

On the Stoney Formula for a Thin Film/Substrate System With Nonuniform Substrate Thickness

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Current methodologies used for the inference of thin film stress through system curvature measurements are strictly restricted to stress and curvature states which are assumed to remain uniform over the entire film/substrate system. Recently Huang, Rosakis, and co-workers [Acta Mech. Sinica, 21, pp. 362–370 (2005); J. Mech. Phys. Solids, 53, 2483–2500 (2005); Thin Solid Films, 515, pp. 2220–2229 (2006); J. Appl. Mech., in press; J. Mech. Mater. Struct., in press] established methods for the film/substrate system subject to nonuniform misfit strain and temperature changes. The film stresses were found to depend nonlocally on system curvatures (i.e., depend on the full-field curvatures). These methods, however, all assume uniform substrate thickness, which is sometimes violated in the thin film/substrate system. Using the perturbation analysis, we extend the methods to nonuniform substrate thickness for the thin film/substrate system subject to nonuniform misfit strain. [DOI: 10.1115/1.2745392]

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1 Introduction

Stoney [1] used a plate system composed of a stress bearing thin film, of uniform thickness h_f , deposited on a relatively thick substrate, of uniform 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:

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

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) 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 involves the following assumptions:

- (i) Both the film thickness h_f and substrate thickness h_s are uniform, the film and substrate have the same radius R , and $h_f \ll h_s \ll R$;
- (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 which is often violated in practice.

Despite the explicitly stated assumptions, 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 system curvature. 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 assumptions (iv) and (v) 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 (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 systems 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

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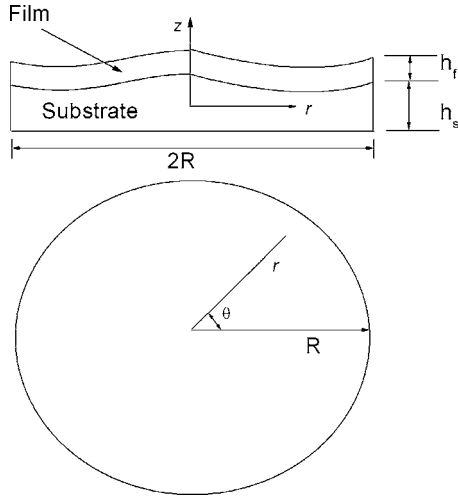


Fig. 1 A schematic diagram of a thin film/substrate system with the cylindrical coordinates (r, θ, z)

avored shape (e.g., ellipsoidal, cylindrical or saddle shapes) that features three different, still spatially constant, curvature components [11,12].

The above-discussed extensions of Stoney's methodology have not relaxed the most restrictive of Stoney's original assumption (vi) of spatial uniformity which does not allow either film stress and 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. 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 subject to non-uniform, axisymmetric misfit strain (in thin film) and temperature change (in both thin film and substrate), respectively, while Ngo et al. [15] 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 substrate curvatures*, i.e., they depend on curvatures of the entire substrate. The relations between film stresses and substrate 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. [16] relaxed part of the assumption (i) to study the thin film and substrate of different radii, i.e., the thin film has a smaller radius than the substrate. Ngo et al. [15] further relaxed the assumption (i) for arbitrarily nonuniform thickness of the thin film. The main purpose of the present paper is to relax the remaining portion in assumption (i), i.e., the uniform thickness of the substrate. To do so we consider the case of thin film/substrate system with nonuniform substrate thickness subject to nonuniform misfit strain field in the thin film. Our goal is to relate film stresses and system curvatures to the misfit strain distribution, and to ultimately derive a relation between the film stresses and the system curvatures that would allow for the accurate experimental inference of film stress from full-field and real-time curvature measurements.

2 Governing Equations and Boundary Conditions

Consider a thin film of uniform thickness h_f which is deposited on a circular substrate of thickness h_s and radius R (Fig. 1). The substrate thickness is nonuniform, but is assumed to be axisymmetric $h_s=h_s(r)$ for simplicity, where r and θ are the polar coordinates. The film is very thin, $h_f \ll h_s$, such that it is modeled as a membrane, and is subject to nonuniform misfit strain ε_m . Here the misfit strain is also assumed to be axisymmetric $\varepsilon_m=\varepsilon_m(r)$ for

simplicity. The substrate is modeled as a plate since $h_s \ll R$. The Young's modulus and Poisson's ratio of the film and substrate are denoted by E_f, ν_f, E_s , and ν_s , respectively.

Let u_f and u_s denote the displacements in the radial direction in the thin film and substrate, respectively. The in-plane membrane strains are obtained from $\varepsilon_{\alpha\beta}=(u_{\alpha,\beta}+u_{\beta,\alpha})/2$ for infinitesimal deformation and rotation, where $\alpha, \beta=r, \theta$. The linear elastic constitutive model, together with the vanishing out-of-plane stress $\sigma_{zz}=0$, give the in-plane stresses as

$$\sigma_{\alpha\beta} = \frac{E}{1-\nu^2} [(1-\nu)\varepsilon_{\alpha\beta} + \nu\varepsilon_{\kappa\kappa}\delta_{\alpha\beta} - (1+\nu)\varepsilon_m\delta_{\alpha\beta}],$$

where $E, \nu=E_f, \nu_f$ in the thin film and E_s, ν_s in the substrate, and the misfit strain ε_m is only in the thin film. The nonvanishing axial forces in the thin film and substrate are

$$N_r = \frac{Eh}{1-\nu^2} \left[\frac{du_r}{dr} + \nu \frac{u_r}{r} - (1+\nu)\varepsilon_m \right]$$

$$N_\theta = \frac{Eh}{1-\nu^2} \left[\nu \frac{du_r}{dr} + \frac{u_r}{r} - (1+\nu)\varepsilon_m \right] \quad (2)$$

where $h=h_f$ in the thin film and $h_s(r)$ in the substrate, and once again the misfit strain ε_m is only in the thin film.

Let w denote the lateral displacement in the normal (z) direction. The curvatures are given by $\kappa_{\alpha\beta}=w_{,\alpha\beta}$. The bending moments in the substrates are

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

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

For nonuniform misfit strain distribution $\varepsilon_m=\varepsilon_m(r)$, the shear stress along the radial direction at the film/substrate interface does not vanish, and is denoted by τ . The in-plane force equilibrium equations for the thin film and substrate, accounting for the effect of interface shear stress τ , becomes

$$\frac{dN_r}{dr} + \frac{N_r - N_\theta}{r} \mp \tau = 0 \quad (4)$$

where the minus sign in front of the interface shear stress is for the thin film, and the plus sign is for the substrate. The moment and out-of-plane force equilibrium equations for the substrate are

$$\frac{dM_r}{dr} + \frac{M_r - M_\theta}{r} + Q - \frac{h_s}{2} \tau = 0 \quad (5)$$

$$\frac{dQ}{dr} + \frac{Q}{r} = 0 \quad (6)$$

where Q is the shear force normal to the neutral axis. Equation (6), together with the requirement of finite Q at $r=0$, gives $Q=0$.

The substitution of Eq. (2) into (4) yields the governing equations for u and τ ,

$$\frac{d^2 u_f}{dr^2} + \frac{1}{r} \frac{du_f}{dr} - \frac{u_f}{r^2} = \frac{1-\nu_f^2}{E_f h_f} \tau + (1+\nu_f) \frac{d\varepsilon_m}{dr} \quad (7)$$

$$\frac{d}{dr} \left[h_s \left(\frac{du_s}{dr} + \frac{u_s}{r} \right) \right] - (1-\nu_s) \frac{dh_s}{dr} \frac{u_s}{r} = - \frac{1-\nu_s^2}{E_s} \tau \quad (8)$$

Equations (3), (5), and (6) give the governing equation for w and τ ,

$$\frac{d}{dr} \left[h_s^3 \left(\frac{d^2 w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right) \right] - (1-\nu_s) \frac{1}{r} \frac{dh_s}{dr} \frac{dw}{dr} = \frac{6(1-\nu_s^2)}{E_s} h_s \tau \quad (9)$$

The continuity of displacements across the film/substrate interface requires

$$u_f = u_s - \frac{h_s}{2} \frac{dw}{dr} \quad (10)$$

Equations (7)–(10) constitute four ordinary differential equations (ODEs) for u_f , u_s , w , and τ . The ODEs are linear, but have non-constant coefficients.

The boundary conditions at the free edge $r=R$ require that the net forces and net moments vanish,

$$N_r^{(f)} + N_r^{(s)} = 0 \quad (11)$$

$$M_r - \frac{h_s}{2} N_r^{(f)} = 0 \quad (12)$$

where the superscripts f and s denote the film and substrate, respectively.

3 Perturbation Method for Small Variation of Substrate Thickness

In the following we assume small variation of substrate thickness

$$h_s = h_{s0} + \Delta h_s = h_{s0} + \beta h_{s1} \quad (13)$$

where h_{s0} (=constant) is the average substrate thickness, and $\Delta h_s(r)$ is the substrate thickness variation which satisfies $|\Delta h_s| \ll h_{s0}$; $\Delta h_s(r)$ is also written as βh_{s1} in (13), where $0 < \beta \ll 1$ is a small, positive constant, and $h_{s1} = h_{s1}(r)$ is on the same order as h_{s0} .

We use the perturbation method to solve the ODEs analytically for $\beta \ll 1$. Two possible scenarios are considered separately in the following:

- (i) The substrate thickness variation Δh_s is on the same order as the thin film thickness h_f , i.e., $\Delta h_s \sim h_f$. This is represented by $\beta = h_f/h_{s0} (\ll 1)$. For this case the film stresses and system curvatures are identical to their counterparts for a constant substrate thickness h_{s0} . This is because the Stoney formula (1), as well as all its extensions, holds only for thin films, $h_f \ll h_s$. As compared to unity (one), terms that are on the order of $O(h_f/h_s)$ are always neglected. In this case the difference between the film stresses (or system curvatures, ...) for nonuniform substrate thickness h_s and those for constant thickness h_{s0} is on the order of $O(\Delta h_s/h_{s0})$ (as compared to unity), which is the same as $O(h_f/h_s)$ since $\Delta h_s \sim h_f$, and is therefore negligible.
- (ii) The substrate thickness variation Δh_s is much larger than the thin film thickness h_f , i.e., $|\Delta h_s| \gg h_f$. This is represented by $h_f/h_{s0} \ll \beta (\ll 1)$. In the following we focus on this case and use the perturbation method (for $\beta \ll 1$) to obtain the analytical solution.

Elimination of τ from (7) and (8) yields an equation for u_f and u_s . For $h_f/h_{s0} \ll 1$, u_f disappears in this equation, which becomes the governing equation for u_s ,

$$\frac{d}{dr} \left[h_s \left(\frac{du_s}{dr} + \frac{u_s}{r} \right) \right] - (1 - \nu_s) \frac{dh_s}{dr} \frac{u_s}{r} = \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s} \frac{d\varepsilon_m}{dr} \quad (14)$$

The above equation, together with (8), gives the interface shear stress

$$\tau = - \frac{E_f h_f}{1 - \nu_f} \frac{d\varepsilon_m}{dr} \quad (15)$$

This is a remarkable result that holds regardless of the substrate thickness and boundary conditions at the edge $r=R$. Therefore, the interface shear stress is proportional to the gradient of misfit strain. For uniform misfit strain $\varepsilon_m(r) = \text{constant}$, the interface

shear stress vanishes (even for nonuniform substrate thickness).

We use the perturbation method to write u_s as

$$u_s = u_{s0} + \beta u_{s1} \quad (16)$$

where $\beta \ll 1$, u_{s0} is the solution for a constant substrate thickness h_{s0} , and is given by Huang et al. [13]

$$u_{s0} = \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_{s0}} \left[\frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1 - \nu_s}{1 + \nu_s} \frac{\overline{\varepsilon_m} r}{2} \right] \quad (17)$$

and

$$\overline{\varepsilon_m} = \frac{2}{\pi R^2} \int_0^R \eta \varepsilon_m d\eta$$

is the average misfit strain in the thin film; u_{s1} in (16) is on the same order as u_{s0} . In the following we use u' to denote du/dr . The substitution of (16) and (17) into (14) and the neglect of $O(\beta^2)$ terms give the following linear ODE with constant coefficients for u_{s1} ,

$$\left(u'_{s1} + \frac{u_{s1}}{r} \right)' = (1 - \nu_s) \frac{h'_{s1}}{h_{s0}} \frac{u_{s0}}{r} - \left[\frac{h_{s1}}{h_{s0}} \left(u'_{s0} + \frac{u_{s0}}{r} \right) \right]' \quad (18)$$

Its general solution is

$$u_{s1}(r) = - \frac{h_{s1}}{h_{s0}} u_{s0} + \frac{1}{2r} \int_0^r \eta \left[1 + \nu_s + (1 - \nu_s) \frac{r^2}{\eta^2} \right] \frac{h'_{s1}(\eta)}{h_{s0}} u_{s0}(\eta) d\eta + \frac{A}{2} \quad (19)$$

where the constant A is to be determined. The total substrate displacement is then given by

$$u_s(r) = \left(2 - \frac{h_s}{h_{s0}} \right) u_{s0} + \frac{1}{2r} \int_0^r \eta \left[1 + \nu_s + (1 - \nu_s) \frac{r^2}{\eta^2} \right] \frac{h'_{s1}(\eta)}{h_{s0}} u_{s0}(\eta) d\eta + \frac{\beta A}{2} \quad (20)$$

The substitution of (15) into (9) yields the governing equation for the displacement w' ,

$$\left[h_s^3 \left(w'' + \frac{w'}{r} \right) \right]' - (1 - \nu_s) (h_s^3)' \frac{w'}{r} = - \frac{6E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s} h_s \varepsilon'_m \quad (21)$$

Its perturbation solution can be written as

$$w' = w'_0 + \beta w'_1 \quad (22)$$

where w'_0 is the solution for a constant substrate thickness h_{s0} , and is given by Huang et al. [13]

$$w'_0 = -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_{s0}^2} \left[\frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1 - \nu_s}{1 + \nu_s} \frac{\overline{\varepsilon_m} r}{2} \right] \quad (23)$$

and once again

$$\overline{\varepsilon_m} = \frac{2}{\pi R^2} \int_0^R \eta \varepsilon_m d\eta$$

is the average misfit strain in the thin film; w'_1 in (22) is on the same order as w'_0 . Equations (21)–(23) give the following linear ODE with constant coefficients for w'_1

$$\left(w_1' + \frac{w_1}{r}\right)' = -\frac{6E_f h_f}{1-\nu_f} \frac{1-\nu_s^2}{E_s h_{s0}^2} \frac{h_{s1}}{h_{s0}} \varepsilon_m' - 3 \left[\frac{h_{s1}}{h_{s0}} \left(w_0'' + \frac{w_0'}{r} \right) \right]' + 3(1-\nu_s) \frac{h_{s1}' w_0'}{h_{s0} r} \quad (24)$$

Its general solution is

$$w_1' = -3 \frac{h_{s1}}{h_{s0}} w_0' + \frac{3}{2r} \int_0^r \eta \left[1 + \nu_s + (1-\nu_s) \frac{r^2}{\eta^2} \right] \frac{h_{s1}'(\eta)}{h_{s0}} w_0'(\eta) d\eta + \frac{B}{2} r + 3 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s^2}{E_s h_{s0}^2} \frac{1}{r} \int_0^r \frac{d}{d\eta} \left[(r^2 - \eta^2) \frac{h_{s1}(\eta)}{h_{s0}} \right] \varepsilon_m(\eta) d\eta \quad (25)$$

where the constant B is to be determined. The complete solution for w' is obtained from (22) as

$$w' = \left(4 - 3 \frac{h_s}{h_{s0}} \right) w_0' + \frac{3}{2r} \int_0^r \eta \left[1 + \nu_s + (1-\nu_s) \frac{r^2}{\eta^2} \right] \frac{h_s'(\eta)}{h_{s0}} w_0'(\eta) d\eta + \frac{\beta B}{2} r + 3 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s^2}{E_s h_{s0}^2} \frac{1}{r} \int_0^r \frac{d}{d\eta} \left\{ (r^2 - \eta^2) \left[\frac{h_s(\eta)}{h_{s0}} - 1 \right] \right\} \times \varepsilon_m(\eta) d\eta \quad (26)$$

The displacement u_f in the thin film is then obtained from u_s in (20) and w' in (26) via (10).

The constants A and B , or equivalently, βA and βB , are determined from the boundary conditions (11) and (12) as

$$\beta A = -\frac{1-\nu_s}{R^2} \int_0^R \frac{R^2 - \eta^2}{\eta} \frac{h_s'(\eta)}{h_{s0}} u_{s0}(\eta) d\eta \quad (27)$$

$$\beta B = -\frac{3(1-\nu_s)}{R^2} \int_0^R \frac{R^2 - \eta^2}{\eta} \frac{h_s'(\eta)}{h_{s0}} w_0'(\eta) d\eta - 6 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s}{E_s h_{s0}^2} \frac{1}{R^2} \times \int_0^R \frac{d}{d\eta} \left\{ [(1+\nu_s)R^2 + (1-\nu_s)\eta^2] \left[\frac{h_s(\eta)}{h_{s0}} - 1 \right] \right\} \varepsilon_m(\eta) d\eta \quad (28)$$

4 Thin-Film Stresses and System Curvatures

The system curvatures $\kappa_{rr} = d^2 w / dr^2$ and $\kappa_{\theta\theta} = (1/r)(dw/dr)$ are obtained from (26). Their sum $\kappa_{\Sigma} \equiv \kappa_{rr} + \kappa_{\theta\theta}$ is given in terms of the misfit strain by

$$\kappa_{\Sigma} = -6 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s^2}{E_s h_{s0}^2} \left\{ \left(3 - 2 \frac{h_s}{h_{s0}} \right) \varepsilon_m + \left[4 - 3 \frac{h_s}{h_{s0}} + \frac{3(1-\nu_s)}{2} \frac{h_s - h_s(0)}{h_{s0}} \right] \frac{1-\nu_s}{1+\nu_s} \varepsilon_m \right. \\ \left. + \int_0^r \left[\frac{3(1-\nu_s)}{\eta^2} \int_0^\eta \rho \varepsilon_m(\rho) d\rho - \varepsilon_m(\eta) \right] \frac{h_s'(\eta)}{h_{s0}} d\eta \right\} \quad (29)$$

where

$$\varepsilon_m = \frac{2}{\pi R^2} \int_0^R \eta \varepsilon_m d\eta$$

is the average misfit strain in the thin film. The difference of system curvatures $\kappa_{\Delta} \equiv \kappa_{rr} - \kappa_{\theta\theta}$ is given by

$$\kappa_{\Delta} = -6 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s^2}{E_s h_{s0}^2} \left\{ \left(4 - 3 \frac{h_s}{h_{s0}} \right) \left(\varepsilon_m - \frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta \right) \right. \\ \left. + \left(\frac{h_s}{h_{s0}} - 1 \right) \varepsilon_m - \frac{2}{r^2} \int_0^r \eta \left[\frac{h_s(\eta)}{h_{s0}} - 1 \right] \varepsilon_m(\eta) d\eta \right. \\ \left. - \frac{1}{r^2} \int_0^r \eta^2 \left[\varepsilon_m(\eta) + \frac{3(1+\nu_s)}{\eta^2} \int_0^\eta \rho \varepsilon_m(\rho) d\rho + \frac{3(1-\nu_s)}{2} \varepsilon_m \right] \frac{h_s'(\eta)}{h_{s0}} d\eta \right\} \quad (30)$$

The thin film stresses are obtained from the constitutive relations

$$\sigma_{rr}^{(f)} = \frac{E_f}{1-\nu_f^2} \left[u_f' + \nu_f \frac{u_f}{r} - (1+\nu_f) \varepsilon_m \right]$$

and

$$\sigma_{\theta\theta}^{(f)} = \frac{E_f}{1-\nu_f^2} \left[\nu_f u_f' + \frac{u_f}{r} - (1+\nu_f) \varepsilon_m \right]$$

where u_f is given in (10). The sum of thin film stresses, up to the $O(\beta^2)$ accuracy (as compared to unity), is related to the misfit strain by

$$\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} = \frac{E_f}{1-\nu_f} (-2\varepsilon_m) \quad (31)$$

The difference of thin film stresses $\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)}$ is on the order of $O((E_f^2/E_s)\varepsilon_m(h_f/h_{s0}))$, which is very small as compared to $\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)}$. Therefore only its leading term is presented

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = 4E_f \frac{E_f h_f}{1-\nu_f^2} \frac{1-\nu_s^2}{E_s h_{s0}} \left[\varepsilon_m - \frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta \right] \quad (32)$$

4.1 Special Case: Uniform Misfit Strain. For uniform misfit strain distribution $\varepsilon_m = \text{constant}$ (and nonuniform substrate thick-

ness), the interface shear stress in (15) vanishes. The thin film stresses become constant and equibiaxial, and are given by

$$\sigma_{rr}^{(f)} = \sigma_{\theta\theta}^{(f)} = \frac{E_f}{1-\nu_f} (-\varepsilon_m) \quad (33)$$

The curvatures in (29) and (30) become

$$\begin{aligned} \kappa_{\Sigma} = & -12 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s}{E_s h_{s0}^2} \left\{ 1 - \frac{5-\nu_s}{2} \left(\frac{h_s}{h_{s0}} - 1 \right) \right. \\ & \left. + (1-2\nu_s) \frac{h_s - h_s(0)}{h_{s0}} \right\} \varepsilon_m \\ \kappa_{\Delta} = & 18 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s^2}{E_s h_{s0}^2} \left\{ \frac{h_s}{h_{s0}} - \frac{2}{r^2} \int_0^r \eta \frac{h_s(\eta)}{h_{s0}} d\eta \right\} \varepsilon_m \end{aligned} \quad (34)$$

which are neither constant nor equibiaxial for varying substrate thickness.

Figure 2 shows a substrate with a step change in thickness; a uniform thickness h in the outer region ($r > R_{in}$) and a slightly different value $h - \Delta h$ in the inner region ($r < R_{in}$), where $|\Delta h| \ll h$. The average thickness becomes $h_{s0} = h - \Delta h (R_{in}^2/R^2)$. The curvature in the circumferential direction is

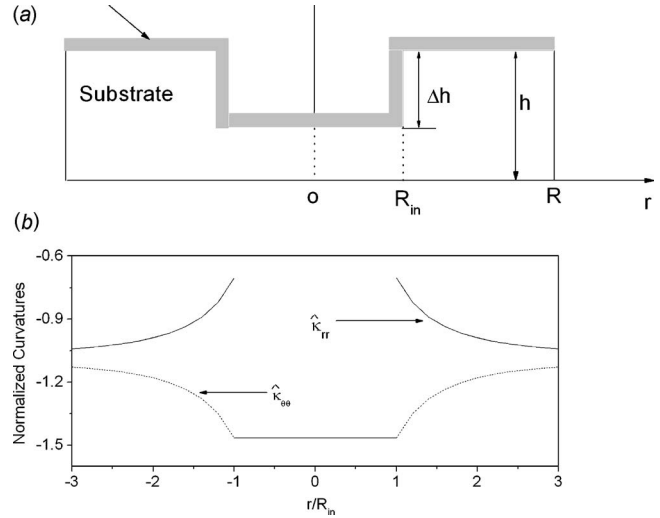


Fig. 2 (a) A schematic diagram of a thin film/substrate system with a step change in substrate thickness. (b) The normalized system curvatures $\hat{\kappa}_{rr} = \kappa_{rr}/\kappa_0$ and $\hat{\kappa}_{\theta\theta} = \kappa_{\theta\theta}/\kappa_0$, where $\kappa_0 = 6(E_f h_f / (1-\nu_f)) / (1-\nu_s / E_s h^2) \varepsilon_m$, $\Delta h/2h = 0.1$, $\nu_s = 0.27$, and $R_{in} = R/3$.

$$\kappa_{\theta\theta} = -6 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s}{E_s h^2} \varepsilon_m \begin{cases} 1 + \frac{\Delta h}{2h} \left[5 - \nu_s - (1-\nu_s) \frac{R_{in}^2}{R^2} \right] & \text{for } r < R_{in} \\ 1 + \frac{\Delta h}{2h} \left[5 - \nu_s - (1-\nu_s) \frac{R_{in}^2}{R^2} - 3(1+\nu_s) \left(1 - \frac{R_{in}^2}{r^2} \right) \right] & \text{for } r > R_{in} \end{cases} \quad (35)$$

which is a constant in the inner region, and is continuous across $r = R_{in}$. The curvature in the radial direction κ_{rr} is the same constant as $\kappa_{\theta\theta}$ in the inner region; however, it is discontinuous across $r = R_{in}$, and is given by

$$\kappa_{rr} = -6 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s}{E_s h^2} \varepsilon_m \begin{cases} 1 + \frac{\Delta h}{2h} \left[5 - \nu_s - (1-\nu_s) \frac{R_{in}^2}{R^2} \right] & \text{for } r < R_{in} \\ 1 + \frac{\Delta h}{2h} \left[5 - \nu_s - (1-\nu_s) \frac{R_{in}^2}{R^2} - 3(1+\nu_s) \left(1 + \frac{R_{in}^2}{r^2} \right) \right] & \text{for } r > R_{in} \end{cases} \quad (36)$$

The continuous $\kappa_{\theta\theta}$ and discontinuous κ_{rr} are illustrated in Fig. 2. Similar discontinuity in κ_{rr} has been observed for varying thin film thickness [17,18].

It should be pointed out that the results in this section hold for discontinuous substrate thickness. This is because the film stresses in (31) and (32) depend only on the misfit strain and are independent of substrate thickness. The system curvatures in (29) and (30) involve the derivative of substrate thickness h'_s , which is not well defined for a discontinuous h_s . However, it appears only in the integration such that (29) and (30) still hold.

In the following, we extend the Stoney formula for arbitrary nonuniform misfit strain distribution and nonuniform substrate thickness.

5 Extension of Stoney Formula for Nonuniform Misfit Strain Distribution and Nonuniform Substrate Thickness

In this section we extend the Stoney formula for arbitrary nonuniform misfit strain distribution and nonuniform substrate thickness by establishing the direct relation between the thin-film stresses and substrate curvatures. We invert the misfit strain from (29) as

$$\varepsilon_m = - \frac{1-\nu_f}{6E_f h_f} \frac{E_s}{1-\nu_s^2} \left\{ \begin{aligned} & h_s^2 \kappa_{\Sigma} - \frac{1-\nu_s}{2} \overline{h_s^2 \kappa_{\Sigma}} \\ & + \frac{1}{2} \int_r^R [(1-3\nu_s)\kappa_{\Sigma}(\eta) - 3(1-\nu_s)\kappa_{\Delta}(\eta)] h_s^2(\eta) \frac{h'_s(\eta)}{h_{s0}} d\eta \\ & - \frac{1-\nu_s}{R^2} \int_0^R \eta^2 [\kappa_{\Sigma}(\eta) - \kappa_{\Delta}(\eta)] h_s^2(\eta) \frac{h'_s(\eta)}{h_{s0}} d\eta \end{aligned} \right\} \quad (37)$$

where

$$\overline{h_s^2 \kappa_{\Sigma}} = \frac{2}{R^2} \int_0^R \eta h_s^2 \kappa_{\Sigma} d\eta$$

is the average of $h_s^2 \kappa_{\Sigma}$, and we have used (30) in establishing (37).

The thin film stresses are obtained by substituting (37) into (31) and (32) as

$$\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} = \frac{E_s}{3(1-\nu_s^2)h_f} \left\{ \begin{aligned} & h_s^2 \kappa_{\Sigma} - \frac{1-\nu_s}{2} h_s^2 \kappa_{\Sigma} \\ & + \frac{1}{2} \int_r^R [(1-3\nu_s)\kappa_{\Sigma}(\eta) - 3(1-\nu_s)\kappa_{\Delta}(\eta)] h_s^2(\eta) \frac{h_s'(\eta)}{h_{s0}} d\eta \\ & - \frac{1-\nu_s}{R^2} \int_0^R \eta^2 [\kappa_{\Sigma}(\eta) - \kappa_{\Delta}(\eta)] h_s^2(\eta) \frac{h_s'(\eta)}{h_{s0}} d\eta \end{aligned} \right\} \quad (38)$$

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = -\frac{2E_f h_{s0}}{3(1+\nu_f)} \kappa_{\Delta} \quad (39)$$

Equations (38) and (39) provide direct relations between film stresses and system curvatures. The system curvatures in (38) always appear together with the square of substrate thickness, i.e., $h_s^2 \kappa_{\Sigma}$ and $h_s^2 \kappa_{\Delta}$. 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 curvatures in the entire substrate (non-local dependence) via the term $h_s^2 \kappa_{\Sigma}$ and the integrals in (38). For uniform substrate thickness, (38) and (39) degenerate to Huang et al. [13]

The interface shear stress τ can also be directly related to system curvatures via (15) and (37)

$$\tau = \frac{E_s}{6(1-\nu_s^2)} \left\{ \frac{d}{dr} (h_s^2 \kappa_{\Sigma}) - \frac{1}{2} [(1-3\nu_s)h_s^2 \kappa_{\Sigma} - 3(1-\nu_s)h_s^2 \kappa_{\Delta}] \frac{h_s'}{h_{s0}} \right\} \quad (40)$$

Equation (40) provides a way to determine the interface shear stresses from the gradients of system curvatures once the full-field curvature information is available. Since the interfacial shear stress is responsible for promoting system failures through delamination of the thin film from the substrate, Eq. (40) has a particular significance. It shows that such stress is related to the gradient of $\kappa_{rr} + \kappa_{\theta\theta}$, as well as to the magnitude of $\kappa_{rr} + \kappa_{\theta\theta}$ and $\kappa_{rr} - \kappa_{\theta\theta}$ for nonuniform substrate thickness.

In summary, (38)–(40) provide a simple way to determine the thin film stresses and interface shear stress from the nonuniform misfit strain in the thin film and nonuniform substrate thickness.

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