Journal of Mechanics of Materials and Structures

THE EFFECT OF THIN FILM/SUBSTRATE RADII ON THE STONEY FORMULA FOR THIN FILM/SUBSTRATE SUBJECTED TO NONUNIFORM AXISYMMETRIC MISFIT STRAIN AND TEMPERATURE

> Xue Feng, Yonggang Huang, Hanqing Jiang, Duc Ngo and Ares J. Rosakis

Volume 1, № 6

June 2006



mathematical sciences publishers

THE EFFECT OF THIN FILM/SUBSTRATE RADII ON THE STONEY FORMULA FOR THIN FILM/SUBSTRATE SUBJECTED TO NONUNIFORM AXISYMMETRIC MISFIT STRAIN AND TEMPERATURE

XUE FENG, YONGGANG HUANG, HANQING JIANG, DUC NGO AND ARES J. ROSAKIS

Current methodologies used for the inference of thin film stress through curvature measurements are strictly restricted to stress and curvature states which are assumed to remain uniform over the entire film/substrate system. There are recent studies of film/substrate systems subjected to nonuniform but axisymmetric misfit strain and temperature changes. The film stresses were found to depend nonlocally on system curvatures (that is, depend on the full-field curvatures). A very simple stress-curvature relation was established, but it is limited to thin film and substrate of same radius. We extend the analysis to thin film and substrate of different radii. Remarkably the same simple stress-curvature relation still holds regardless of the film/substrate radii mismatch.

1. Introduction

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:

$$\sigma^{(f)} = \frac{E_s h_s^2 \kappa}{6h_f (1 - \nu_s)}.$$
(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) 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 [Stoney 1909; Freund and Suresh 2004].

Stoney's formula involves a number of assumptions given in the following:

- (i) both the film thickness h_f and the 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 equi-biaxial (two equal stress components in any two, mutually orthogonal in-plane directions) while the out-of-plane direct stress and all shear stresses vanish;

Keywords: thin film radius, nonuniform misfit strain, nonuniform wafer curvatures, stress-curvature relations, nonlocal effects, interfacial shears.

- (v) the system's curvature components are equi-biaxial (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 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 equi-biaxiality [Freund and Suresh 2004]. Related analyses treating discontinuous films in the form of bare periodic lines [Wikstrom et al. 1999b] or composite films with periodic line structures (for example, bare or encapsulated periodic lines) have also been derived [Shen et al. 1996; Wikstrom et al. 1999a; Park and Suresh 2000]. These latter analyses have removed the assumptions (iv) and (v) of equi-biaxiality 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 [Masters and Salamon 1993; Salamon and Masters 1995; Finot et al. 1997; Freund 2000]. These analyses have removed both the restrictions of an equi-biaxial 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 which have also been observed experimentally [Lee et al. 2001; Park et al. 2003; Fahnline et al. 1991]. These bifurcations are transformations from an initially equi-biaxial 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, that is, 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 (for example, ellipsoidal, cylindrical or saddle shapes) which features three different, still spatially constant, curvature components [Lee et al. 2001; Park et al. 2003; Masters and Salamon 1993; Salamon and Masters 1995].

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 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 [Masters and Salamon 1994]. Recently Huang et al. [2005] and Huang and Rosakis [2005] relaxed the assumption (vi) (and also (iv) and (v)) to study the thin film/substrate system subject to nonuniform,



Figure 1. A schematic diagram of the thin film/substrate system with different film and substrate radii. The cylindrical coordinates (r, θ, z) are used.

axisymmetric misfit strain (in thin film) and temperature change (in both thin film and substrate), respectively. The axisymmetric variation in particular is often present in film/substrate systems due to the circular wafer geometry and the axisymmetric geometries of most processing equipment used to manufacture such wafers. Their most important result is that the film stresses depend *nonlocally* on the substrate curvatures, that is, they depend on curvatures of the entire substrate. Huang et al. [2005] and Huang and Rosakis [2005] established very simple relations between film stresses and substrate curvatures for arbitrarily nonuniform, axisymmetric misfit strain and temperature change, respectively, and such relations degenerate to Stoney's formula for uniform, equi-iaxial stresses and curvatures.

The main purpose of the present paper is to extend their work by relaxing the assumption (i) such that the thin film and substrate may have different radii. To do so we consider the case of a thin film and substrate with different radii subjected to arbitrary, radially symmetric misfit strain field $\varepsilon_m(r)$ in the thin film or temperature field T(r) in the thin film and substrate. Our goal is to relate film stresses and system curvatures to the misfit strain (or temperature) 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. Nonuniform misfit strain

2.1. Governing equations. A circular thin film of radius R_f is deposited on a substrate of a larger radius $R_s > R_f$ (see Figure 1). The film thickness h_f is much less than the substrate thickness h_s , that is, $h_f \ll h_s$. The Young's modulus and Poisson's ratio of the film and substrate are denoted by E_f , v_f , E_s and v_s , respectively. The thin film is subjected to axisymmetric misfit strain distribution $\varepsilon_m(r)$, where r is the radial coordinate. The cylindrical coordinates (r, θ, z) are used (Figure 1) for this axisymmetric problem.



Figure 2. A schematic diagram of the nonuniform shear traction distribution at the interface between the film and the substrate.

The thin film and substrate are modeled as a membrane and a plate, respectively, since the film is very thin and has the negligible bending stiffness. Let u_f and u_s denote the radial displacements in the thin film and substrate (at the neutral axis). The strains are $\varepsilon_{rr} = du/dr$ and $\varepsilon_{\theta\theta} = u/r$, where u is u_f in the thin film and u_s in the substrate. The axial forces in the film and substrate can be obtained from the linear elastic constitutive model as

$$N_r = \frac{Eh}{1 - \nu^2} \left(\frac{du}{dr} + \nu \frac{u}{r} - (1 + \nu)\varepsilon_{\text{misfit}} \right), \qquad N_\theta = \frac{Eh}{1 - \nu^2} \left(\nu \frac{du}{dr} + \frac{u}{r} - (1 + \nu)\varepsilon_{\text{misfit}} \right), \tag{2}$$

where E, v, h and $\varepsilon_{\text{misfit}}$ are E_f , v_f , h_f and ε_m in the thin film and E_s , v_s , h_s and 0 in the substrate.

The shear stress traction σ_{rz} at the film/substrate interface is denoted by $\tau(r)$ as shown in Figure 2. The normal stress traction σ_{zz} vanishes because the thin film cannot be subjected to bending. The equilibrium of forces requires

$$\frac{dN_r}{dr} + \frac{N_r - N_\theta}{r} \mp \tau = 0, \tag{3}$$

where $-\tau$ and $+\tau$ are for the thin film and substrate within the film portion $(r \le R_f)$, respectively, and τ vanishes for the substrate outside the film $(R_f < r \le R_s)$. The substitution of Equation (2) into Equation (3) yields the following governing equations for u_f , u_s and τ

$$\frac{d^2 u_f}{dr^2} + \frac{1}{r} \frac{d u_f}{dr} - \frac{u_f}{r^2} = \frac{1 - \nu_f^2}{E_f h_f} \tau + (1 + \nu_f) \frac{d\varepsilon_m}{dr}, \qquad \text{for } r \le R_f,$$
(4)

$$\frac{d^2 u_s}{dr^2} + \frac{1}{r} \frac{du_s}{dr} - \frac{u_s}{r^2} = \begin{cases} -\frac{1-\nu_s^2}{E_s h_s} \tau, & \text{for } r \le R_f, \\ 0, & \text{for } R_f < r \le R_s. \end{cases}$$
(5)

Let w denote the lateral displacement of the substrate in the normal (z) direction. The bending moments in the substrate are given in terms of w by

$$M_r = \frac{E_s h_s^3}{12(1-v_s^2)} \left(\frac{d^2 w}{dr^2} + \frac{v_s}{r} \frac{dw}{dr}\right), \qquad M_\theta = \frac{E_s h_s^3}{12(1-v_s^2)} \left(v_s \frac{d^2 w}{dr^2} + \frac{1}{r} \frac{dw}{dr}\right). \tag{6}$$

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

$$\frac{dM_r}{dr} + \frac{M_r - M_\theta}{r} + Q - \frac{h_s}{2}\tau = 0, \qquad \frac{dQ}{dr} + \frac{Q}{r} = 0, \tag{7}$$

where Q is the shear force normal to the neutral axis, $h_s \tau/2$ is the contribution from the shear stress τ at the film/substrate interface within the film portion $(r \le R_f)$, and it vanishes for the substrate outside the film $(R_f < r \le R_s)$. The second equation in Equation (7) and the requirement of finite Q at the center r = 0 give Q = 0 in the entire substrate. The substitution of Equation (6) into the first equation in Equation (7) then gives the following governing equation for w and τ

$$\frac{d^3w}{dr^3} + \frac{1}{r}\frac{d^2w}{dr^2} - \frac{1}{r^2}\frac{dw}{dr} = \begin{cases} \frac{6(1-v_s^2)}{E_s h_s^2}\tau, & \text{for } r \le R_f, \\ 0, & \text{for } R_f < r \le R_s. \end{cases}$$
(8)

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

$$u_f = u_s - \frac{1}{2}h_s \frac{dw}{dr}, \qquad \text{for } r \le R_f.$$
(9)

Equations (4), (5), (8) and (9) constitute four ordinary differential equations for u_f , u_s , w and τ within the film portion ($r \le R_f$). Outside the film ($R_f < r \le R_s$) Equations (5) and (8) govern u_s and w.

The shear stress at the film/substrate interface can be obtained by eliminating u_f , u_s and w from these four equations as

$$\tau = -\frac{E_f h_f}{1 - \nu_f} \frac{d\varepsilon_m}{dr} \left(1 + \mathbb{O}\left(\frac{h_f}{h_s}\right) \right),\tag{10}$$

where the higher-order terms for $h_f/h_s \ll 1$ are neglected. That the interface shear stress is proportional to the gradient of misfit strain is a remarkable result. Equations (5) and (8) can then be solved analytically as

$$\frac{dw}{dr} = \begin{cases}
-6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{B_1}{2} r, & \text{for } r \le R_f, \\
A_1 r + \frac{C_1}{r}, & \text{for } R_f < r \le R_s,
\end{cases}$$

$$\mu = \begin{cases}
\frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s} \frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{B_2}{2} r, & \text{for } r \le R_f,
\end{cases}$$
(11)

where only the leading terms for $h_f/h_s \ll 1$ are shown, and B_1 , A_1 , C_1 , B_2 , A_2 and C_2 are constants to be determined by the continuity conditions across the edge of thin film $(r = R_f)$ and boundary conditions at the edge of substrate $(r = R_s)$ to be given in the next section. The displacement u_f in the thin film can be obtained from interface continuity condition in Equation (9).

2.2. Continuity conditions and boundary conditions. The displacement continuity conditions at the edge of thin film require

$$\left[\frac{dw}{dr}\right]_{r=R_f} = 0 \quad \text{and} \quad [u_s]_{r=R_f} = 0, \tag{13}$$

where $[\cdots]$ stands for the jump. The jump of the axial force in substrate $[N_r^{(s)}]$ is related to the axial force in thin film $N_r^{(f)}$ by

$$N_r^{(f)}\Big|_{r=R_f} - \left(N_r^{(s)}\right)_{r=R_f} = 0,$$

such that the net external force vanishes. Similarly, the jump of the bending moment in substrate $[M_r]$ is related to the bending moment produced by the axial force in thin film with respect to the neutral axis of substrate by

$$-[M_r]_{r=R_f} - \frac{1}{2}(h_s + h_f)N_r^{(f)}\Big|_{r=R_f} = 0$$

such that the net external moment vanishes.

The traction-free boundary conditions at the edge of substrate are

$$N_r^{(s)}\Big|_{r=R_s} = 0$$
 and $M_r\Big|_{r=R_s} = 0.$ (14)

Equations (13)–(14) are 6 linear algebraic equations to determine B_1 , A_1 , C_1 , B_2 , A_2 and C_2 . The displacements in Equations (11), (12) and (9) are then given by

$$\frac{dw}{dr} = \begin{cases} -6 \frac{E_f h_f}{1 - v_f} \frac{1 - v_s^2}{E_s h_s^2} \left(\frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1 - v_s}{1 + v_s} \frac{\overline{\varepsilon_m}}{2} r\right), & \text{for } r \le R_f, \\ -6 \frac{E_f h_f}{1 - v_f} \frac{1 - v_s^2}{E_s h_s^2} \left(\frac{\overline{\varepsilon_m}}{2} \frac{R_s^2}{r} + \frac{1 - v_s}{1 + v_s} \frac{\overline{\varepsilon_m}}{2} r\right), & \text{for } R_f < r \le R_s. \end{cases}$$
$$u_s = \begin{cases} \frac{E_f h_f}{1 - v_f} \frac{1 - v_s^2}{E_s h_s} \left(\frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1 - v_s}{1 + v_s} \frac{\overline{\varepsilon_m}}{2} \cdot r\right), & \text{for } r \le R_f, \\ \frac{E_f h_f}{1 - v_f} \frac{1 - v_s^2}{E_s h_s} \left(\frac{\overline{\varepsilon_m}}{2} \frac{R_s^2}{r} + \frac{1 - v_s}{1 + v_s} \frac{\overline{\varepsilon_m}}{2} r\right), & \text{for } R_f < r \le R_s, \end{cases}$$

 $u_f = 4u_s, \qquad \text{for } r \le R_f,$

where

$$\overline{\varepsilon_m} = \frac{2}{R_s^2} \int_0^{R_f} \eta \varepsilon_m(\eta) d\eta = \frac{1}{A_{\text{substrate}}} \int_{A_{\text{film}}} \varepsilon_m dA$$

is the average misfit strain, that is, the misfit strain of the thin film averaged over the entire substrate.

2.3. *Thin film stresses and substrate curvatures.* The substrate curvatures can be obtained from the displacement w as

$$\kappa_{rr} = \frac{d^2 w}{dr^2} = \begin{cases} -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \left(\varepsilon_m - \frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) \, d\eta + \frac{1 - \nu_s}{1 + \nu_s} \frac{\overline{\varepsilon_m}}{2} \right), & \text{for } r \le R_f, \\ -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \left(-\frac{\overline{\varepsilon_m}}{2} \frac{R_s^2}{r^2} + \frac{1 - \nu_s}{1 + \nu_s} \frac{\overline{\varepsilon_m}}{2} \right), & \text{for } R_f < r \le R_s, \end{cases}$$
(15)

$$\kappa_{\theta\theta} = \frac{1}{r} \frac{dw}{dr} = \begin{cases} -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \left(\frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) \, d\eta + \frac{1 - \nu_s}{1 + \nu_s} \frac{\overline{\varepsilon_m}}{2}\right), & \text{for } r \le R_f, \\ -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \left(\frac{\overline{\varepsilon_m}}{2} \frac{R_s^2}{r^2} + \frac{1 - \nu_s}{1 + \nu_s} \frac{\overline{\varepsilon_m}}{2}\right), & \text{for } R_f < r \le R_s. \end{cases}$$
(16)

The circumferential curvature $\kappa_{\theta\theta}$ is continuous across the edge of thin film $(r = R_f)$, but the radial curvature has a jump. The sum of these two curvatures is

$$\kappa_{rr} + \kappa_{\theta\theta} = \begin{cases} -12 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s}{E_s h_s^2} \left(\varepsilon_m - \frac{1 - \nu_s}{2} \left(\varepsilon_m - \overline{\varepsilon_m} \right) \right), & \text{for } r \le R_f, \\ -6 \frac{E_f h_f}{1 - \nu_f} \frac{(1 - \nu_s)^2}{E_s h_s^2} \overline{\varepsilon_m}, & \text{for } R_f < r \le R_s. \end{cases}$$

where the first term on the right hand side of the first line corresponds to the local misfit strain ε_m , while the second term gives the deviation from the local misfit strain and is proportional to the difference between the local misfit strain and the average misfit strain $\varepsilon_m - \overline{\varepsilon_m}$. The difference between two curvatures in Equations (15)–(16) is

$$\kappa_{rr} - \kappa_{\theta\theta} = \begin{cases} -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \left(\varepsilon_m - \frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) \, d\eta \right), & \text{for } r \le R_f, \\ 6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \frac{R_s^2}{r^2} \overline{\varepsilon_m}, & \text{for } R_f < r \le R_s. \end{cases}$$
(17)

The stresses in the thin film are obtained from Equation (2) as

$$\sigma_{rr}^{(f)} = \frac{E_f}{1 - \nu_f} \bigg\{ -\varepsilon_m + 4 \frac{E_f h_f}{1 - \nu_f^2} \frac{1 - \nu_s^2}{E_s h_s} \left(\varepsilon_m - (1 - \nu_f) \frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) \, d\eta + \frac{1 + \nu_f}{2} \frac{1 - \nu_s}{1 + \nu_s} \, \overline{\varepsilon_m} \right) \bigg\},$$

$$\sigma_{\theta\theta}^{(f)} = \frac{E_f}{1 - \nu_f} \bigg\{ -\varepsilon_m + 4 \frac{E_f h_f}{1 - \nu_f^2} \frac{1 - \nu_s^2}{E_s h_s} \left(\nu_f \varepsilon_m + (1 - \nu_f) \frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) \, d\eta + \frac{1 + \nu_f}{2} \frac{1 - \nu_s}{1 + \nu_s} \, \overline{\varepsilon_m} \right) \bigg\}.$$

The sum and difference of these stresses have the following simple expressions

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

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = 4E_f \frac{E_f h_f}{1 - \nu_f^2} \frac{1 - \nu_s^2}{E_s h_s} \Big(\varepsilon_m - \frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) \, d\eta \Big).$$
(18)

For uniform misfit strain ε_m = constant, the substrate curvatures from Equations (15)–(17) become

$$\begin{aligned} \kappa &= \kappa_{rr} = \kappa_{\theta\theta} = -6 \, \frac{E_f h_f}{1 - v_f} \, \frac{1 - v_s}{E_s h_s^2} \left(1 - \frac{1 - v_s}{2} \left(1 - \frac{R_f^2}{R_s^2} \right) \right) \varepsilon_m, \qquad \text{for } r \le R_f, \\ \kappa_{rr} &= 3 \, \frac{E_f h_f}{1 - v_f} \, \frac{1 - v_s}{E_s h_s^2} \left((1 + v_s) \frac{R_f^2}{r^2} - (1 - v_s) \frac{R_f^2}{R_s^2} \right) \varepsilon_m, \qquad \text{for } R_f < r \le R_s, \\ \kappa_{\theta\theta} &= -3 \, \frac{E_f h_f}{1 - v_f} \, \frac{1 - v_s}{E_s h_s^2} \left((1 + v_s) \frac{R_f^2}{r^2} + (1 - v_s) \frac{R_f^2}{R_s^2} \right) \varepsilon_m, \qquad \text{for } R_f < r \le R_s. \end{aligned}$$

The curvature state is constant and equi-biaxial only within film portion $r \le R_f$. It can be easily verified that the circumferential curvature is continuous across the edge of thin film, but the radial curvature has

a jump. The thin film stresses from (18) become

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

For this special case only, the stress state becomes equi-biaxial. Elimination of misfit strain ε_m from the above two equations yields a simple relation

$$\sigma = \frac{E_s h_s^2}{6(1-\nu_s)h_f \left(1-\frac{1-\nu_s}{2}\left(1-\frac{R_f^2}{R_s^2}\right)\right)} \kappa,$$

where κ is the constant curvature within the film portion $r \leq R_f$. For the thin film and substrate of same radii, the above relation degenerates Stoney's formula in Equation (1) which has been used to estimate the thin-film stress σ from the substrate curvature κ , if the misfit strain, stress and curvature are all constants, and if the plate system shape is spherical. For the thin film and substrate of different radii, the radius effect clearly comes into play. In the following, we establish a simple relation between film stress and substrate curvature for nonuniform misfit strain distribution.

2.4. *Extension of Stoney formula for nonuniform misfit strain distribution.* We extend the Stoney formula by establishing the direct relation between the thin-film stresses and substrate curvatures for the thin film and substrate of different radii subjected nonuniform misfit distribution. Both $\kappa_{rr} - \kappa_{\theta\theta}$ in Equation (17) and $\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)}$ in Equation (18) are proportional to $\varepsilon_m(r) - \frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta$. Therefore, elimination of misfit strain gives the difference $\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)}$ in thin-film stresses directly proportional to the difference $\kappa_{rr} - \kappa_{\theta\theta}$ in substrate curvatures,

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = -\frac{2E_f h_s}{3(1+\nu_f)} (\kappa_{rr} - \kappa_{\theta\theta}).$$
⁽¹⁹⁾

This relation is independent of the thin film and substrate radii, and is identical to its counterpart for the thin film and substrate with the same radii subjected to nonuniform misfit strain [Huang et al. 2005]. The above relation clearly shows that the radial and circumferential stress components will be equal only if the equivalent curvature components are also equal.

We now focus on the sum of thin-film stresses $\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)}$ and sum of substrate curvatures $\kappa_{rr} + \kappa_{\theta\theta}$. We define the average substrate curvature $\overline{\kappa_{rr} + \kappa_{\theta\theta}}$ as

$$\overline{\kappa_{rr} + \kappa_{\theta\theta}} = \frac{1}{A_{\text{substrate}}} \int \int_{A_{\text{substrate}}} \left(\kappa_{rr} + \kappa_{\theta\theta} \right) \eta \, d\eta d\theta = \frac{2}{R_s^2} \int_0^{R_s} \eta \left(\kappa_{rr} + \kappa_{\theta\theta} \right) d\eta,$$

where the integration is over the entire area $A_{\text{substrate}}$ of the substrate. The average substrate curvature can be related to the average misfit strain $\overline{\varepsilon_m}$ by averaging both sides of Equation (17), that is,

$$\overline{\kappa_{rr} + \kappa_{\theta\theta}} = 12 \, \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s}{E_s h_s^2} \left(-\overline{\varepsilon_m} \right).$$

Elimination of misfit strain ε_m and average misfit strain $\overline{\varepsilon_m}$ gives the sum of thin-film stresses in terms of curvatures as

$$\sigma_{rr} + \sigma_{\theta\theta} = \frac{E_s h_s^2}{6(1 - \nu_s)h_f} \left(\kappa_{rr} + \kappa_{\theta\theta} + \frac{1 - \nu_s}{1 + \nu_s} \left(\kappa_{rr} + \kappa_{\theta\theta} - \overline{\kappa_{rr} + \kappa_{\theta\theta}} \right) \right). \tag{20}$$

The above equation is once again independent of the thin film and substrate radii, and is identical to its counterpart for the thin film and substrate with the same radii subjected to nonuniform misfit strain [Huang et al. 2005]. Equations (19) and (20) provide direct relations between thin-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 average curvature in the entire substrate (nonlocal dependence).

The interface stress $\tau(r)$ given in Equation (10) can also be directly related to substrate curvatures via

$$\tau = \frac{E_s h_s^2}{6(1 - \nu_s^2)} \frac{d}{dr} \left(\kappa_{rr} + \kappa_{\theta\theta} \right).$$
(21)

This provides a remarkably simple way to estimate the interface shear stress from the radial gradient of the sum of two substrate curvatures. Equation (21) is independent of the thin film and substrate radii, and is identical to its counterpart for the thin film and substrate with the same radii subjected to nonuniform misfit strain [Huang et al. 2005].

Since interfacial shear stresses are responsible for promoting system failures through delamination of the thin film from the substrate, Equation (21) has particular significance. It shows that such stresses are proportional to the radial gradient 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 Equation (21) 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, this interfacial shear stress τ vanishes as is the case for all Stoney-like formulations described in the introduction.

3. Nonuniform temperature

We now consider the thin film and substrate of radii R_f and $R_s > R_f$ subjected to nonuniform temperature change T(r). The problem is still axisymmetric.

The linear elastic constitutive model given in Equation (2) still holds except that the misfit strain $\varepsilon_{\text{misfit}}$ is replaced by $\alpha_f T$ for the thin film and $\alpha_s T$ for the substrate, where α_f and α_s are the coefficients of thermal expansion. The equilibrium equations (3) and (7), moment-curvature relation (6), displacement continuity (9) across the thin film/substrate interface, and continuity and boundary conditions in Section 2.2 also hold.

The shear stress at the film/substrate interface is given by

$$\tau = \frac{E_f h_f}{1 - \nu_f^2} \left((1 + \nu_s) \alpha_s - (1 + \nu_f) \alpha_f \right) \frac{dT}{dr}.$$

This is a remarkable result that the interface shear stress is proportional to the gradient of temperature change. The displacements are given by

$$\frac{dw}{dr} = \begin{cases} \frac{6E_{f}h_{f}}{1-v_{f}^{2}} \frac{1-v_{s}^{2}}{E_{s}h_{s}^{2}} \left((1+v_{s}) \alpha_{s} - (1+v_{f}) \alpha_{f} \right) \frac{1}{r} \int_{0}^{r} \eta T(\eta) d\eta + \frac{B_{1}}{2}r, & \text{for } r \leq R_{f}, \\ \frac{3E_{f}h_{f}}{2(1-v_{f})} \frac{1-v_{s}^{2}}{E_{s}h_{s}^{2}} \times \left\{ \left((1+v_{s}) \alpha_{s} - 2\alpha_{f} \right) \overline{T_{f}} + (1-v_{s}) \alpha_{s} \overline{T_{s}} \right\} \left(\frac{1-v_{s}}{1+v_{s}} \frac{R_{f}^{2}}{R_{s}^{2}}r + \frac{R_{f}^{2}}{r} \right), & \text{for } R_{f} < r \leq R_{s}, \\ u_{s} = (1+v_{s}) \alpha_{s} \frac{1}{r} \int_{0}^{r} \eta T(\eta) d\eta + \frac{1}{2} (1-v_{s}) \alpha_{s} \overline{T_{s}}, & \text{for } r \leq R_{s}, \\ u_{f} = u_{s}, & \text{for } r \leq R_{f}, \end{cases}$$

where

$$\overline{T_f} = \frac{1}{A_{\text{film}}} \iint_{A_{\text{film}}} T\eta \, d\eta \, d\theta = \frac{2}{R_f^2} \int_0^{R_f} \eta T \, d\eta \qquad \text{and} \qquad \overline{T_s} = \frac{1}{A_{\text{substrate}}} \iint_{A_{\text{substrate}}} T\eta \, d\eta \, d\theta = \frac{2}{R_s^2} \int_0^{R_s} \eta T \, d\eta$$

are the average temperatures in the film and substrate, respectively, and

$$\frac{B_1}{2} = \frac{3E_f h_f}{1 - v_f^2} \frac{1 - v_s^2}{E_s h_s^2} \times \left\{ \frac{1 + v_f}{2} \left(\frac{1 - v_s}{1 + v_s} \frac{R_f^2}{R_s^2} + 1 \right) \left\{ \left((1 + v_s)\alpha_s - 2\alpha_f \right) \overline{T_f} + (1 - v_s)\alpha_s \overline{T_s} \right\} - \left((1 + v_s)\alpha_s - (1 + v_f)\alpha_f \right) \overline{T_f} \right\}.$$

The sum of two substrate curvatures is

$$\kappa_{rr} + \kappa_{\theta\theta} = \begin{cases} \frac{6E_f h_f}{1 - v_f^2} \frac{1 - v_s^2}{E_s h_s^2} \left((1 + v_s) \alpha_s - (1 + v_f) \alpha_f \right) T + B_1, & \text{for } r \le R_f, \\ \frac{3E_f h_f}{1 - v_f} \frac{(1 - v_s)^2}{E_s h_s^2} \frac{R_f^2}{R_s^2} \left\{ \left((1 + v_s) \alpha_s - 2\alpha_f \right) \overline{T_f} + (1 - v_s) \alpha_s \overline{T_s} \right\}, & \text{for } R_f < r \le R_s, \end{cases}$$

and the difference between two substrate curvatures is

$$\kappa_{rr} - \kappa_{\theta\theta} = \begin{cases} \frac{6E_f h_f}{1 - v_f^2} \frac{1 - v_s^2}{E_s h_s^2} \times \left((1 + v_s) \alpha_s - (1 + v_f) \alpha_f \right) \left(T - \frac{1}{r^2} \int_0^r \eta T(\eta) \, d\eta \right), & \text{for } r \le R_f, \\ -\frac{3E_f h_f}{1 - v_f} \frac{1 - v_s^2}{E_s h_s^2} \times \left\{ \left((1 + v_s) \alpha_s - 2\alpha_f \right) \overline{T_f} + (1 - v_s) \alpha_s \overline{T_s} \right\} \frac{R_f^2}{r^2}, & \text{for } R_f < r \le R_s. \end{cases}$$

Similarly, the sum and difference of thin-film stresses are given by

$$\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} = \frac{E_f}{1 - \nu_f} \Big\{ \Big((1 + \nu_s)\alpha_s - 2\alpha_f \Big) T + (1 - \nu_s)\alpha_s \overline{T_s} \Big\},$$

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = \frac{E_f}{1 + \nu_f} (1 + \nu_s)\alpha_s \Big(T - \frac{2}{r^2} \int_0^r \eta T(\eta) d\eta \Big).$$

Elimination of temperature change gives the difference $\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)}$ in thin-film stresses directly proportional to the difference $\kappa_{rr} - \kappa_{\theta\theta}$ in substrate curvatures,

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = \frac{E_s h_s^2}{6(1 - v_s)h_f} \frac{(1 - v_f)\alpha_s}{(1 + v_s)\alpha_s - (1 + v_f)\alpha_f} (\kappa_{rr} - \kappa_{\theta\theta}).$$
(22)

This relation is independent of the thin film and substrate radii, and is identical to its counterpart for the thin film and substrate with the same radii subjected to nonuniform temperature change [Huang and Rosakis 2005]. The sum of thin-film stresses $\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)}$ is related to the sum of substrate curvatures $\kappa_{rr} + \kappa_{\theta\theta}$ by

$$\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} = \frac{E_s h_s^2}{6(1 - v_s)h_f} \times \left\{ \kappa_{rr} + \kappa_{\theta\theta} + \left(\frac{1 - v_s}{1 + v_s} - \frac{(1 - v_f)\alpha_s}{(1 + v_s)\alpha_s - (1 + v_f)\alpha_f}\right) \times (\kappa_{rr} + \kappa_{\theta\theta} - \overline{\kappa_{rr} + \kappa_{\theta\theta}}) - \frac{1 + v_s}{2} \frac{(1 - v_f)\alpha_s}{(1 + v_s)\alpha_s - (1 + v_f)\alpha_f} \left(1 - \frac{R_f^2}{R_s^2}\right) \overline{\kappa_{rr} + \kappa_{\theta\theta}} \right\},$$
(23)

where

$$\overline{\kappa_{rr} + \kappa_{\theta\theta}} = \frac{1}{A_{\text{substrate}}} \iint_{A_{\text{substrate}}} (\kappa_{rr} + \kappa_{\theta\theta}) \eta \, d\eta \, d\theta$$

is the average substrate curvature. The above equation depends on the thin film and substrate radii, and is different from its counterpart for the thin film and substrate with the same radii subjected to nonuniform temperature change [Huang and Rosakis 2005].

The interface stress $\tau(r)$ can be directly related to substrate curvatures via

$$\tau = \frac{E_s h_s^2}{6(1-v_s^2)} \frac{d}{dr} \left(\kappa_{rr} + \kappa_{\theta\theta}\right).$$

This once again provides a remarkably simple way to estimate the interface shear stress from the radial gradient of the sum of two substrate curvatures. Equation (23) is independent of the thin film and substrate radii, and is identical to its counterpart for the thin film and substrate with the same radii subjected to temperature change [Huang and Rosakis 2005].

4. Discussion and conclusions

The recent work of [Huang et al. 2005] and [Huang and Rosakis 2005] shows that, unlike Stoney's formula in Equation (1), the thin film stresses depend on the substrate curvatures *nonlocally*—that is, the stress components at a point on the film 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). This demonstrates that analytical 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. The presence of nonlocal contributions, and the stress dependence on all curvature components, necessitates the use of full-field curvature measurement (over the entire surface of the plate system) in order to determine the film stresses. Furthermore, the

shear stress along the film/substrate interface is proportional to the radial derivative of the first curvature invariant $\kappa_{rr} + \kappa_{\theta\theta}$. This provides a means to determine the interface shear stress that is responsible for the delamination of thin film/substrate systems.

The results of [Huang et al. 2005] and [Huang and Rosakis 2005], however, are limited to thin film and substrate of the same radius. They are extended to thin film and substrate of different radii in the present paper. The most remarkable result is that, for thin film subjected to nonuniform, axisymmetric misfit strain, the film and substrate radii have no effect on the relation between thin film stresses and substrate curvatures, i.e., the stress-curvature relation is identical to that for thin film and substrate of the same radius. This conclusion is particularly useful to the determination of thin film stresses from substrate curvatures since one only needs to know the local and average curvatures of the substrate, and not the thin film and substrate radii.

For thin film and substrate subjected to nonuniform, axisymmetric temperature change, the film and substrate radii still do not affect the difference in film stresses $\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)}$, but they influence the sum of film stresses $\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)}$. The reason for this difference between misfit strain and temperature change is the former occurs only in the film, while the latter occurs in both the thin film and substrate, and the nonuniform temperature change in the substrate leads to stresses and curvatures that depend on the radii.

For both axisymmetric misfit strain and temperature change, the interface shear stress is always proportional to the radial gradient of curvature sum, and is independent of the thin film and substrate radii.

References

- [Fahnline et al. 1991] D. E. Fahnline, C. B. Masters, and N. J. Salamon, "Thin film stresses from nonspherical substrate bending measurements", *J. Vac. Sci. Technol. A* **9**:4 (1991), 2483–2487.
- [Finot et al. 1997] M. Finot, I. Blech, S. S., and H. Fijimoto, "Large deformation and geometric instability of substrates with thin-film deposits", *J. Appl. Phys.* **81**:8 (1997), 3457–3464.
- [Freund 2000] L. B. Freund, "Substrate curvature due to thin film mismatch strain in the nonlinear deformation range", *J. Mech. Phys. Solids* **48**:6-7 (2000), 1159–1174. MR 2001c:74029
- [Freund and Suresh 2004] L. B. Freund and S. Suresh, *Thin film materials; Stress, defect formation and surface evolution*, Cambridge University Press, New York, 2004.
- [Huang and Rosakis 2005] Y. Huang and A. J. Rosakis, "Extension of Stoney's formula to non-uniform temperature distributions in thin film/substrate systems: The case of radial symmetry", *J. Mech. Phys. Solids* **53**:11 (2005), 2483–2500.
- [Huang et al. 2005] Y. Huang, D. Ngo, and A. J. Rosakis, "Non-uniform, axisymmetric misfit strain: in thin films bonded on plate substrates/substrate systems: the relation between non-uniform film stresses and system curvatures", *Acta. Mech. Sinica* **21**:4 (2005), 362–370.
- [Lee et al. 2001] H. Lee, A. J. Rosakis, and L. B. Freund, "Full field optical measurement of curvatures in ultra-thin film/substrate systems in the range of geometrically nonlinear deformations", *J. Appl. Phys.* **89**:11 (2001), 6116–6129.
- [Masters and Salamon 1993] C. B. Masters and N. J. Salamon, "Geometrically nonlinear stress-deflection relations for thin film/substrate systems", *Int. J. Engrg. Sci.* **31**:6 (1993), 915–925.
- [Masters and Salamon 1994] C. B. Masters and N. J. Salamon, "Geometrically nonlinear stress-deflection relations for thin film/substrate systems with a finite element comparison", *J. Appl. Mech. (ASME)* **61** (1994), 872–878.
- [Park and Suresh 2000] T. S. Park and S. Suresh, "Effects of line and passivation geometry on curvature evolution during processing and thermal cycling in copper interconnect lines", *Acta Mater.* **48**:12 (2000), 3169–3175.
- [Park et al. 2003] T. S. Park, S. Suresh, A. J. Rosakis, and J. Ryu, "Measurement of full field curvature and geometrical instability of thin film-substrate systems through CGS interferometry", *J. Mech. Phys. Solids* **51**:11-12 (2003), 2191–2211.

- [Salamon and Masters 1995] N. J. Salamon and C. B. Masters, "Bifurcation in isotropic thin film/substrate plates", *Int. J. Solids Struct.* **32**:3-4 (1995), 473–481.
- [Shen et al. 1996] Y. L. Shen, S. Suresh, and I. A. Blech, "Stresses, curvatures, and shape changes arising from patterned lines on silicon wafers", *J. Appl. Phys.* **80**:3 (1996), 1388–1398.
- [Stoney 1909] G. G. Stoney, "The tension of metallic films deposited by electrolysis", *Proc. R. Soc. Lond.* 82:553 (1909), 172–175.
- [Wikstrom et al. 1999a] A. Wikstrom, P. Gudmundson, and S. Suresh, "Analysis of average thermal stresses in passivated metal interconnects", *J. Appl. Phys.* 86:11 (1999), 6088–6095.
- [Wikstrom et al. 1999b] A. Wikstrom, P. Gudmundson, and S. Suresh, "Thermoelastic analysis of periodic thin lines deposited on a substrate", J. Mech. Phys. Solids 47:5 (1999), 1113–1130.

Received 27 Dec 2005.

XUE FENG: xuefeng@uiuc.edu Department of Mechanical and Industrial Engineering, University of Illinois, Urbana, IL 61801, United States

YONGGANG HUANG: huang9@uiuc.edu Department of Mechanical and Industrial Engineering, University of Illinois, Urbana, IL 61801, United States

HANQING JIANG: hqjiang@uiuc.edu Department of Mechanical and Aerospace Engineering, Arizona State University, Tempe, AZ 85287, United States

DUC NGO: ducngo2@uiuc.edu Department of Mechanical and Industrial Engineering, University of Illinois, Urbana, IL 61801, United States

ARES J. ROSAKIS: rosakis@aero.caltech.edu Graduate Aeronautical Laboratory, California Institute of Technology, Pasadena, CA 91125, United States