

Thin film/substrate systems featuring arbitrary film thickness and misfit strain distributions. Part I: Analysis for obtaining film stress from non-local curvature information

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Abstract

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. Recently Huang, Rosakis and co-workers [Huang, Y., Ngo, D., Rosakis, A.J., 2005. 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. Sin.* 21, 362–370; Huang, Y., Rosakis A.J., 2005. 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, 2483–2500; Ngo, D., Huang, Y., Rosakis, A. J., Feng, X. 2006. Spatially non-uniform, isotropic misfit strain in thin films bonded on plate substrates: the relation between non-uniform film stresses and system curvatures. *Thin Solid Films* (in press)] established methods for film/substrate system subject to non-uniform misfit strain and temperature changes. The film stresses were found to depend non-locally on system curvatures (i.e., depend on the full-field curvatures). The existing methods, however, all assume uniform film thickness which is often violated in the thin film/substrate system. We extend these methods to arbitrarily non-uniform film thickness for the thin film/substrate system subject to non-uniform misfit strain. Remarkably the stress-curvature relation for uniform film thickness still holds if the film thickness is replaced by its local value at the point where the stress is evaluated. This result has been experimentally validated in Part II of this paper.

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1. Introduction

Stoney (1909) 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:

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

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. Eq. (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 (e.g., Freund and Suresh, 2004).

Stoney formula involve 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 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;
- (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 point-wise 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 non-uniformity 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 equi-biaxiality as well as the assumption of small deformations/deflections. A biaxial form of Stoney formula (with different direct stress values and non-zero in-plane shear stress) was derived by relaxing the assumption (v) of curvature equi-biaxiality (e.g., Freund and Suresh, 2004). Related analyses treating discontinuous films in the form of bare periodic lines (Wikstrom et al., 1999a) or composite films with periodic line structures (e.g., bare or encapsulated periodic lines) have also been derived (Shen et al., 1996; Wikstrom et al., 1999b; 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, non-equal, 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 that have also been observed experimentally (Lee et al., 2001; Park and Suresh, 2000). 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, i.e., the ratio of in-plane to thickness dimension and the elastic stiffness. These analyses also retain the assumption (vi) of spatial curvature and stress uniformity across the system. However, they allow for deformations to evolve from an initially spherical shape to an energetically favored shape (e.g., ellipsoidal, cylindrical or saddle shapes) that features three different, still spatially constant, curvature components (Lee et al., 2001; Park and Suresh, 2000).

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 non-uniformly distributed over the plate area. 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 non-uniform, axisymmetric misfit strain (in thin film) and temperature change (in both thin film and substrate), respectively, while Ngo et al. (2006) studied the thin film/substrate system subject to arbitrarily non-uniform (e.g., non-axisymmetric) misfit strain and temperature. The most important result is that the film stresses depend non-locally 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 non-uniform misfit strain and temperature change, and such relations degenerate to Stoney formula for uniform, equi-biaxial stresses and curvatures.

Feng et al. (2006) relaxed part of the assumption (i) to study the thin film and substrate of different radii. The main purpose of the present paper is to further relax the assumption (i) to study arbitrarily non-uniform thickness of the thin film. To do so we consider the case of non-uniform film thickness and the thin film/substrate system subject to arbitrary misfit strain field in the thin film. Our goal is to relate film stresses and system curvatures to the misfit strain distribution for arbitrarily non-uniform film thickness, 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

Consider a thin film of non-uniform thickness $h_f(r, \theta)$ which is deposited on a circular substrate of constant thickness h_s and radius R , where r and θ are the polar coordinates (Fig. 1). The film is very thin, $h_f \ll h_s$, such that it is modeled as a membrane, and is subject to arbitrary misfit strain distribution $\varepsilon^m(r, \theta)$. 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 $u_r^{(f)}, u_\theta^{(f)}, u_r^{(s)}$ and $u_\theta^{(s)}$ denote the in-plane displacements in the thin film and substrate along the radial (r) and circumferential (θ) directions, respectively. The in-plane membrane strains are obtained from

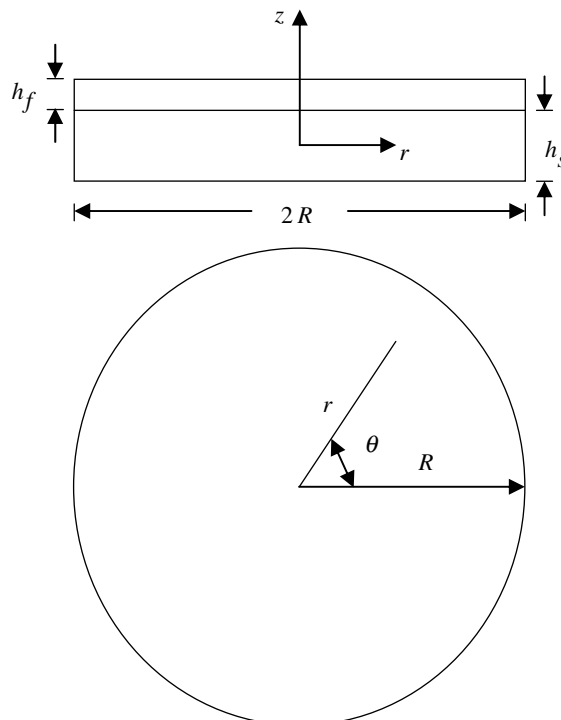


Fig. 1. A schematic diagram of a thin film/substrate system with the cylindrical coordinates (r, θ, z).

$\varepsilon = [\nabla u + (\nabla u)^T]/2$ 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 axial forces in the thin film and substrate are

$$\begin{aligned} N_r &= \frac{Eh}{1-\nu^2} \left[\frac{\partial u_r}{\partial r} + \nu \left(\frac{u_r}{r} + \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} \right) - (1+\nu)\varepsilon^m \right], \\ N_\theta &= \frac{Eh}{1-\nu^2} \left[\nu \frac{\partial u_r}{\partial r} + \frac{u_r}{r} + \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} - (1+\nu)\varepsilon^m \right], \\ N_{r\theta} &= \frac{Eh}{2(1+\nu)} \left(\frac{1}{r} \frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r} \right), \end{aligned} \quad (2.1)$$

where $h = h_f$ in the thin film and h_s 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 $\kappa = \nabla \nabla w$. The bending moments in the substrates are

$$\begin{aligned} M_r &= \frac{E_s h_s^3}{12(1-\nu_s^2)} \left[\frac{\partial^2 w}{\partial r^2} + \nu_s \left(\frac{1}{r} \frac{\partial w}{\partial r} + \frac{1}{r^2} \frac{\partial^2 w}{\partial \theta^2} \right) \right], \\ M_\theta &= \frac{E_s h_s^3}{12(1-\nu_s^2)} \left(\nu_s \frac{\partial^2 w}{\partial r^2} + \frac{1}{r} \frac{\partial w}{\partial r} + \frac{1}{r^2} \frac{\partial^2 w}{\partial \theta^2} \right), \\ M_{r\theta} &= \frac{E_s h_s^3}{12(1+\nu_s)} \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial w}{\partial \theta} \right). \end{aligned} \quad (2.2)$$

For non-uniform misfit strain distribution $\varepsilon^m = \varepsilon^m(r, \theta)$, the shear stresses at the film/substrate interface do not vanish, and are denoted by τ_r and τ_θ . The in-plane force equilibrium equations for the thin film and substrate, accounting for the effect of interface shear stresses τ_r and τ_θ , become

$$\begin{aligned} \frac{\partial N_r}{\partial r} + \frac{N_r - N_\theta}{r} + \frac{1}{r} \frac{\partial N_{r\theta}}{\partial \theta} \mp \tau_r &= 0, \\ \frac{\partial N_{r\theta}}{\partial r} + \frac{2}{r} N_{r\theta} + \frac{1}{r} \frac{\partial N_\theta}{\partial \theta} \mp \tau_\theta &= 0, \end{aligned} \quad (2.3)$$

where the minus sign in front of the interface shear stresses 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

$$\begin{aligned} \frac{\partial M_r}{\partial r} + \frac{M_r - M_\theta}{r} + \frac{1}{r} \frac{\partial M_{r\theta}}{\partial \theta} + Q_r - \frac{h_s}{2} \tau_r &= 0, \\ \frac{\partial M_{r\theta}}{\partial r} + \frac{2}{r} M_{r\theta} + \frac{1}{r} \frac{\partial M_\theta}{\partial \theta} + Q_\theta - \frac{h_s}{2} \tau_\theta &= 0, \end{aligned} \quad (2.4)$$

$$\frac{\partial Q_r}{\partial r} + \frac{Q_r}{r} + \frac{1}{r} \frac{\partial Q_\theta}{\partial \theta} = 0, \quad (2.5)$$

where Q_r and Q_θ are the shear forces normal to the neutral axis.

The substitution of Eqs. (2.1)–(2.3) yields the governing equations for u_r, u_θ, τ_r and τ_θ

$$\begin{aligned} \frac{\partial}{\partial r} \left\{ h_f \left[\frac{\partial u_r^{(f)}}{\partial r} + \frac{u_r^{(f)}}{r} + \frac{1}{r} \frac{\partial u_\theta^{(f)}}{\partial \theta} \right] \right\} + \frac{1-\nu_f}{2} \frac{h_f}{r^2} \left\{ \frac{\partial^2 u_r^{(f)}}{\partial \theta^2} - \frac{\partial}{\partial r} \left[r \frac{\partial u_\theta^{(f)}}{\partial \theta} \right] \right\} \\ + \frac{1-\nu_f}{2} \left\langle \frac{\partial h_f}{\partial \theta} \left\{ \frac{\partial}{\partial r} \left[\frac{u_\theta^{(f)}}{r} \right] + \frac{1}{r^2} \frac{\partial u_r^{(f)}}{\partial \theta} \right\} - \frac{2}{r} \frac{\partial h_f}{\partial r} \left[u_r^{(f)} + \frac{\partial u_\theta^{(f)}}{\partial \theta} \right] \right\rangle \\ = \frac{1-\nu_f^2}{E_f} \tau_r + (1+\nu_f) \frac{\partial (h_f \varepsilon^m)}{\partial r}, \end{aligned} \quad (2.6a)$$

$$\begin{aligned} & \frac{1}{r} \frac{\partial}{\partial \theta} \left\{ h_f \left[\frac{\partial u_r^{(f)}}{\partial r} + \frac{u_r^{(f)}}{r} + \frac{1}{r} \frac{\partial u_\theta^{(f)}}{\partial \theta} \right] \right\} + \frac{1 - \nu_f}{2} h_f \left\langle -\frac{\partial}{\partial r} \left[\frac{1}{r} \frac{\partial u_r^{(f)}}{\partial \theta} \right] + \frac{\partial}{\partial r} \left\{ \frac{1}{r} \frac{\partial}{\partial r} [r u_\theta^{(f)}] \right\} \right\rangle \\ & + \frac{1 - \nu_f}{2} \left\langle \frac{\partial h_f}{\partial r} \left\{ \frac{1}{r} \frac{\partial u_r^{(f)}}{\partial \theta} + r \frac{\partial}{\partial r} \left[\frac{u_\theta^{(f)}}{r} \right] \right\} - \frac{2}{r} \frac{\partial h_f}{\partial \theta} \frac{\partial u_r^{(f)}}{\partial r} \right\rangle \\ & = \frac{1 - \nu_f^2}{E_f} \tau_\theta + (1 + \nu_f) \frac{1}{r} \frac{\partial (h_f \varepsilon^m)}{\partial \theta}, \end{aligned} \tag{2.6b}$$

$$\frac{\partial}{\partial r} \left[\frac{\partial u_r^{(s)}}{\partial r} + \frac{u_r^{(s)}}{r} + \frac{1}{r} \frac{\partial u_\theta^{(s)}}{\partial \theta} \right] + \frac{1 - \nu_s}{2} \frac{1}{r^2} \left\{ \frac{\partial^2 u_r^{(s)}}{\partial \theta^2} - \frac{\partial}{\partial r} \left[r \frac{\partial u_\theta^{(s)}}{\partial \theta} \right] \right\} = -\frac{1 - \nu_s^2}{E_s h_s} \tau_r, \tag{2.7a}$$

$$\frac{1}{r} \frac{\partial}{\partial \theta} \left[\frac{\partial u_r^{(s)}}{\partial r} + \frac{u_r^{(s)}}{r} + \frac{1}{r} \frac{\partial u_\theta^{(s)}}{\partial \theta} \right] + \frac{1 - \nu_s}{2} \left\langle -\frac{\partial}{\partial r} \left[\frac{1}{r} \frac{\partial u_r^{(s)}}{\partial \theta} \right] + \frac{\partial}{\partial r} \left\{ \frac{1}{r} \frac{\partial}{\partial r} [r u_\theta^{(s)}] \right\} \right\rangle = -\frac{1 - \nu_s^2}{E_s h_s} \tau_\theta. \tag{2.7b}$$

Elimination of Q_r and Q_θ from Eqs. (2.4) and (2.5), together with Eq. (2.2), give the governing equation for w , τ_r and τ_θ

$$\nabla^2 (\nabla^2 w) = \frac{6(1 - \nu_s^2)}{E_s h_s^2} \left(\frac{\partial \tau_r}{\partial r} + \frac{\tau_r}{r} + \frac{1}{r} \frac{\partial \tau_\theta}{\partial \theta} \right), \tag{2.8}$$

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 film/substrate interface requires

$$u_r^{(f)} = u_r^{(s)} - \frac{h_s}{2} \frac{\partial w}{\partial r}, \quad u_\theta^{(f)} = u_\theta^{(s)} - \frac{h_s}{2} \frac{1}{r} \frac{\partial w}{\partial \theta}. \tag{2.9}$$

Eqs. (2.6)–(2.9) 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 . For the limit $h_f/h_s \ll 1$, these equations are decoupled such that we can solve $u_r^{(s)}$, $u_\theta^{(s)}$ first, then w , followed by $u_r^{(f)}$ and $u_\theta^{(f)}$, and finally τ_r and τ_θ .

- (i) Elimination of τ_r and τ_θ from Eqs. (2.6) and (2.7) 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 give the governing equations for $u_r^{(s)}$ and $u_\theta^{(s)}$

$$\frac{\partial}{\partial r} \left[\frac{\partial u_r^{(s)}}{\partial r} + \frac{u_r^{(s)}}{r} + \frac{1}{r} \frac{\partial u_\theta^{(s)}}{\partial \theta} \right] + \frac{1 - \nu_s}{2} \frac{1}{r^2} \left\{ \frac{\partial^2 u_r^{(s)}}{\partial \theta^2} - \frac{\partial}{\partial r} \left[r \frac{\partial u_\theta^{(s)}}{\partial \theta} \right] \right\} = \frac{E_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s} \frac{\partial}{\partial r} (h_f \varepsilon^m), \tag{2.10a}$$

$$\begin{aligned} & \frac{1}{r} \frac{\partial}{\partial \theta} \left[\frac{\partial u_r^{(s)}}{\partial r} + \frac{u_r^{(s)}}{r} + \frac{1}{r} \frac{\partial u_\theta^{(s)}}{\partial \theta} \right] + \frac{1 - \nu_s}{2} \left\langle -\frac{\partial}{\partial r} \left[\frac{1}{r} \frac{\partial u_r^{(s)}}{\partial \theta} \right] + \frac{\partial}{\partial r} \left\{ \frac{1}{r} \frac{\partial}{\partial r} [r u_\theta^{(s)}] \right\} \right\rangle \\ & = \frac{E_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s} \frac{1}{r} \frac{\partial}{\partial \theta} (h_f \varepsilon^m). \end{aligned} \tag{2.10b}$$

- (ii) Elimination of $u_r^{(f)}$ and $u_\theta^{(f)}$ from Eqs. (2.6) and (2.9) gives τ_r and τ_θ in terms of $u_r^{(s)}$, $u_\theta^{(s)}$ and w (and ε^m). Substitution of τ_r and τ_θ into Eq. 2.8 yields the following governing equation for w

$$\nabla^2 (\nabla^2 w) = -6 \frac{E_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \nabla^2 (h_f \varepsilon^m). \tag{2.11}$$

- (iii) The continuity condition Eq. 2.9 gives $u_r^{(f)}$ and $u_\theta^{(f)}$. The leading terms of the interface shear stresses τ_r and τ_θ are then obtained from Eqs. 2.6 as

$$\tau_r = -\frac{E_f}{1 - \nu_f} \frac{\partial (h_f \varepsilon^m)}{\partial r}, \quad \tau_\theta = -\frac{E_f}{1 - \nu_f} \frac{1}{r} \frac{\partial (h_f \varepsilon^m)}{\partial \theta}. \tag{2.12}$$

Eqs. (2.10)–(2.12) show that the film thickness h_f always appears together with the misfit strain ε^m . The interface shear stresses are proportional to the gradients of $h_f\varepsilon^m$, and they vanish only for uniform misfit strain and uniform film thickness. The boundary conditions at the free edge $r = R$ require that the net forces and net moments vanish,

$$N_r^{(f)} + N_r^{(s)} = 0 \quad \text{and} \quad N_{r\theta}^{(f)} + N_{r\theta}^{(s)} = 0, \tag{2.13}$$

$$M_r - \frac{h_s}{2} N_r^{(f)} = 0 \quad \text{and} \quad Q_r - \frac{1}{r} \frac{\partial}{\partial \theta} \left(M_{r\theta} - \frac{h_s}{2} N_{r\theta}^{(f)} \right) = 0. \tag{2.14}$$

3. Thin-film stresses and substrate curvatures

Eqs. (2.10)–(2.12) and boundary conditions Eqs. (2.13) and (2.14) can be solved in the same way as that for the uniform film thickness but non-uniform misfit strain (Ngo et al., 2006) by replacing the misfit strain ε^m with $h_f\varepsilon^m$, where h_f is the film thickness. We expand $h_f\varepsilon^m$ to the Fourier series as

$$h_f\varepsilon^m = \sum_{n=0}^{\infty} (h_f\varepsilon^m)_c^{(n)}(r) \cos n\theta + \sum_{n=1}^{\infty} (h_f\varepsilon^m)_s^{(n)}(r) \sin n\theta, \tag{3.1}$$

where $(h_f\varepsilon^m)_c^{(0)}(r) = \frac{1}{2\pi} \int_0^{2\pi} h_f\varepsilon^m d\theta$, $(h_f\varepsilon^m)_c^{(n)}(r) = \frac{1}{\pi} \int_0^{2\pi} h_f\varepsilon^m \cos n\theta d\theta$ ($n \geq 1$) and $(h_f\varepsilon^m)_s^{(n)}(r) = \frac{1}{\pi} \int_0^{2\pi} h_f\varepsilon^m \sin n\theta d\theta$ ($n \geq 1$).

The substrate curvatures $\kappa_{rr} = \frac{\partial^2 w}{\partial r^2}$, $\kappa_{\theta\theta} = \frac{1}{r} \frac{\partial w}{\partial r} + \frac{1}{r^2} \frac{\partial^2 w}{\partial \theta^2}$ and $\kappa_{r\theta} = \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial w}{\partial \theta} \right)$ are related to $h_f\varepsilon^m$ by

$$\kappa_{rr} + \kappa_{\theta\theta} = -12 \frac{E_f}{1 - \nu_f} \frac{1 - \nu_s}{E_s h_s^2} * \left\{ \begin{aligned} & h_f\varepsilon^m - \frac{1-\nu_s}{2} (\overline{h_f\varepsilon^m} - \overline{h_f\varepsilon^m}) \\ & + \frac{1-\nu_s}{3+\nu_s} \sum_{n=1}^{\infty} (n+1) \frac{r^n}{R^{2n+2}} \left[\cos n\theta \int_0^R \eta^{n+1} (h_f\varepsilon^m)_c^{(n)}(\eta) d\eta \right. \\ & \left. + \sin n\theta \int_0^R \eta^{n+1} (h_f\varepsilon^m)_s^{(n)}(\eta) d\eta \right] \end{aligned} \right\}, \tag{3.2a}$$

$$\kappa_{rr} - \kappa_{\theta\theta} = -6 \frac{E_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} * \left\{ \begin{aligned} & h_f\varepsilon^m - \frac{2}{r^2} \int_0^r \eta (h_f\varepsilon^m)_c^{(0)} d\eta \\ & + \frac{1-\nu_s}{3+\nu_s} \sum_{n=1}^{\infty} \frac{n+1}{R^{n+2}} \left[n \frac{r^n}{R^{n-2}} - (n-1) \frac{r^{n-2}}{R^{n-2}} \right] \left[\cos n\theta \int_0^R \eta^{n+1} (h_f\varepsilon^m)_c^{(n)} d\eta \right. \\ & \left. + \sin n\theta \int_0^R \eta^{n+1} (h_f\varepsilon^m)_s^{(n)} d\eta \right] \\ & - \sum_{n=1}^{\infty} \frac{n+1}{r^{n+2}} \left[\cos n\theta \int_0^r \eta^{n+1} (h_f\varepsilon^m)_c^{(n)} d\eta + \sin n\theta \int_0^r \eta^{n+1} (h_f\varepsilon^m)_s^{(n)} d\eta \right] \\ & - \sum_{n=1}^{\infty} (n-1) r^{n-2} \left[\cos n\theta \int_r^R \eta^{1-n} (h_f\varepsilon^m)_c^{(n)} d\eta + \sin n\theta \int_r^R \eta^{1-n} (h_f\varepsilon^m)_s^{(n)} d\eta \right] \end{aligned} \right\}, \tag{3.2b}$$

$$\kappa_{r\theta} = 3 \frac{E_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} * \left\{ \begin{aligned} & \frac{1-\nu_s}{3+\nu_s} \sum_{n=1}^{\infty} \frac{n+1}{R^{n+2}} \left[n \frac{r^n}{R^{n-2}} - (n-1) \frac{r^{n-2}}{R^{n-2}} \right] \left[\sin n\theta \int_0^R \eta^{n+1} (h_f\varepsilon^m)_c^{(n)} d\eta \right. \\ & \left. - \cos n\theta \int_0^R \eta^{n+1} (h_f\varepsilon^m)_s^{(n)} d\eta \right] \\ & + \sum_{n=1}^{\infty} \frac{n+1}{r^{n+2}} \left[\sin n\theta \int_0^r \eta^{n+1} (h_f\varepsilon^m)_c^{(n)} d\eta - \cos n\theta \int_0^r \eta^{n+1} (h_f\varepsilon^m)_s^{(n)} d\eta \right] \\ & - \sum_{n=1}^{\infty} (n-1) r^{n-2} \left[\sin n\theta \int_r^R \eta^{1-n} (h_f\varepsilon^m)_c^{(n)} d\eta - \cos n\theta \int_r^R \eta^{1-n} (h_f\varepsilon^m)_s^{(n)} d\eta \right] \end{aligned} \right\}, \tag{3.2c}$$

where $\overline{h_f\varepsilon^m} = \frac{1}{\pi R^2} \int_A h_f\varepsilon^m dA$ is the average of $h_f\varepsilon^m$ over the entire area A of the thin film, and $\overline{h_f\varepsilon^m}$ is also related to $(h_f\varepsilon^m)_c^{(0)}$ by $\overline{h_f\varepsilon^m} = \frac{2}{R^2} \int_0^R \eta (h_f\varepsilon^m)_c^{(0)}(\eta) d\eta$. The stresses in the thin film are related to $h_f\varepsilon^m$ by

$$\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} = \frac{E_f}{1 - \nu_f} (-2\varepsilon^m), \tag{3.3a}$$

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = 4E_f \frac{E_f}{1 - \nu_f^2} \frac{1 - \nu_s^2}{E_s h_s} * \left\{ \begin{aligned} & h_f \varepsilon^m - \frac{2}{r^2} \int_0^r \eta (h_f \varepsilon^m)_c^{(0)} d\eta \\ & - \sum_{n=1}^{\infty} \frac{n+1}{r^{n+2}} \left[\cos n\theta \int_0^r \eta^{n+1} (h_f \varepsilon^m)_c^{(n)} d\eta + \sin n\theta \int_0^r \eta^{n+1} (h_f \varepsilon^m)_s^{(n)} d\eta \right] \\ & - \sum_{n=1}^{\infty} (n-1) r^{n-2} \left[\cos n\theta \int_r^R \eta^{1-n} (h_f \varepsilon^m)_c^{(n)} d\eta + \sin n\theta \int_r^R \eta^{1-n} (h_f \varepsilon^m)_s^{(n)} d\eta \right] \\ & - \frac{\nu_s}{3 + \nu_s} \sum_{n=1}^{\infty} \frac{n+1}{R^{n+2}} \left[n \frac{r^n}{R^n} - (n-1) \frac{r^{n-2}}{R^{n-2}} \right] \left[\cos n\theta \int_0^R \eta^{n+1} (h_f \varepsilon^m)_c^{(n)} d\eta \right. \\ & \left. + \sin n\theta \int_0^R \eta^{n+1} (h_f \varepsilon^m)_s^{(n)} d\eta \right] \end{aligned} \right\}, \tag{3.3b}$$

$$\sigma_{r\theta}^{(f)} = 2E_f \frac{E_f}{1 - \nu_f^2} \frac{1 - \nu_s^2}{E_s h_s} * \left\{ \begin{aligned} & - \sum_{n=1}^{\infty} \frac{n+1}{r^{n+2}} \left[\sin n\theta \int_0^r \eta^{n+1} (h_f \varepsilon^m)_c^{(n)} d\eta - \cos n\theta \int_0^r \eta^{n+1} (h_f \varepsilon^m)_s^{(n)} d\eta \right] \\ & + \sum_{n=1}^{\infty} (n-1) r^{n-2} \left[\sin n\theta \int_r^R \eta^{1-n} (h_f \varepsilon^m)_c^{(n)} d\eta - \cos n\theta \int_r^R \eta^{1-n} (h_f \varepsilon^m)_s^{(n)} d\eta \right] \\ & + \frac{\nu_s}{3 + \nu_s} \sum_{n=1}^{\infty} \frac{n+1}{R^{n+2}} \left[n \frac{r^n}{R^n} - (n-1) \frac{r^{n-2}}{R^{n-2}} \right] \left[\sin n\theta \int_0^R \eta^{n+1} (h_f \varepsilon^m)_c^{(n)} d\eta \right. \\ & \left. - \cos n\theta \int_0^R \eta^{n+1} (h_f \varepsilon^m)_s^{(n)} d\eta \right] \end{aligned} \right\}. \tag{3.3c}$$

For uniform misfit strain distribution $\varepsilon^m = constant$ and uniform film thickness $h_f = constant$, the interface shear stresses in Eq. (2.12) vanish. The curvatures in Eqs. (3.2) become

$$\kappa = \kappa_{rr} = \kappa_{\theta\theta} = -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s}{E_s h_s^2} \varepsilon^m, \quad \kappa_{r\theta} = 0.$$

The stresses in the thin film in Eqs. (3.3) become

$$\sigma^{(f)} = \sigma_{rr}^{(f)} = \sigma_{\theta\theta}^{(f)} = \frac{E_f}{1 - \nu_f} (-\varepsilon^m), \quad \sigma_{r\theta}^{(f)} = 0.$$

For this special case only, both stress and curvature states become equi-biaxial. The elimination of misfit strain ε^m and film thickness h_f from the above two equations yields a simple relation $\sigma^{(f)} = \frac{E_s h_s^2}{6(1 - \nu_s) h_f} \kappa$, 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 misfit strain, film thickness, stress and curvature are all constant and if the plate system shape is spherical. In the following, we extend such a relation for arbitrary non-uniform misfit strain distribution and non-uniform film thickness.

4. Extension of Stoney formula for non-uniform misfit strain distribution and non-uniform film thickness

The stresses and curvatures are all given in terms of misfit strain in the previous section. We extend the Stoney formula for arbitrary non-uniform misfit strain distribution and non-uniform film thickness in this section by establishing the direct relation between the thin-film stresses and substrate curvatures.

Following Ngo et al. (2006), we first define the coefficients C_n and S_n related to the substrate curvatures by

$$\begin{aligned} C_n &= \frac{1}{\pi R^2} \int \int_A (\kappa_{rr} + \kappa_{\theta\theta}) \left(\frac{\eta}{R}\right)^n \cos n\varphi dA, \\ S_n &= \frac{1}{\pi R^2} \int \int_A (\kappa_{rr} + \kappa_{\theta\theta}) \left(\frac{\eta}{R}\right)^n \sin n\varphi dA, \end{aligned} \tag{4.1}$$

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 misfit strain ε^m and film thickness h_f , elimination of $h_f \varepsilon^m$ gives the film stress in terms of substrate curvatures by

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = -\frac{E_f h_s}{6(1 + \nu_f)} \left\{ 4(\kappa_{rr} - \kappa_{\theta\theta}) - \sum_{n=1}^{\infty} (n+1) \left[n \left(\frac{r}{R}\right)^n - (n-1) \left(\frac{r}{R}\right)^{n-2} \right] (C_n \cos n\theta + S_n \sin n\theta) \right\}, \tag{4.2a}$$

$$\sigma_{r\theta}^{(f)} = -\frac{E_f h_s}{6(1 + \nu_f)} \left\{ 4\kappa_{r\theta} + \frac{1}{2} \sum_{n=1}^{\infty} (n+1) \left[n \left(\frac{r}{R}\right)^n - (n-1) \left(\frac{r}{R}\right)^{n-2} \right] (C_n \sin n\theta - S_n \cos n\theta) \right\}, \tag{4.2b}$$

$$\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} = \frac{E_s h_s^2}{6h_f(1 - \nu_s)} \left[\begin{aligned} &\kappa_{rr} + \kappa_{\theta\theta} + \frac{1-\nu_s}{1+\nu_s} (\kappa_{rr} + \kappa_{\theta\theta} - \overline{\kappa_{rr} + \kappa_{\theta\theta}}) \\ &- \frac{1-\nu_s}{1+\nu_s} \sum_{n=1}^{\infty} (n+1) \left(\frac{r}{R}\right)^n (C_n \cos n\theta + S_n \sin n\theta) \end{aligned} \right], \tag{4.2c}$$

where $\overline{\kappa_{rr} + \kappa_{\theta\theta}} = C_0 = \frac{1}{\pi R^2} \int \int_A (\kappa_{rr} + \kappa_{\theta\theta}) dA$ is the average curvature over entire area A of the thin film. Eqs. (4.2) provides 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 (non-local dependence) via the coefficients C_n and S_n . It is also important to note that Eq. 4.2b for shear stress $\sigma_{r\theta}^{(f)}$ and Eq. 4.2a for the difference in normal stresses $\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)}$ are independent of the thin film thickness h_f , but Eq. 4.2c for the sum of normal stresses $\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)}$ is inversely proportional to the local film thickness h_f at the same point.

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

$$\tau_r = \frac{E_s h_s^2}{6(1 - \nu_s^2)} \left[\frac{\partial}{\partial r} (\kappa_{rr} + \kappa_{\theta\theta}) - \frac{1 - \nu_s}{2R} \sum_{n=1}^{\infty} n(n+1) (C_n \cos n\theta + S_n \sin n\theta) \left(\frac{r}{R}\right)^{n-1} \right], \tag{4.3a}$$

$$\tau_\theta = \frac{E_s h_s^2}{6(1 - \nu_s^2)} \left[\frac{1}{r} \frac{\partial}{\partial \theta} (\kappa_{rr} + \kappa_{\theta\theta}) + \frac{1 - \nu_s}{2R} \sum_{n=1}^{\infty} n(n+1) (C_n \sin n\theta - S_n \cos n\theta) \left(\frac{r}{R}\right)^{n-1} \right], \tag{4.3b}$$

which is also independent of the film thickness h_f . Eq. (4.3) provides a way to determine the interface shear stresses from the gradients of substrate curvatures, and it also displays a non-local 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, Eq. (4.3) has particular significance. It shows 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. Eq. (4.3) 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 can be shown that the relations between the film stresses and substrate curvatures given in the form of infinite series in Eqs. (4.2) and (4.3) can be equivalently expressed in the form of integration as (Ngo et al., 2006)

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = -\frac{E_f h_s}{6(1 + \nu_f)} \left\{ 4(\kappa_{rr} - \kappa_{\theta\theta}) - \frac{1}{\pi R^2} \int \int_A (\kappa_{rr} + \kappa_{\theta\theta}) \frac{\frac{\eta}{R} F_{\text{minus}}\left(\frac{r}{R}, \frac{\eta}{R}, \varphi - \theta\right)}{\left[1 - 2\frac{\eta r}{R^2} \cos(\varphi - \theta) + \frac{\eta^2 r^2}{R^4}\right]^3} dA \right\}, \tag{4.4a}$$

$$\sigma_{r\theta}^{(f)} = -\frac{E_f h_s}{6(1 + \nu_f)} \left\{ 4\kappa_{r\theta} - \frac{1}{2} \frac{1}{\pi R^2} \int \int_A (\kappa_{rr} + \kappa_{\theta\theta}) \frac{\frac{\eta}{R} F_{\text{shear}}\left(\frac{r}{R}, \frac{\eta}{R}, \varphi - \theta\right)}{\left[1 - 2\frac{\eta r}{R^2} \cos(\varphi - \theta) + \frac{\eta^2 r^2}{R^4}\right]^3} dA \right\}, \tag{4.4b}$$

$$\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} = \frac{E_s h_s^2}{6h_f(1 - \nu_s)} * \left\{ \begin{aligned} &\kappa_{rr} + \kappa_{\theta\theta} + \frac{1-\nu_s}{1+\nu_s} (\kappa_{rr} + \kappa_{\theta\theta} - \overline{\kappa_{rr} + \kappa_{\theta\theta}}) \\ &- \frac{1-\nu_s}{1+\nu_s} \frac{r}{\pi R^3} \int \int_A (\kappa_{rr} + \kappa_{\theta\theta}) \frac{\frac{\eta}{R} F_{\text{plus}}\left(\frac{r}{R}, \frac{\eta}{R}, \varphi - \theta\right)}{\left[1 - 2\frac{\eta r}{R^2} \cos(\varphi - \theta) + \frac{\eta^2 r^2}{R^4}\right]^2} dA \end{aligned} \right\}, \tag{4.4c}$$

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

$$\begin{aligned}
F_{\text{minus}}(r_1, \eta_1, \varphi_1) &= -r_1^2 \eta_1 (6 + 9\eta_1^2 + r_1^2 \eta_1^4) + r_1 (2 + 9\eta_1^2 + 6r_1^2 \eta_1^2 + 6r_1^2 \eta_1^4) \cos \varphi_1 \\
&\quad - \eta_1 (3 + 3r_1^2 \eta_1^2 + 2r_1^4 \eta_1^2) \cos 2\varphi_1 + r_1 \eta_1^2 \cos 3\varphi_1, \\
F_{\text{shear}}(r_1, \eta_1, \varphi_1) &= r_1 (2 + 9\eta_1^2 - 6r_1^2 \eta_1^2) \sin \varphi_1 - \eta_1 (3 + 3r_1^2 \eta_1^2 - 2r_1^4 \eta_1^2) \sin 2\varphi_1 + r_1 \eta_1^2 \sin 3\varphi_1, \\
F_{\text{plus}}(r_1, \eta_1, \varphi_1) &= 2(1 + 2r_1^2 \eta_1^2) \cos \varphi_1 - r_1 \eta_1 \cos 2\varphi_1 - r_1 \eta_1 (4 + r_1^2 \eta_1^2).
\end{aligned} \tag{4.5}$$

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

$$\tau_r = \frac{E_s h_s^2}{6(1 - \nu_s^2)} \left\{ \frac{\partial}{\partial r} (\kappa_{rr} + \kappa_{\theta\theta}) - \frac{1 - \nu_s}{\pi R^3} \iint_A (\kappa_{rr} + \kappa_{\theta\theta}) \frac{\frac{r}{R} F_{\text{radial}}\left(\frac{r}{R}, \frac{r}{R}, \varphi - \theta\right)}{\left[1 - 2\frac{r}{R^2} \cos(\varphi - \theta) + \frac{r^2}{R^4}\right]^3} dA \right\}, \tag{4.6a}$$

$$\tau_\theta = \frac{E_s h_s^2}{6(1 - \nu_s^2)} \left\{ \frac{1}{r} \frac{\partial}{\partial \theta} (\kappa_{rr} + \kappa_{\theta\theta}) - \frac{1 - \nu_s}{\pi R^3} \iint_A (\kappa_{rr} + \kappa_{\theta\theta}) \frac{\frac{r}{R} F_{\text{circumferential}}\left(\frac{r}{R}, \frac{r}{R}, \varphi - \theta\right)}{\left[1 - 2\frac{r}{R^2} \cos(\varphi - \theta) + \frac{r^2}{R^4}\right]^3} dA \right\}, \tag{4.6b}$$

where

$$\begin{aligned}
F_{\text{radial}}(r_1, \eta_1, \varphi_1) &= (1 + 3r_1^2 \eta_1^2) \cos \varphi_1 - r_1 \eta_1 (3 + r_1^2 \eta_1^2 \cos 2\varphi_1), \\
F_{\text{circumferential}}(r_1, \eta_1, \varphi_1) &= (1 - 3r_1^2 \eta_1^2) \sin \varphi_1 + r_1^3 \eta_1^3 \sin 2\varphi_1.
\end{aligned} \tag{4.7}$$

5. Discussion and conclusions

The Stoney formula Eq. (1.1) has been extended for non-uniform but axisymmetric temperature (Huang and Rosakis, 2005) and misfit strain (Huang et al., 2005) as well as for arbitrarily non-uniform (e.g., non-axisymmetric) temperature and misfit strain (Ngo et al., 2006). The dependence of film stresses on substrate curvatures is non-local, i.e., the stress components at a point on the film depend on both the curvature components at the same point and on the curvatures of all other points on the plate system. The presence of non-local 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 non-local 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 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.

The non-uniformities also result in the shear stresses along the thin film/substrate interface. Such interface shear stresses vanish for the special case of uniform $\kappa_{rr} + \kappa_{\theta\theta}$ in the Stoney formula 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.

The present analysis provides a very simple way to account for the effect of non-uniform film thickness on the Stoney formula. The most remarkable result is that, for arbitrarily non-uniform film thickness, the stress-curvature relations are identical to their counterparts for uniform film thickness (Huang and Rosakis, 2005; Huang et al., 2005; Ngo et al., 2006) except that thickness is replaced by its local value. For example, the sum of normal stresses $\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)}$ at a point on the film is inversely proportional to the local film thickness at the same point. Part II of this paper provides the experimental validation of this result. Feng et al. (2006) extended the Stoney formula for a thin film with uniform thickness and a radius that is smaller than the substrate radius. This can be considered as a special case of the present analysis with the film thickness being a constant in the thin film and zero (outside the film).

There may exist misfit or threading dislocations on the film/substrate interfaces at large misfit strains (e.g., Freund, 1990; Gillard et al., 1994). The results in this paper are based on linear elasticity for both the thin film and substrate, and have not accounted for the effects of misfit or threading dislocations.

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