{rr} \varepsilon_{\theta\theta} + \frac{1-\nu}{2} \gamma_{r\theta}^2 - 2(1+\nu)\alpha T (\varepsilon_{rr} + \varepsilon_{\theta\theta}) \right] \tag{3.6}
$$

where E, ν, and α take their corresponding values in the thin film (i.e., E_f, ν_f, and α_f for $h_s/2 + h_f \geq z \geq h_s/2$) and in the substrate (i.e., E_s, ν_s, and α_s for $h_s/2 \geq z \geq -h_s/2$). For the displacement fields in Sec. 2 and the associated strain fields, the potential energy Π in Eq. (3.5) becomes a quadratic function of parameters A_0, D_0, A_1, and B_1. The principle of minimum potential energy requires

$$
\frac{\partial \Pi}{\partial A_0} = 0 \quad \frac{\partial \Pi}{\partial D_0} = 0 \quad \frac{\partial \Pi}{\partial A_1} = 0 \quad \frac{\partial \Pi}{\partial B_1} = 0 \tag{3.7}
$$

It can be shown that, as expected in the limit $h_f/h_s \ll 1$, the above four conditions in Eq. (3.7) are equivalent to the vanishing of net forces in Eq. (3.1) and net moments in Eq. (3.3).

4 Thin Film Stresses and Substrate Curvatures

We provide the general solution that includes both cosine and sine terms in this section. The substrate curvatures are

$$
\kappa_{rr} = \frac{\partial^2 w}{\partial r^2} \quad \kappa_{\theta\theta} = \frac{1}{r} \frac{\partial w}{\partial r} + \frac{1}{r^2} \frac{\partial^2 w}{\partial \theta^2} \quad \kappa_{r\theta} = \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial w}{\partial \theta} \right) \tag{4.1}
$$

The sum of substrate curvatures is related to the temperature by

$$\kappa_{rr}+\kappa_{\theta\theta}=12\frac{E_fh_f}{1-\nu_f}\frac{1-\nu_s}{E_sh_s^2}\left\{(\alpha_s-\alpha_f)T+\left[\frac{(1+\nu_s)^2}{2(1+\nu_f)}-1\right]\alpha_s(T-\bar{T})+\frac{(1-\nu_s)}{2}\alpha_f(T-\bar{T})+(1+\nu_s)\left[\frac{1-\nu_s}{3+\nu_s}(\alpha_s-\alpha_f)-\frac{\nu_s-\nu_f}{1+\nu_f}\alpha_s\right]\sum_{n=1}^{\infty}(n+1)\frac{r^n}{R^{2n+2}}\left[\cos n\theta\int_0^R\eta^{n+1}T_c^{(n)}(\eta)d\eta+\sin n\theta\int_0^R\eta^{n+1}T_s^{(n)}(\eta)d\eta\right]\right\} \tag{4.2}$$

where $\bar{T}=(1/\pi R^2)\int\int_A T(\eta,\varphi)dA$ is the average temperature over the entire area A of the thin film, $dA=\eta d\eta d\varphi$, and $\bar{T}$ is also related to $T_c^{(0)}$ by $\bar{T}=(2/R^2)\int_0^R\eta T_c^{(0)}(\eta)d\eta$. The difference between two curvatures $(\kappa_{rr}-\kappa_{\theta\theta})$ and the twist $\kappa_{r\theta}$ are given by

$$\kappa_{rr}-\kappa_{\theta\theta}=6\frac{E_fh_f}{1-\nu_f^2}\frac{1-\nu_s^2}{E_sh_s^2}[(1+\nu_s)\alpha_s-(1+\nu_f)\alpha_f]\times\left[T-\frac{2}{r^2}\int_0^r\eta T_c^{(0)}d\eta-\sum_{n=1}^{\infty}\frac{n+1}{r^{n+2}}\left(\cos n\theta\int_0^r\eta^{n+1}T_c^{(n)}d\eta+\sin n\theta\int_0^r\eta^{n+1}T_s^{(n)}d\eta\right)-\sum_{n=1}^{\infty}(n-1)r^{n-2}\left(\cos n\theta\int_r^R\eta^{1-n}T_c^{(n)}d\eta+\sin n\theta\int_r^R\eta^{1-n}T_s^{(n)}d\eta\right)\right]+6\frac{E_fh_f}{1-\nu_f^2}\frac{1-\nu_s^2}{E_sh_s^2}\frac{1}{3+\nu_s}\times\{(1-\nu_s)[(1+\nu_s)\alpha_s-(1+\nu_f)\alpha_f]-4(\nu_s-\nu_f)\alpha_s\}\sum_{n=1}^{\infty}\frac{n+1}{R^{n+2}}\left[n\left(\frac{r}{R}\right)^n-(n-1)\left(\frac{r}{R}\right)^{n-2}\right]\times\left(\cos n\theta\int_0^R\eta^{n+1}T_c^{(n)}d\eta+\sin n\theta\int_0^R\eta^{n+1}T_s^{(n)}d\eta\right) \tag{4.3}$$

$$\kappa_{r\theta}=3\frac{E_fh_f}{1-\nu_f^2}\frac{1-\nu_s^2}{E_sh_s^2}[(1+\nu_s)\alpha_s-(1+\nu_f)\alpha_f]\times\left[-\sum_{n=1}^{\infty}\frac{n+1}{r^{n+2}}\left(\sin n\theta\int_0^r\eta^{n+1}T_c^{(n)}d\eta-\cos n\theta\int_0^r\eta^{n+1}T_s^{(n)}d\eta\right)+\sum_{n=1}^{\infty}(n-1)r^{n-2}\left(\sin n\theta\int_r^R\eta^{1-n}T_c^{(n)}d\eta-\cos n\theta\int_r^R\eta^{1-n}T_s^{(n)}d\eta\right)\right]-3\frac{E_fh_f}{1-\nu_f^2}\frac{1-\nu_s^2}{E_sh_s^2}\frac{1}{3+\nu_s}\{(1-\nu_s)\times[(1+\nu_s)\alpha_s-(1+\nu_f)\alpha_f]-4(\nu_s-\nu_f)\alpha_s\}\sum_{n=1}^{\infty}\frac{n+1}{R^{n+2}}\left[n\left(\frac{r}{R}\right)^n-(n-1)\left(\frac{r}{R}\right)^{n-2}\right]\times\left(\sin n\theta\int_0^R\eta^{n+1}T_c^{(n)}d\eta-\cos n\theta\int_0^R\eta^{n+1}T_s^{(n)}d\eta\right) \tag{4.4}$$

The stresses in the thin film are obtained from Eq. (2.1). Specifically, the sum of stresses $\sigma_{rr}^{(f)}+\sigma_{\theta\theta}^{(f)}$ is related to the temperature by

$$\sigma_{rr}^{(f)}+\sigma_{\theta\theta}^{(f)}=\frac{E_f}{1-\nu_f}\left[2(\alpha_s-\alpha_f)T-(1-\nu_s)\alpha_s(T-\bar{T})+2(1-\nu_s)\alpha_s\sum_{n=1}^{\infty}\frac{n+1}{R^{2n+2}}r^n\left(\cos n\theta\int_0^R\eta^{n+1}T_c^{(n)}d\eta+\sin n\theta\int_0^R\eta^{n+1}T_s^{(n)}d\eta\right)\right] \tag{4.5}$$

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

$$\sigma_{rr}^{(f)}-\sigma_{\theta\theta}^{(f)}=\frac{E_f}{1+\nu_f}(1+\nu_s)\alpha_s\left\{T-\frac{2}{r^2}\int_0^r\eta T_c^{(0)}d\eta-\sum_{n=1}^{\infty}\frac{n+1}{r^{n+2}}\left(\cos n\theta\int_0^r\eta^{n+1}T_c^{(n)}d\eta+\sin n\theta\int_0^r\eta^{n+1}T_s^{(n)}d\eta\right)-\sum_{n=1}^{\infty}(n-1)r^{n-2}\left(\cos n\theta\int_r^R\eta^{1-n}T_c^{(n)}d\eta+\sin n\theta\int_r^R\eta^{1-n}T_s^{(n)}d\eta\right)-\sum_{n=1}^{\infty}\frac{n+1}{R^{n+2}}\left[n\left(\frac{r}{R}\right)^n-(n-1)\left(\frac{r}{R}\right)^{n-2}\right]\left(\cos n\theta\int_0^R\eta^{n+1}T_c^{(n)}d\eta+\sin n\theta\int_0^R\eta^{n+1}T_s^{(n)}d\eta\right)\right\} \tag{4.6}$$

$$\sigma_{r\theta}^{(f)}=\frac{E_f}{2(1+\nu_f)}(1+\nu_s)\alpha_s\left\{-\sum_{n=1}^{\infty}\frac{n+1}{r^{n+2}}\left(\sin n\theta\int_0^r\eta^{n+1}T_c^{(n)}d\eta-\cos n\theta\int_0^r\eta^{n+1}T_s^{(n)}d\eta\right)+\sum_{n=1}^{\infty}(n-1)r^{n-2}\left(\sin n\theta\int_r^R\eta^{1-n}T_c^{(n)}d\eta-\cos n\theta\int_r^R\eta^{1-n}T_s^{(n)}d\eta\right)+\sum_{n=1}^{\infty}\frac{n+1}{R^{n+2}}\left[n\left(\frac{r}{R}\right)^n-(n-1)\left(\frac{r}{R}\right)^{n-2}\right]\left(\sin n\theta\int_0^R\eta^{n+1}T_c^{(n)}d\eta-\cos n\theta\int_0^R\eta^{n+1}T_s^{(n)}d\eta\right)\right\} \tag{4.7}$$

The interface shear stresses τ_r and τ_θ are related to the temperature by

$$\tau_r = \frac{E_f h_f}{1-\nu_f^2}\left[[(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f]\frac{\partial T}{\partial r} - 2(\nu_s-\nu_f)\alpha_s \sum_{n=1}^{\infty} n(n+1)\frac{r^{n-1}}{R^{2n+2}}\left(\cos n\theta \int_0^R \eta^{n+1} T_c^{(n)} d\eta + \sin n\theta \int_0^R \eta^{n+1} T_s^{(n)} d\eta\right)\right] \quad (4.8)$$

$$\tau_\theta = \frac{E_f h_f}{1-\nu_f^2}\left\{ [(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f]\frac{1}{r}\frac{\partial T}{\partial \theta} + 2(\nu_s-\nu_f)\alpha_s \sum_{n=1}^{\infty} n(n+1)\frac{r^{n-1}}{R^{2n+2}}\left(\sin n\theta \int_0^R \eta^{n+1} T_c^{(n)} d\eta - \cos n\theta \int_0^R \eta^{n+1} T_s^{(n)} d\eta\right)\right\} \quad (4.9)$$

For uniform temperature distribution T=constant, the curvatures in the substrate obtained from Eqs. (4.2)–(4.4) become

$$\kappa = \kappa_{rr} = \kappa_{\theta\theta} = 6\frac{E_f h_f}{1-\nu_f}\frac{1-\nu_s}{E_s h_s^2}(\alpha_s - \alpha_f)T$$

The stresses in the thin film obtained from Eqs. (4.5)–(4.7) become

$$\sigma^{(f)} = \sigma_{rr}^{(f)} = \sigma_{\theta\theta}^{(f)} = \frac{E_f}{1-\nu_f}(\alpha_s - \alpha_f)T$$

For this special case only, both stress and curvature states become equibiaxial. The elimination of temperature T from the above two equations yields a simple relation $\sigma^{(f)} = (E_s h_s^2 / 6(1-\nu_s)h_f)\kappa$, which is exactly the Stoney formula in Eq. (1.1), and it has been used to estimate the thin-film stress $\sigma^{(f)}$ from the substrate curvature κ, if the temperature, stress, and curvature are all constant and if the plate system shape is spherical. In the following, we extend such a relation for arbitrary nonaxisymmetric temperature distribution.

5 Extension of Stoney Formula for Nonaxisymmetric Temperature Distribution

The stresses and curvatures are all given in terms of temperature in the previous section. We extend the Stoney formula for arbitrary nonuniform and nonaxisymmetric temperature distribution in this section by establishing the direct relation between the thinfilm stresses and substrate curvatures.

We first define the coefficients C_n and S_n related to the substrate curvatures by

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

where the integration is over the entire area A of the thin film, and $dA = \eta d\eta d\varphi$. Since both the substrate curvatures and film stresses depend on the temperature T, elimination of temperature gives the film stress in terms of substrate curvatures by

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = \frac{E_s h_s^2}{1-\nu_s}\frac{1-\nu_f}{6h_f}\frac{\alpha_s}{(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f}\left\{\kappa_{rr} - \kappa_{\theta\theta} - \sum_{n=1}^{\infty}(n+1)\left[n\left(\frac{r}{R}\right)^n - (n-1)\left(\frac{r}{R}\right)^{n-2}\right](C_n \cos n\theta + S_n \sin n\theta)\right\} \quad (5.2)$$

$$\sigma_{r\theta}^{(f)} = \frac{E_s h_s^2}{1-\nu_s}\frac{1-\nu_f}{6h_f}\frac{\alpha_s}{(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f}\left\{\kappa_{r\theta} + \frac{1}{2}\sum_{n=1}^{\infty}(n+1) \times \left[n\left(\frac{r}{R}\right)^n - (n-1)\left(\frac{r}{R}\right)^{n-2}\right](C_n \sin n\theta - S_n \cos n\theta)\right\} \quad (5.3)$$

$$\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} = \frac{E_s h_s^2}{6h_f(1-\nu_s)}\left\{\kappa_{rr}+\kappa_{\theta\theta} + \left[\frac{1-\nu_s}{1+\nu_s} - \frac{(1-\nu_f)\alpha_s}{(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f}\right](\kappa_{rr}+\kappa_{\theta\theta} - \overline{\kappa_{rr}+\kappa_{\theta\theta}}) - \left[\frac{1-\nu_s}{1+\nu_s} - \frac{2(1-\nu_f)\alpha_s}{(1+\nu_s)\alpha_s - (1+\nu_f)\alpha_f}\right]\sum_{n=1}^{\infty}(n+1) \times \left(\frac{r}{R}\right)^n (C_n \cos n\theta + S_n \sin n\theta)\right\} \quad (5.4)$$

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. Equations (5.2)–(5.4) provide direct relations between individual film stresses and substrate curvatures. It is important to note that stresses at a point in the 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_n and S_n.

The interface shear stresses τ_r and τ_θ can also be directly related to substrate curvatures via

$$\tau_r = \frac{E_s h_s^2}{6(1-\nu_s^2)}\left[\frac{\partial}{\partial r}(\kappa_{rr}+\kappa_{\theta\theta}) - \frac{1-\nu_s}{2R}\sum_{n=1}^{\infty} n(n+1)(C_n \cos n\theta + S_n \sin n\theta)\left(\frac{r}{R}\right)^{n-1}\right] \quad (5.5)$$

$$\tau_\theta = \frac{E_s h_s^2}{6(1-\nu_s^2)}\left[\frac{1}{r}\frac{\partial}{\partial \theta}(\kappa_{rr}+\kappa_{\theta\theta}) + \frac{1-\nu_s}{2R}\sum_{n=1}^{\infty} n(n+1)(C_n \sin n\theta - S_n \cos n\theta)\left(\frac{r}{R}\right)^{n-1}\right] \quad (5.6)$$

This provides a way to estimate the interface shear stresses from the gradients of substrate curvatures. It also displays a nonlocal dependence via the coefficients C_n and S_n.

Since interfacial shear stresses are responsible for promoting system failures through delamination of the thin film from the substrate, Eqs. (5.5) and (5.6) have particular significance. They show that such stresses are related to the gradients of $\kappa_{rr}+\kappa_{\theta\theta}$ and not to its magnitude, as might have been expected of a local, Stoney-like formulation. The implementation value of Eqs. (5.5) and (5.6) is that it provides an easy way of inferring these special interfacial shear stresses once the full-field curvature information is available. As a result, the methodology also provides a way to evaluate the risk of and to mitigate such important forms of failure. It should be noted that for the special case of spatially constant curvatures, the interfacial shear stresses vanish as is the case for all Stoney-like formulations described in Sec. 1.

It can be shown that the relations between the film stresses and substrate curvatures given in the form of infinite series in Eqs. (5.2)–(5.4) can be equivalently expressed in the form of integration as

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = \frac{E_s h_s^2}{1-\nu_s}\frac{1-\nu_f}{6h_f}\frac{\alpha_s}{(1+\nu_s)\alpha_s-(1+\nu_f)\alpha_f} \times \left\{ \kappa_{rr} - \kappa_{\theta\theta} - \frac{1}{\pi R^2}\int\int_A (\kappa_{rr}+\kappa_{\theta\theta}) \times \frac{\frac{\eta}{R}F_{\text{minus}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2 r^2}{R^4}\right]^3}dA \right\} \quad (5.7)$$

$$\sigma_{r\theta}^{(f)} = \frac{E_s h_s^2}{1-\nu_s}\frac{1-\nu_f}{6h_f}\frac{\alpha_s}{(1+\nu_s)\alpha_s-(1+\nu_f)\alpha_f} \left\{ \kappa_{r\theta} - \frac{1}{2}\frac{1}{\pi R^2}\int\int_A (\kappa_{rr} + \kappa_{\theta\theta}) \frac{\frac{\eta}{R}F_{\text{shear}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2 r^2}{R^4}\right]^3}dA \right\} \quad (5.8)$$

$$\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} = \frac{E_s h_s^2}{6h_f(1-\nu_s)} \left\{ \kappa_{rr} + \kappa_{\theta\theta} + \left[\frac{1-\nu_s}{1+\nu_s} - \frac{(1-\nu_f)\alpha_s}{(1+\nu_s)\alpha_s-(1+\nu_f)\alpha_f}\right](\kappa_{rr}+\kappa_{\theta\theta}-\overline{\kappa_{rr}+\kappa_{\theta\theta}}) - \left[\frac{1-\nu_s}{1+\nu_s} - \frac{2(1-\nu_f)\alpha_s}{(1+\nu_s)\alpha_s-(1+\nu_f)\alpha_f}\right]\frac{r}{\pi R^3}\int\int_A (\kappa_{rr} + \kappa_{\theta\theta}) \frac{\frac{\eta}{R}F_{\text{plus}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2 r^2}{R^4}\right]^4}dA \right\} \quad (5.9)$$

where functions F_{minus}, F_{shear}, and F_{plus} are given by

$$F_{\text{minus}}(r_1,\eta_1,\varphi_1) = -r_1^2\eta_1(6+9\eta_1^2+r_1^2\eta_1^4) + r_1(2+9\eta_1^2+6r_1^2\eta_1^2 + 6r_1^2\eta_1^4)\cos\varphi_1 - \eta_1(3+3r_1^2\eta_1^2+2r_1^4\eta_1^2)\cos 2\varphi_1 + r_1\eta_1^2\cos 3\varphi_1$$

$$F_{\text{shear}}(r_1,\eta_1,\varphi_1) = r_1(2+9\eta_1^2-6r_1^2\eta_1^2)\sin\varphi_1 - \eta_1(3+3r_1^2\eta_1^2 - 2r_1^4\eta_1^2)\sin 2\varphi_1 + r_1\eta_1^2\sin 3\varphi_1 \quad (5.10)$$

$$F_{\text{plus}}(r_1,\eta_1,\varphi_1) = 2(1+2r_1^2\eta_1^2)\cos\varphi_1 - r_1\eta_1\cos 2\varphi_1 - r_1\eta_1(4+r_1^2\eta_1^2)$$

The interface shear stresses can also be related to substrate curvatures via integrals as

$$\tau_r = \frac{E_s h_s^2}{6(1-\nu_s^2)}\left\{ \frac{\partial}{\partial r}(\kappa_{rr}+\kappa_{\theta\theta}) - \frac{1-\nu_s}{\pi R^3}\int\int_A (\kappa_{rr} + \kappa_{\theta\theta}) \frac{\frac{\eta}{R}F_{\text{radial}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2 r^2}{R^4}\right]^3}dA \right\} \quad (5.11)$$

$$\tau_\theta = \frac{E_s h_s^2}{6(1-\nu_s^2)}\left\{ \frac{1}{r}\frac{\partial}{\partial \theta}(\kappa_{rr}+\kappa_{\theta\theta}) - \frac{1-\nu_s}{\pi R^3}\int\int_A (\kappa_{rr} + \kappa_{\theta\theta}) \frac{\frac{\eta}{R}F_{\text{circumferential}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2 r^2}{R^4}\right]^3}dA \right\} \quad (5.12)$$

where

$$F_{\text{radial}}(r_1,\eta_1,\varphi_1) = (1+3r_1^2\eta_1^2)\cos\varphi_1 - r_1\eta_1(3+r_1^2\eta_1^2\cos 2\varphi_1) \quad (5.13)$$

$$F_{\text{circumferential}}(r_1,\eta_1,\varphi_1) = (1-3r_1^2\eta_1^2)\sin\varphi_1 + r_1^3\eta_1^3\sin 2\varphi_1$$

Finally it should be noted that Eq. (5.4) also reduces to Stoney's result for the case of spatial curvature uniformity. Indeed for this case, Eq. (5.4) reduces to:

$$\sigma_{rr} + \sigma_{\theta\theta} = \frac{E_s h_s^2}{6(1-\nu_s)h_f}(\kappa_{rr}+\kappa_{\theta\theta}) \quad (5.14)$$

If in addition the curvature state is equibiaxial ($\kappa_{rr}=\kappa_{\theta\theta}$), as assumed by Stoney, Eq. (1.1) is recovered while relation (5.2) furnishes $\sigma_{rr}=\sigma_{\theta\theta}$ (stress equibiaxiality) as a special case.

6 Discussion and Conclusions

Unlike Stoney's original analysis and its extensions discussed in Sec. 1, the present analysis, together with Huang and Rosakis [13] and Huang et al. [14] for the special case of axisymmetry, show that the dependence of film stresses on substrate curvatures is not generally "local." Here the stress components at a point on the film will, in general, depend on both the local value of the curvature components (at the same point) and on the value of curvatures of all other points on the plate system (nonlocal dependence). The more pronounced the curvature nonuniformities are, the more important such nonlocal effects become in accurately determining film stresses from curvature measurements. This demonstrates that analyses methods based on Stoney's approach and its various extensions cannot handle the nonlocality of the stress/curvature dependence and may result in substantial stress prediction errors if such analyses are applied locally in cases where spatial variations of system curvatures and stresses are present.

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 κ_{rr}, $\kappa_{\theta\theta}$, and $\kappa_{r\theta}$) from the entire plate surface.

Regarding the curvature-temperature (Eqs. (4.2)–(4.4)) and stress-temperature (Eqs. (4.5)–(4.7)) relations, the following points are noteworthy. These relations also generally feature a dependence of local temperature $T(r,\theta)$ which is "Stoney-like" as well as a "nonlocal" contribution from the temperature of other points on the plate system. Furthermore, the stress and curvature states are always nonequibiaxial (i.e., $\sigma_{rr}^{(f)} \neq \sigma_{\theta\theta}^{(f)}$ and $\kappa_{rr} \neq \kappa_{\theta\theta}$) in the presence of temperature nonuniformities. Only if T=constant these states become equibiaxial, the "nonlocal" contributions vanish, and Stoney's original results are recovered as a special case.

Finally, it should be noted that the existence of nonuniformities also results in the establishment of shear stresses along the film/substrate interface. These stresses are in general related to the derivatives of the first curvature invariant $\kappa_{rr}+\kappa_{\theta\theta}$ (Eqs. (5.11) and (5.12)). In terms of temperature, these interfacial shear stresses are also related to the gradients of the temperature distribution $T(r,\theta)$. The occurrence of such stresses is ultimately related to spatial nonuniformities, and as a result, such stresses vanish for the special case of uniform $\kappa_{rr}+\kappa_{\theta\theta}$ or T considered by Stoney and its various extensions. 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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