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Spatially non-uniform, isotropic misfit strain in thin films bonded on plate substrates: The relation between non-uniform film stresses and system curvatures

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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. By considering a circular thin-film/substrate system subject to arbitrarily non-uniform misfit strain distributions, we derive relations between the film stresses and the misfit strain, and between the plate system's curvatures and the misfit strain. These relations feature a "local" part which involves a direct dependence of the stress or curvature components on the misfit strain at the same point, and a "non-local" part which reflects the effect of misfit strain of other points on the location of scrutiny. Most notably, we also derive relations between components of the film stress and those of system curvatures which allow for the experimental inference of such stresses from full-field curvature measurements in the presence of arbitrary non-uniformities. These relations also feature a "non-local" dependence on curvatures making full-field measurements of curvature a necessity for the correct inference of stress. Finally, it is shown that the interfacial shear tractions between the film and the substrate are related to the gradients of the first curvature invariant and can also be inferred experimentally.

Keywords: Thin films; Non-uniform misfit strain; Non-local stress-curvature relations; Interfacial shears

1. Introduction

Various substrates formed of suitable solid-state materials may be used as platforms to support various thin film structures. Integrated electronic circuits, integrated optical devices and optoelectronic circuits, micro-electro-mechanical systems deposited on wafers, three-dimensional electronic circuits, systems-on-a-chip structures, lithographic reticles, and flat panel display systems are examples of such thin film structures integrated on various types of plate substrates.

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

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

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Gradient Sensing) interferometry have been used to measure the spatial distribution of stresses (or strains) [2].

Stress changes in thin films following discrete process steps or occurring during thermal excursions may be calculated in principle from changes in the film/substrate systems curvatures or "bow" based on analytical correlations between such quantities. Early attempts to provide such correlations are well documented [3]. Various formulations have been developed for this purpose and most of these are essentially extensions of Stoney's approximate plate analysis [4].

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

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

In the above the subscripts "f" and "s" denote the thin film and substrate, respectively, and E and ν are the Young's modulus and Poisson's ratio. Eq. (1.1), known as Stoney formula, has been extensively used in the literature to infer film stress changes from experimental measurement of system curvature changes [3].

Stoney's formula was derived for an isotropic "thin" solid film of uniform thickness deposited on a much "thicker" plate substrate based on a number of assumptions. Stoney's assumptions include the following: (1) both the film thickness h_f and the substrate thickness h_s are uniform and $h_f \ll h_s \ll R$, where R represents the characteristic length in the lateral direction (e.g., system radius R shown in Fig. 1); (2) the strains and rotations of the plate system are infinitesimal; (3) both the film and substrate are homogeneous, isotropic, and linearly elastic; (4) the film stress states are in-plane isotropic or 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; (5) the system's curvature components are equi-biaxial (two equal direct curvatures) while the twist curvature vanishes in all directions; and (6) all surviving stress and curvature components are spatially constant over the plate system's surface, a situation which is often violated in practice.

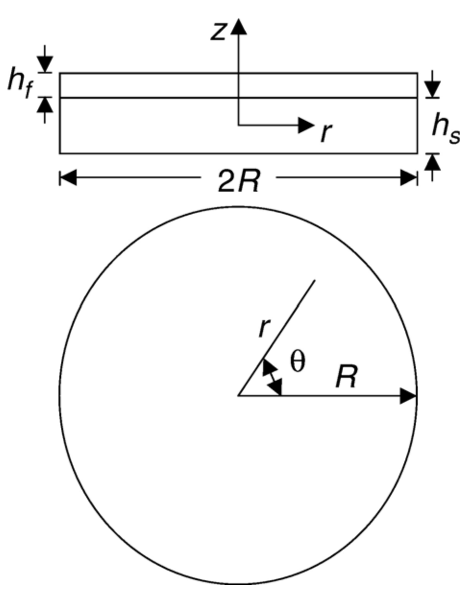

Fig. 1. A schematic diagram of the thin film/substrate system, showing the cylindrical coordinates (r, θ, z).

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

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

Following the initial formulation by Stoney, a number of extensions have been derived by various researchers who have relaxed some of the other assumptions (other than the assumption of uniformity) made by his analysis. 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, appropriate for anisotropic film stresses, including different stress values at two different directions and non-zero, in-plane shear stresses, was derived by relaxing the assumption of curvature equi-biaxiality [3]. Related analyses treating discontinuous films in the form of bare periodic lines [5] or composite films with periodic line structures (e.g., bare or encapsulated periodic lines) have also been derived [6–8]. These latter analyses have also removed the assumption 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 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 [9–12]. These analyses have removed both the restrictions of an equi-biaxial curvature state as well as the assumption of infinitesimal deformations. They have allowed for the prediction of kinematically nonlinear behavior and bifurcations in curvature states. These bifurcations are transformations from an initially 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 of spatial curvature and stress uniformity across the system. However, they allow for deformations to evolve from an initially spherical shape to an energetically favored shape (e.g., ellipsoidal, cylindrical or saddle shapes) which features three different, still spatially constant, curvature components [13].

None of the above-discussed extensions of Stoney's methodology have relaxed the most restrictive of Stoney's original assumption of spatial uniformity which does not allow either film stress or curvature components to vary across the plate surface. This crucial assumption is often violated in practice since film stresses and the associated system curvatures are non-uniformly distributed over the plate area. Huang and Rosakis [14] and Huang et al. [15] have recently made progress to remove the two restrictive assumptions of the Stoney analysis relating to spatial uniformity and equi-biaxiality. They have studied the cases of thin film/substrate systems subject to non-uniform but axisymmetric temperature distribution $T(r)$ and misfit strain $\varepsilon_m(r)$, respectively. Their results show that the relations between film stresses and substrate curvatures feature not only a "local" part which involves a direct dependence of stresses on curvatures at the same point, but also a "non-local" part which reflects of the effect of curvatures at other points on the location of scrutiny. The "non-local" effect comes into play in the axisymmetric analysis via the average curvature in the thin film. The most recent and perhaps the most comprehensive analysis to date of non-uniformities can be found in the work of Huang et al. [15] where the most general case of temperature induced spatial non-uniformities was analyzed. In this case the cause of film and substrate stresses as well as system curvatures was an "arbitrary" temperature distribution $T(r,\theta)$ acting on the system. The results of this generalization are substantially much more complicated than those of the axisymmetric case $T(r)$ but have a very similar structure. As perhaps expected they can be decomposed to a "local" or "Stoney-like" part, and a non-local part. The first term of the non-local part is identical in structure to that of the axisymmetric prediction while the rest is given in terms of an infinite series of terms of diminishing strength.

The generalization of the axisymmetric misfit strain $\varepsilon_m(r)$ to an arbitrarily varying misfit strain $\varepsilon_m(r,\theta)$ is the subject of the present investigation. Indeed, the main purpose of the present paper is to remove the two restrictive assumptions of the Stoney analysis relating to stress and curvature spatial uniformity and to in-plane isotropic equi-biaxiality for the general case of a thin film/substrate system subject to an arbitrarily varying misfit strain distribution $\varepsilon_m(r,\theta)$ whose presence will create an arbitrary stress and curvature field as well as arbitrarily large stress and curvature gradients. It should be noted that although spatially varying, this misfit strain is locally assumed to be in-plane isotropic. As we will see later, and as obvious from the axisymmetric case, this does not imply that the stress state is also in-plane isotropic. 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 for spatially varying, in-plane isotropic misfit strain distributions. Such a relation would allow for the accurate experimental inference of accumulated film stress from full-field curvature measurements which may take place following various processing steps (on-line monitoring).

Although many important features of the two solutions, corresponding to $T(r,\theta)$ or $\varepsilon_m(r,\theta)$ non-uniformities are expected to be similar, some fundamental differences between these two situations are also anticipated. Perhaps the easiest way to rationalize this from a physical point of view is to recall that for the former case the driving force for system curvature is the temperature distribution while for the latter case it is the misfit strain between film and substrate. In the former case, both the film and the substrate are each subjected to $T(r,\theta)$ and even if not bonded they independently develop non-uniform deformation and stress states. These states need to be further reconsidered due to eventual film/substrate bonding (continuity of displacements across the interface). In the latter case however, it is the film misfit strain which induces the system deformations and the film and substrate stress. In the limit of zero film thickness the system and substrate stresses and deformations vanish. This is not true however when instead a non-uniform temperature is prescribed. When the limit is considered in this case the bare substrate still involves non-zero stresses and deformations. As a result of this there seems to be "additional" interactions and coupling between the film and the substrate which are only active when a non-uniform temperature film is in existence. The practical implications of the above are as follows: during processes, such as various anneal or cooling steps when the temperature varies with time and across a film/substrate system, the former analysis is appropriate and should be used for the in-situ, real-time monitoring of film stress, through full-field curvature measurement. However, after the end of a process when the temperature field has equilibrated to a uniform state, the latter analysis is of relevance. Here the goal is the measurement of permanent (residual) stresses which have been locked in the film through the process and its non-uniformities. The latter analysis is also relevant for the study of non-uniform stress build up or relieve in cases where temperature is not involved. These include certain types of film deposition, etching or polishing process all of which can be monitored by means of on-line full field curvature measurement methods.

2. Governing equations

Consider a thin film of thickness h_f which is deposited on a circular substrate of thickness h_s and radius R such that $h_f \ll h_s \ll R$. A thin film is subject to arbitrary misfit strain distribution $\varepsilon^m(r,\theta)$, where r and θ are the polar coordinates (Fig. 1). 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. The substrate is modeled as a plate since it can be subjected to bending, and $h_s \ll R$. The thin film is modeled as a membrane which cannot be subject to bending due to its small thickness $h_f \ll h_s$.

Let $u_r^{(\mathrm{f})}$ and $u_\theta^{(\mathrm{f})}$ denote the displacements in the radial (r) and circumferential (θ) directions. The strains in the thin film are $\varepsilon_{rr}=\frac{\partial u_r^{(\mathrm{f})}}{\partial r}$, $\varepsilon_{\theta\theta}=\frac{u_r^{(\mathrm{f})}}{r}+\frac{1}{r}\frac{\partial u_\theta^{(\mathrm{f})}}{\partial\theta}$, and $\gamma_{r\theta}=\frac{1}{r}\frac{\partial u_r^{(\mathrm{f})}}{\partial\theta}+\frac{\partial u_\theta^{(\mathrm{f})}}{\partial r}-\frac{u_\theta^{(\mathrm{f})}}{r}$. The strains in the film are related to the stresses and the misfit strain ε^m by $\varepsilon_{ij}=\frac{1}{E_\mathrm{f}}[(1+v_f)\sigma_{ij}-v_f\sigma_{kk}\delta_{ij}]+\varepsilon^m\delta_{ij}$ via the linear elastic constitutive model, which can be equivalently written as

$$\begin{aligned}
\sigma_{rr}&=\frac{E_\mathrm{f}}{1-v_\mathrm{f}^2}\left[\frac{\partial u_r^{(\mathrm{f})}}{\partial r}+v_\mathrm{f}\left(\frac{u_r^{(\mathrm{f})}}{r}+\frac{1}{r}\frac{\partial u_\theta^{(\mathrm{f})}}{\partial\theta}\right)-(1+v_f)\varepsilon^m\right],\\
\sigma_{\theta\theta}&=\frac{E_\mathrm{f}}{1-v_\mathrm{f}^2}\left[v_\mathrm{f}\frac{\partial u_r^{(\mathrm{f})}}{\partial r}+\frac{u_r^{(\mathrm{f})}}{r}+\frac{1}{r}\frac{\partial u_\theta^{(\mathrm{f})}}{\partial\theta}-(1+v_\mathrm{f})\varepsilon^m\right],\\
\sigma_{r\theta}&=\frac{E_\mathrm{f}}{2(1+v_\mathrm{f})}\left(\frac{1}{r}\frac{\partial u_r^{(\mathrm{f})}}{\partial\theta}+\frac{\partial u_\theta^{(\mathrm{f})}}{\partial r}-\frac{u_\theta^{(\mathrm{f})}}{r}\right).
\end{aligned}\tag{2.1}$$

The membrane forces in the thin film are

$$N_r^{(\mathrm{f})}=h_\mathrm{f}\sigma_{rr},N_\theta^{(\mathrm{f})}=h_\mathrm{f}\sigma_{\theta\theta},N_{r\theta}^{(\mathrm{f})}=h_\mathrm{f}\sigma_{r\theta}.\tag{2.2}$$

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

$$\begin{aligned}
&\frac{\partial N_r^{(\mathrm{f})}}{\partial r}+\frac{N_r^{(\mathrm{f})}-N_\theta^{(\mathrm{f})}}{r}+\frac{1}{r}\frac{\partial N_{r\theta}^{(\mathrm{f})}}{\partial\theta}-\tau_r=0,\\
&\frac{\partial N_{r\theta}^{(\mathrm{f})}}{\partial r}+\frac{2}{r}N_{r\theta}^{(\mathrm{f})}+\frac{1}{r}\frac{\partial N_\theta^{(\mathrm{f})}}{\partial\theta}-\tau_\theta=0.
\end{aligned}\tag{2.3}$$

The substitution of Eqs. (2.1) and (2.2) into (2.3) yields the following governing equations for $u_r^{(\mathrm{f})}$,$u_\theta^{(\mathrm{f})}$,τ_r and τ_θ

$$\begin{aligned}
&\frac{\partial^2 u_r^{(\mathrm{f})}}{\partial r^2}+\frac{1}{r}\frac{\partial u_r^{(\mathrm{f})}}{\partial r}-\frac{u_r^{(\mathrm{f})}}{r^2}+\frac{1-v_\mathrm{f}}{2}\frac{1}{r^2}\frac{\partial^2 u_r^{(\mathrm{f})}}{\partial\theta^2}+\frac{1+v_\mathrm{f}}{2}\frac{1}{r}\frac{\partial^2 u_\theta^{(\mathrm{f})}}{\partial r\partial\theta}\\
&\qquad-\frac{3-v_\mathrm{f}}{2}\frac{1}{r^2}\frac{\partial u_\theta^{(\mathrm{f})}}{\partial\theta}=\frac{1-v_\mathrm{f}^2}{E_\mathrm{f}h_\mathrm{f}}\tau_r+(1+v_\mathrm{f})\frac{\partial\varepsilon^m}{\partial r},\\
&\frac{1+v_\mathrm{f}}{2}\frac{1}{r}\frac{\partial^2 u_r^{(\mathrm{f})}}{\partial r\partial\theta}+\frac{3-v_\mathrm{f}}{2}\frac{1}{r^2}\frac{\partial u_r^{(\mathrm{f})}}{\partial\theta}\\
&\qquad+\frac{1-v_\mathrm{f}}{2}\left(\frac{\partial^2 u_\theta^{(\mathrm{f})}}{\partial r^2}+\frac{1}{r}\frac{\partial u_\theta^{(\mathrm{f})}}{\partial r}-\frac{u_\theta^{(\mathrm{f})}}{r^2}\right)\\
&\qquad+\frac{1}{r^2}\frac{\partial^2 u_\theta^{(\mathrm{f})}}{\partial\theta^2}=\frac{1-v_\mathrm{f}^2}{E_\mathrm{f}h_\mathrm{f}}\tau_\theta+(1+v_\mathrm{f})\frac{1}{r}\frac{\partial\varepsilon^m}{\partial\theta}.
\end{aligned}\tag{2.4}$$

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

$$\begin{aligned}
\varepsilon_{rr}&=\frac{\partial u_r^{(\mathrm{s})}}{\partial r}-z\frac{\partial^2 w}{\partial r^2},\\
\varepsilon_{\theta\theta}&=\frac{u_r^{(\mathrm{s})}}{r}+\frac{1}{r}\frac{\partial u_\theta^{(\mathrm{s})}}{\partial\theta}-z\left(\frac{1}{r}\frac{\partial w}{\partial r}+\frac{1}{r^2}\frac{\partial^2 w}{\partial\theta^2}\right),\\
\gamma_{r\theta}&=\frac{1}{r}\frac{\partial u_r^{(\mathrm{s})}}{\partial\theta}+\frac{\partial u_\theta^{(\mathrm{s})}}{\partial r}-\frac{u_\theta^{(\mathrm{s})}}{r}-2z\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial w}{\partial\theta}\right).
\end{aligned}\tag{2.5}$$

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

$$\begin{aligned}
\sigma_{rr}&=\frac{E_\mathrm{s}}{1-v_\mathrm{s}^2}\left\{\frac{\partial u_r^{(\mathrm{s})}}{\partial r}+v_\mathrm{s}\left(\frac{u_r^{(\mathrm{s})}}{r}+\frac{1}{r}\frac{\partial u_\theta^{(\mathrm{s})}}{\partial\theta}\right)-z\left[\frac{\partial^2 w}{\partial r^2}+v_\mathrm{s}\left(\frac{1}{r}\frac{\partial w}{\partial r}+\frac{1}{r^2}\frac{\partial^2 w}{\partial\theta^2}\right)\right]\right\},\\
\sigma_{\theta\theta}&=\frac{E_\mathrm{s}}{1-v_\mathrm{s}^2}\left[v_\mathrm{s}\frac{\partial u_r^{(\mathrm{s})}}{\partial r}+\frac{u_r^{(\mathrm{s})}}{r}+\frac{1}{r}\frac{\partial u_\theta^{(\mathrm{s})}}{\partial\theta}-z\left(v_\mathrm{s}\frac{\partial^2 w}{\partial r^2}+\frac{1}{r}\frac{\partial w}{\partial r}+\frac{1}{r^2}\frac{\partial^2 w}{\partial\theta^2}\right)\right],\\
\sigma_{r\theta}&=\frac{E_\mathrm{s}}{2(1+v_\mathrm{s})}\left[\frac{1}{r}\frac{\partial u_r^{(\mathrm{s})}}{\partial\theta}+\frac{\partial u_\theta^{(\mathrm{s})}}{\partial r}-\frac{u_\theta^{(\mathrm{s})}}{r}-2z\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial w}{\partial\theta}\right)\right].
\end{aligned}\tag{2.6}$$

The forces and bending moments in the substrate are

$$\begin{aligned}
N_r^{(\mathrm{s})}&=\int_{-\frac{h_\mathrm{s}}{2}}^{\frac{h_\mathrm{s}}{2}}\sigma_{rr}\mathrm{d}z=\frac{E_\mathrm{s}h_\mathrm{s}}{1-v_\mathrm{s}^2}\left[\frac{\partial u_r^{(\mathrm{s})}}{\partial r}+v_\mathrm{s}\left(\frac{u_r^{(\mathrm{s})}}{r}+\frac{1}{r}\frac{\partial u_\theta^{(\mathrm{s})}}{\partial\theta}\right)\right],\\
N_\theta^{(\mathrm{s})}&=\int_{-\frac{h_\mathrm{s}}{2}}^{\frac{h_\mathrm{s}}{2}}\sigma_{\theta\theta}\mathrm{d}z=\frac{E_\mathrm{s}h_\mathrm{s}}{1-v_\mathrm{s}^2}\left(v_\mathrm{s}\frac{\partial u_r^{(\mathrm{s})}}{\partial r}+\frac{u_r^{(\mathrm{s})}}{r}+\frac{1}{r}\frac{\partial u_\theta^{(\mathrm{s})}}{\partial\theta}\right),\\
N_{r\theta}^{(\mathrm{s})}&=\int_{-\frac{h_\mathrm{s}}{2}}^{\frac{h_\mathrm{s}}{2}}\sigma_{r\theta}\mathrm{d}z=\frac{E_\mathrm{s}h_\mathrm{s}}{2(1+v_\mathrm{s})}\left(\frac{1}{r}\frac{\partial u_r^{(\mathrm{s})}}{\partial\theta}+\frac{\partial u_\theta^{(\mathrm{s})}}{\partial r}-\frac{u_\theta^{(\mathrm{s})}}{r}\right).
\end{aligned}\tag{2.7}$$

$$\begin{aligned}
M_r&=-\int_{-\frac{h_\mathrm{s}}{2}}^{\frac{h_\mathrm{s}}{2}}z\sigma_{rr}\mathrm{d}z=\frac{E_\mathrm{s}h_\mathrm{s}^3}{12(1-v_\mathrm{s}^2)}\left[\frac{\partial^2 w}{\partial r^2}+v_\mathrm{s}\left(\frac{1}{r}\frac{\partial w}{\partial r}+\frac{1}{r^2}\frac{\partial^2 w}{\partial\theta^2}\right)\right],\\
M_\theta&=-\int_{-\frac{h_\mathrm{s}}{2}}^{\frac{h_\mathrm{s}}{2}}z\sigma_{\theta\theta}\mathrm{d}z=\frac{E_\mathrm{s}h_\mathrm{s}^3}{12(1-v_\mathrm{s}^2)}\left(v_\mathrm{s}\frac{\partial^2 w}{\partial r^2}+\frac{1}{r}\frac{\partial w}{\partial r}+\frac{1}{r^2}\frac{\partial^2 w}{\partial\theta^2}\right),\\
M_{r\theta}&=-\int_{-\frac{h_\mathrm{s}}{2}}^{\frac{h_\mathrm{s}}{2}}z\sigma_{r\theta}\mathrm{d}z=\frac{E_\mathrm{s}h_\mathrm{s}^3}{12(1+v_\mathrm{s})}\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial w}{\partial\theta}\right).
\end{aligned}\tag{2.8}$$

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

$$\begin{aligned}
&\frac{\partial N_r^{(\mathrm{s})}}{\partial r}+\frac{N_r^{(\mathrm{s})}-N_\theta^{(\mathrm{s})}}{r}+\frac{1}{r}\frac{\partial N_{r\theta}^{(\mathrm{s})}}{\partial\theta}+\tau_r=0,\\
&\frac{\partial N_{r\theta}^{(\mathrm{s})}}{\partial r}+\frac{2}{r}N_{r\theta}^{(\mathrm{s})}+\frac{1}{r}\frac{\partial N_{\theta\theta}^{(\mathrm{s})}}{\partial\theta}+\tau_\theta=0.
\end{aligned}\tag{2.9}$$

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

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

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

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

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

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

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

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

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

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

Eqs. (2.4) and Please split and link these to Eqs. (2.12)–(2.14) constitute seven ordinary differential equations for seven variables, namely $u_r^{(f)}$, $u_\theta^{(f)}$, $u_r^{(s)}$, $u_\theta^{(s)}$, w, τ_r and τ_θ. We discuss in the following how to decouple these seven equations under the limit $h_f/h_s\ll 1$ such that we can solve $u_r^{(s)}$, $u_\theta^{(s)}$ first, then 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 force equilibrium equations (2.4) for the thin film and (2.12) for the substrate yields two equations for $u_r^{(f)}$, $u_\theta^{(f)}$, $u_r^{(s)}$ and $u_\theta^{(s)}$. For $h_f/h_s\ll 1$, $u_r^{(f)}$ and $u_\theta^{(f)}$ disappear in these two equations, which become the following governing equations for $u_r^{(s)}$ and $u_\theta^{(s)}$ only,

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

The substrate displacements $u_r^{(s)}$ and $u_\theta^{(s)}$ are on the order of h_f/h_s.

(ii) Elimination of $u_r^{(f)}$ and $u_\theta^{(f)}$ from the continuity condition (2.14) and equilibrium equation (2.4) for the thin film gives τ_r and τ_θ in terms of $u_r^{(s)}$, $u_\theta^{(s)}$ and w (and ε^m).

(iii) The substitution of the above τ_r and τ_θ into the moment equilibrium Eq. (2.13) yields the governing equation for the normal displacement w. For $h_f/h_s\ll 1$, this governing equation takes the form

$$\nabla^2(\nabla^2 w)=-6\frac{E_fh_f}{1-\nu_f}\frac{1-\nu_s^2}{E_sh_s^2}\nabla^2\varepsilon^m.\tag{2.16}$$

This is a biharmonic equation which can be solved analytically. The substrate displacement w is on the order of h_f/h_s.

(iv) The displacements $u_r^{(f)}$ and $u_\theta^{(f)}$ in the thin film are obtained from Eq. (2.14), and they are also on the same order h_f/h_s as $u_r^{(s)}$, $u_\theta^{(s)}$ and w. The leading terms of the interface shear stresses τ_r and τ_θ are then obtained from Eq. (2.4) as

$$\tau_r=-\frac{E_fh_f}{1-\nu_f}\frac{\partial\varepsilon^m}{\partial r},\quad \tau_\theta=-\frac{E_fh_f}{1-\nu_f}\frac{1}{r}\frac{\partial\varepsilon^m}{\partial\theta}.\tag{2.17}$$

These are remarkable results that hold regardless of boundary conditions at the edge $r=R$. Therefore the interface shear stresses are proportional to the gradients of misfit strain. For uniform misfit strain the interface shear stresses vanish.

We expand the arbitrary non-uniform misfit strain distribution $\varepsilon^m(r,\theta)$ to the Fourier series,

$$\varepsilon^m(r,\theta)=\sum_{n=0}^{\infty}\varepsilon_c^{m(n)}(r)\cos n\theta+\sum_{n=1}^{\infty}\varepsilon_s^{m(n)}(r)\sin n\theta,\tag{2.18}$$

where$\varepsilon_c^{m(0)}(r)=\frac{1}{2\pi}\int_0^{2\pi}\varepsilon^m(r,\theta)\mathrm{d}\theta$,$\varepsilon_c^{m(n)}(r)=\frac{1}{\pi}\int_0^{2\pi}\varepsilon^m(r,\theta)\cos n\theta\mathrm{d}\theta$ ($n\geq 1$) and $\varepsilon_s^{m(n)}(r)=\frac{1}{\pi}\int_0^{2\pi}\varepsilon^m(r,\theta)\sin n\theta\mathrm{d}\theta$ ($n\geq 1$). Without losing generality, we focus on the cos $n\theta$ term here. The corresponding displacements can be expressed as

$$\begin{aligned}&u_r^{(s)}=u_r^{(sn)}(r)\cos n\theta,\ u_\theta^{(s)}=u_\theta^{(sn)}(r)\sin n\theta,\\&w=w^{(n)}(r)\cos n\theta.\end{aligned}\tag{2.19}$$

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

$$\begin{aligned}\begin{Bmatrix}u_r^{(sn)}\\u_\theta^{(sn)}\end{Bmatrix}=&\begin{Bmatrix}1-\nu_s-\frac{1+\nu_s}{2}n\\\frac{1+\nu_s}{2}n+2\end{Bmatrix}\left[A_0r^{n+1}+\frac{E_fh_f}{1-\nu_f}\frac{1+\nu_s}{E_sh_s}\frac{1}{4(n+1)}r\varepsilon_c^{m(n)}\right]\\&+\begin{Bmatrix}1\\1\end{Bmatrix}\left\langle\frac{E_fh_f}{1+\nu_f}\frac{1+\nu_s}{E_sh_s}\frac{1}{4(n+1)}\begin{Bmatrix}-\left[1-\nu_s-\frac{n}{2}(1+\nu_s)\right]r\varepsilon_c^{m(n)}\\+2(1-\nu_s)(n+1)\frac{1}{r^{n+1}}\int_0^r\eta^{1+n}\varepsilon_c^{m(n)}(\eta)\mathrm{d}\eta\end{Bmatrix}\right\rangle\\&-\begin{Bmatrix}1-\nu_s+\frac{1+\nu_s}{2}n\\\frac{1+\nu_s}{2}n-2\end{Bmatrix}\frac{E_fh_f}{1-\nu_f}\frac{1+\nu_s}{E_sh_s}\frac{1}{4(n-1)}r\varepsilon_c^{m(n)}\\&+\begin{Bmatrix}-1\\1\end{Bmatrix}\left\langle D_0r^{n-1}-\frac{E_fh_f}{1-\nu_f}\frac{1+\nu_s}{E_sh_s}\frac{1}{4(n-1)}\begin{Bmatrix}\left[1-\nu_s+\frac{n}{2}(1+\nu_s)\right]r\varepsilon_c^{m(n)}\\-2(1-\nu_s)(n-1)r^{n-1}\int_r^R\eta^{1-n}\varepsilon_c^{m(n)}(\eta)\mathrm{d}\eta\end{Bmatrix}\right\rangle\\&+O\left(\frac{h_f^2}{h_s^2}\right),\end{aligned}\tag{2.20}$$

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

The normal displacement w is obtained from the biharmonic Eq. (2.16) as

$$w^{(n)} = A_1 r^{n+2} + B_1 r^n + \frac{3}{n}\frac{1-\nu_s^2}{E_s h_s^2}\frac{E_f h_f}{1-\nu_f}\left[r^n \int_r^R \eta^{1-n}\varepsilon_c^{m(n)}(\eta)\mathrm{d}\eta + r^{-n}\int_0^r \eta^{n+1}\varepsilon_c^{m(n)}(\eta)\mathrm{d}\eta\right] + O\left(\frac{h_f^2}{h_s^2}\right), \quad (2.21)$$

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

3. Boundary conditions

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

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

which give A_0 and D_0 as

$$A_0 = \frac{E_f h_f}{1-\nu_f}\frac{1-\nu_s}{E_s h_s}\frac{1}{R^{2n+2}}\int_0^R \eta^{n+1}\varepsilon_c^{m(n)}(\eta)\mathrm{d}\eta + O\left(\frac{h_f^2}{h_s^2}\right),$$
$$D_0 = -\frac{E_f h_f}{1-\nu_f}\frac{1-\nu_s^2}{E_s h_s}\frac{n+1}{2R^{2n}}\int_0^R \eta^{n+1}\varepsilon_c^{m(n)}(\eta)\mathrm{d}\eta + O\left(\frac{h_f^2}{h_s^2}\right) \quad (3.2)$$

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

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

which give A_1 and B_1 as

$$A_1 = -\frac{3(1-\nu_s)}{3+\nu_s}\frac{E_f h_f}{1-\nu_f}\frac{1-\nu_s^2}{E_s h_s^2}\frac{1}{R^{2n+2}}\int_0^R \eta^{n+1}\varepsilon_c^{m(n)}(\eta)\mathrm{d}\eta + O\left(\frac{h_f^2}{h_s^2}\right),$$
$$B_1 = -\frac{n+1}{n}R^2 A_1 + O\left(\frac{h_f^2}{h_s^2}\right). \quad (3.4)$$

It is important to point out that the boundary conditions can also be established from the variational principle [12]. The total potential energy in the thin film/substrate system with the free edge at $r=R$ is

$$\Pi = \int_0^R r\mathrm{d}r \int_0^{2\pi} \mathrm{d}\theta \int_{-\frac{h_s}{2}}^{\frac{h_s}{2}+h_f} U\mathrm{d}z, \quad (3.5)$$

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

$$U = \frac{E}{2(1-\nu^2)}\left[\varepsilon_{rr}^2 + \varepsilon_{\theta\theta}^2 + 2\nu\varepsilon_{rr}\varepsilon_{\theta\theta} + \frac{1-\nu}{2}\gamma_{r\theta}^2 - 2(1+\nu)\varepsilon^m(\varepsilon_{rr}+\varepsilon_{\theta\theta})\right], \quad (3.6)$$

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

$$\frac{\partial \Pi}{\partial A_0} = 0, \frac{\partial \Pi}{\partial D_0} = 0, \frac{\partial \Pi}{\partial A_1} = 0 \text{ and } \frac{\partial \Pi}{\partial B_1} = 0. \quad (3.7)$$

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

4. Thin-film stresses and substrate curvatures

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

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

The sum of substrate curvatures is related to the misfit strain by

$$\kappa_{rr} + \kappa_{\theta\theta} = -12\frac{E_f h_f}{1-\nu_f}\frac{1-\nu_s}{E_s h_s^2} * \left\{ \begin{array}{l} \varepsilon^m - \frac{1-\nu_s}{2}(\varepsilon^m - \overline{\varepsilon^m}) + \frac{1-\nu_s^2}{3+\nu_s}\sum_{n=1}^{\infty}(n+1)\frac{r^n}{R^{2n+2}} \\ \times\left[\cos n\theta \int_0^R \eta^{n+1}\varepsilon_c^{m(n)}(\eta)\mathrm{d}\eta + \sin n\theta \int_0^R \eta^{n+1}\varepsilon_s^{m(n)}(\eta)\mathrm{d}\eta\right] \end{array} \right\}, \quad (4.2)$$

where $\overline{\varepsilon^m} = \frac{1}{\pi R^2}\iint_A \varepsilon^m(\eta,\varphi)\mathrm{d}A$ is the average misfit strain over the entire area A of the thin film, $\mathrm{d}A = \eta\mathrm{d}\eta\mathrm{d}\varphi$, and ε^m is also related to $\varepsilon_c^{m(0)}$ by $\overline{\varepsilon^m} = \frac{2}{R^2}\int_0^R \eta\varepsilon_c^{m(0)}(\eta)\mathrm{d}\eta$. The difference between two curvatures, $\kappa_{rr} - \kappa_{\theta\theta}$, and the twist $\kappa_{r\theta}$ are given by

$$\kappa_{rr} - \kappa_{\theta\theta} = -6\frac{E_f h_f}{1-\nu_f}\frac{1-\nu_s^2}{E_s h_s^2} * \left\{ \begin{array}{l} \varepsilon^m - \frac{2}{r^2}\int_0^r \eta\varepsilon_c^{m(0)}\mathrm{d}\eta + \frac{1-\nu_s}{3+\nu_s}\sum_{n=1}^{\infty}\frac{n+1}{R^{n+2}}\left[n\frac{r^n}{R^n} - (n-1)\frac{r^{n-2}}{R^{n-2}}\right] \\ \times\left(\cos n\theta\int_0^R \eta^{n+1}\varepsilon_c^{m(n)}\mathrm{d}\eta + \sin n\theta\int_0^R \eta^{n+1}\varepsilon_s^{m(n)}\mathrm{d}\eta\right) \\ -\sum_{n=1}^{\infty}\frac{n+1}{r^{n+2}}\left(\cos n\theta\int_0^r \eta^{n+1}\varepsilon_c^{m(n)}\mathrm{d}\eta + \sin n\theta\int_0^r \eta^{n+1}\varepsilon_s^{m(n)}\mathrm{d}\eta\right) \\ -\sum_{n=1}^{\infty}(n-1)r^{n-2}\left(\cos n\theta\int_0^R \eta^{1-n}\varepsilon_c^{m(n)}\mathrm{d}\eta + \sin n\theta\int_r^R \eta^{1-n}\varepsilon_s^{m(n)}\mathrm{d}\eta\right) \end{array} \right\} \quad (4.3)$$

$$\kappa_{r\theta} = 3\frac{E_f h_f}{1-\nu_f}\frac{1-\nu_s^2}{E_s h_s^2} * \left\{ \begin{array}{l} \frac{1-\nu_s}{3+\nu_s}\sum_{n=1}^{\infty}\frac{n+1}{R^{n+2}}\left[n\frac{r^n}{R^n} - (n-1)\frac{r^{n-2}}{R^{n-2}}\right] \\ \times\left(\sin n\theta\int_0^R \eta^{n+1}\varepsilon_c^{m(n)}\mathrm{d}\eta - \cos n\theta\int_0^R \eta^{n+1}\varepsilon_s^{m(n)}\mathrm{d}\eta\right) \\ +\sum_{n=1}^{\infty}\frac{n+1}{r^{n+2}}\left(\sin n\theta\int_0^r \eta^{n+1}\varepsilon_c^{m(n)}\mathrm{d}\eta - \cos n\theta\int_0^r \eta^{n+1}\varepsilon_s^{m(n)}\mathrm{d}\eta\right) \\ -\sum_{n=1}^{\infty}(n-1)r^{n-2}\left(\sin n\theta\int_r^R \eta^{1-n}\varepsilon_c^{m(n)}\mathrm{d}\eta - \cos n\theta\int_r^R \eta^{1-n}\varepsilon_s^{m(n)}\mathrm{d}\eta\right) \end{array} \right\} \quad (4.4)$$

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

$$\sigma_{rr}^{(f)}+\sigma_{\theta\theta}^{(f)}=\frac{E_f}{1-\nu_f}(-2\varepsilon^m). \tag{4.5}$$

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

$$\sigma_{rr}^{(f)}-\sigma_{\theta\theta}^{(f)}=4E_f\frac{E_fh_f}{1-\nu_f^2}\frac{1-\nu_s^2}{E_sh_s} * \left\{\begin{array}{l}\varepsilon^m-\frac{2}{r^2}\int_0^r\eta\varepsilon_c^{m(0)}d\eta-\sum_{n=1}^{\infty}\frac{n+1}{r^{n+2}}\\ \times\left(\cos n\theta\int_0^r\eta^{n+1}\varepsilon_c^{m(n)}d\eta+\sin n\theta\int_0^r\eta^{n+1}\varepsilon_s^{m(n)}d\eta\right)\\ -\sum_{n=1}^{\infty}(n-1)r^{n-2}\left(\cos n\theta\int_r^R\eta^{1-n}\varepsilon_c^{m(n)}d\eta+\sin n\theta\int_r^R\eta^{1-n}\varepsilon_s^{m(n)}d\eta\right)\\ -\frac{\nu_s}{3+\nu_s}\sum_{n=1}^{\infty}\frac{n+1}{R^{n+2}}\left[n\frac{r^n}{R^n}-(n-1)\frac{r^{n-2}}{R^{n-2}}\right]\\ \times\left(\cos n\theta\int_0^R\eta^{n+1}\varepsilon_c^{m(n)}d\eta+\sin n\theta\int_0^R\eta^{n+1}\varepsilon_s^{m(n)}d\eta\right)\end{array}\right\} \tag{4.6}$$

$$\sigma_{r\theta}^{(f)}=2E_f\frac{E_fh_f}{1-\nu_f^2}\frac{1-\nu_s^2}{E_sh_s} * \left\{\begin{array}{l}-\sum_{n=1}^{\infty}\frac{n+1}{r^{n+2}}\left(\sin n\theta\int_0^r\eta^{n+1}\varepsilon_c^{m(n)}d\eta-\cos n\theta\int_0^r\eta^{n+1}\varepsilon_s^{m(n)}d\eta\right)\\ +\sum_{n=1}^{\infty}(n-1)r^{n-2}\left(\sin n\theta\int_r^R\eta^{1-n}\varepsilon_c^{m(n)}d\eta-\cos n\theta\int_r^R\eta^{1-n}\varepsilon_s^{m(n)}d\eta\right)\\ +\frac{\nu_s}{3+\nu_s}\sum_{n=1}^{\infty}\frac{n+1}{R^{n+2}}\left[n\frac{r^n}{R^n}-(n-1)\frac{r^{n-2}}{R^{n-2}}\right]\\ \times\left(\sin n\theta\int_0^R\eta^{n+1}\varepsilon_c^{m(n)}d\eta-\cos n\theta\int_0^R\eta^{n+1}\varepsilon_s^{m(n)}d\eta\right)\end{array}\right\} \tag{4.7}$$

For uniform misfit strain distribution ε^m=constant, the interface shear stresses in Eq. (2.17) vanish. The curvatures in the substrate obtained from Eqs. (4.2)–(4.4)] become

$$\kappa=\kappa_{rr}=\kappa_{\theta\theta}=-6\frac{E_fh_f}{1-\nu_f}\frac{1-\nu_s}{E_sh_s^2}\varepsilon^m,\ \kappa_{r\theta}=0.$$

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

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

For this special case only, both stress and curvature states become equi-biaxial. The elimination of misfit strain ε^m from the above two equations yields a simple relation $\sigma^{(f)}=\frac{E_sh_s^2}{6(1-\nu_s)h_f}\kappa$, 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, 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-axisymmetric misfit strain distribution.

5. Extension of Stoney formula for non-axisymmetric misfit strain distribution

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 and non-axisymmetric misfit strain distribution in this section by establishing the direct relation between the thin-film stresses and substrate curvatures.

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

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

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

$$\sigma_{rr}^{(f)}-\sigma_{\theta\theta}^{(f)}=-\frac{E_fh_s}{6(1+\nu_f)} * \left\{4(\kappa_{rr}-\kappa_{\theta\theta})-\sum_{n=1}^{\infty}(n+1)\left[n\left(\frac{r}{R}\right)^n-(n-1)\left(\frac{r}{R}\right)^{n-2}\right](C_n\cos n\theta+S_n\sin n\theta)\right\}, \tag{5.2}$$

$$\sigma_{r\theta}^{(f)}=-\frac{E_fh_s}{6(1+\nu_f)}\left\{4\kappa_{r\theta}+\frac{1}{2}\sum_{n=1}^{\infty}(n+1)\left[n\left(\frac{r}{R}\right)^n-(n-1)\left(\frac{r}{R}\right)^{n-2}\right](C_n\sin n\theta-S_n\cos n\theta)\right\}, \tag{5.3}$$

$$\sigma_{rr}^{(f)}+\sigma_{\theta\theta}^{(f)}=\frac{E_sh_s^2}{6h_f(1-\nu_s)}\left[\begin{array}{l}\kappa_{rr}+\kappa_{\theta\theta}+\frac{1-\nu_s}{1+\nu_s}\left(\kappa_{rr}+\kappa_{\theta\theta}-\overline{\kappa_{rr}+\kappa_{\theta\theta}}\right)\\ -\frac{1-\nu_s}{1+\nu_s}\sum_{n=1}^{\infty}(n+1)\left(\frac{r}{R}\right)^n(C_n\cos n\theta+S_n\sin n\theta)\end{array}\right], \tag{5.4}$$

where $\overline{\kappa_{rr}+\kappa_{\theta\theta}}=C_0=\frac{1}{\pi R^2}\iint_A(\kappa_{rr}+\kappa_{\theta\theta})dA$ is the average curvature over entire area A of the thin film. Eqs. (5.2)–(5.4) provide direct relations between individual film stresses and substrate curvatures. It is important to note that stresses at a point in the thin film depend not only on curvatures at the same point (local dependence), but also on the curvatures in the entire substrate (non-local dependence) via the coefficients C_n and S_n.

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

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

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

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

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

$$\sigma_{rr}^{(\mathrm{f})}-\sigma_{\theta\theta}^{(\mathrm{f})}=-\frac{E_{\mathrm{f}}h_{\mathrm{s}}}{6(1+\nu_{\mathrm{f}})} \times\left\{4(\kappa_{rr}-\kappa_{\theta\theta})-\frac{1}{\pi R^2}\iint_A(\kappa_{rr}+\kappa_{\theta\theta})\frac{\frac{\eta}{R}F_{\mathrm{minus}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2r^2}{R^4}\right]^3}\mathrm{d}A\right\}, \tag{5.7}$$

$$\sigma_{r\theta}^{(\mathrm{f})}=-\frac{E_{\mathrm{f}}h_{\mathrm{s}}}{6(1+\nu_{\mathrm{f}})}\left\{4\kappa_{r\theta}-\frac{1}{2}\frac{1}{\pi R^2}\iint_A(\kappa_{rr}+\kappa_{\theta\theta})\frac{\frac{\eta}{R}F_{\mathrm{shear}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2r^2}{R^4}\right]^3}\mathrm{d}A\right\}, \tag{5.8}$$

$$\sigma_{rr}^{(\mathrm{f})}+\sigma_{\theta\theta}^{(\mathrm{f})}=\frac{E_{\mathrm{s}}h_{\mathrm{s}}^2}{6h_{\mathrm{f}}(1-\nu_{\mathrm{s}})} * \left\{\begin{array}{l}\kappa_{rr}+\kappa_{\theta\theta}+\frac{1-\nu_{\mathrm{s}}}{1+\nu_{\mathrm{s}}}\left(\kappa_{rr}+\kappa_{\theta\theta}-\overline{\kappa_{rr}+\kappa_{\theta\theta}}\right)\\ -\frac{1-\nu_{\mathrm{s}}}{1+\nu_{\mathrm{s}}}\frac{r}{\pi R^3}\iint_A(\kappa_{rr}+\kappa_{\theta\theta})\frac{\frac{\eta}{R}F_{\mathrm{plus}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2r^2}{R^4}\right]^2}\mathrm{d}A\end{array}\right\}, \tag{5.9}$$

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

$$F_{\mathrm{minus}}(r_1,\eta_1,\varphi_1)=-r_1^2\eta_1(6+9\eta_1^2+r_1^2\eta_1^4)+r_1(2+9\eta_1^2+6r_1^2\eta_1^2+6r_1^2\eta_1^4)\cos\varphi_1 -\eta_1(3+3r_1^2\eta_1^2+2r_1^4\eta_1^2)\cos2\varphi_1+r_1\eta_1^2\cos3\varphi_1, \tag{5.10}$$

$$F_{\mathrm{shear}}(r_1,\eta_1,\varphi_1)=r_1(2+9\eta_1^2-6r_1^2\eta_1^2)\sin\varphi_1-\eta_1(3+3r_1^2\eta_1^2-2r_1^4\eta_1^2)\sin2\varphi_1+r_1\eta_1^2\sin3\varphi_1,$$

$$F_{\mathrm{plus}}(r_1,\eta_1,\varphi_1)=2(1+2r_1^2\eta_1^2)\cos\varphi_1-r_1\eta_1\cos2\varphi_1-r_1\eta_1(4+r_1^2\eta_1^2).$$

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

$$\tau_r=\frac{E_{\mathrm{s}}h_{\mathrm{s}}^2}{6(1-\nu_{\mathrm{s}}^2)}\left\{\frac{\partial}{\partial r}(\kappa_{rr}+\kappa_{\theta\theta})-\frac{1-\nu_{\mathrm{s}}}{\pi R^3}\iint_A(\kappa_{rr}+\kappa_{\theta\theta})\frac{\frac{\eta}{R}F_{\mathrm{radial}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2r^2}{R^4}\right]^3}\mathrm{d}A\right\}, \tag{5.11}$$

$$\tau_\theta=\frac{E_{\mathrm{s}}h_{\mathrm{s}}^2}{6(1-\nu_{\mathrm{s}}^2)}\left\{\frac{1}{r}\frac{\partial}{\partial r}(\kappa_{rr}+\kappa_{\theta\theta})-\frac{1-\nu_{\mathrm{s}}}{\pi R^3}\iint_A(\kappa_{rr}+\kappa_{\theta\theta})\frac{\frac{\eta}{R}F_{\mathrm{circumferential}}\left(\frac{r}{R},\frac{\eta}{R},\varphi-\theta\right)}{\left[1-2\frac{\eta r}{R^2}\cos(\varphi-\theta)+\frac{\eta^2r^2}{R^4}\right]^3}\mathrm{d}A\right\}, \tag{5.12}$$

where

$$\begin{aligned}F_{\mathrm{radial}}(r_1,\eta_1,\varphi_1)&=(1+3r_1^2\eta_1^2)\cos\varphi_1-r_1\eta_1(3+r_1^2\eta_1^2\cos2\varphi_1),\\ F_{\mathrm{circumferantial}}(r_1,\eta_1,\varphi_1)&=(1-3r_1^2\eta_1^2)\sin\varphi_1+r_1^3\eta_1^3\sin2\varphi_1.\end{aligned} \tag{5.13}$$

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

$$\sigma_{rr}+\sigma_{\theta\theta}=\frac{E_{\mathrm{s}}h_{\mathrm{s}}^2}{6(1-\nu_{\mathrm{s}})h_{\mathrm{f}}}(\kappa_{rr}+\kappa_{\theta\theta}). \tag{5.14}$$

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

6. An example

In this section we present an example to illustrate the difference between the stresses given by Eqs. (5.2)–(5.4) and by the Stoney formula (1.1). We adopt a displacement profile

$$w=w_0\left(\frac{r}{R}\right)^n\cos n\theta, \tag{6.1}$$

where w_0 is the maximum displacement, and n is an integer. For $n=2$, the displacement corresponds to the saddle shape. Such a displacement gives the curvatures

$$\begin{aligned}\kappa_{rr}&=-\kappa_{\theta\theta}=n(n-1)\frac{w_0}{R^2}\left(\frac{r}{R}\right)^{n-2}\cos n\theta,\\ \kappa_{r\theta}&=-n(n-1)\frac{w_0}{R^2}\left(\frac{r}{R}\right)^{n-2}\sin n\theta.\end{aligned} \tag{6.2}$$

The stresses determined from Eqs. (5.2)–(5.4) are

$$\sigma_{rr}^{(\mathrm{f})}=-\sigma_{\theta\theta}^{(\mathrm{f})}=-\frac{2E_{\mathrm{f}}h_{\mathrm{s}}}{3(1+\nu_{\mathrm{f}})}n(n-1)\frac{w_0}{R^2}\left(\frac{r}{R}\right)^{n-2}\cos n\theta, \tag{6.3}$$

$$\sigma_{r\theta}^{(\mathrm{f})}=\frac{2E_{\mathrm{f}}h_{\mathrm{s}}}{3(1+\nu_{\mathrm{f}})}n(n-1)\frac{w_0}{R^2}\left(\frac{r}{R}\right)^{n-2}\sin n\theta. \tag{6.4}$$

Fig. 2 shows the contour of normal stress $\sigma_{rr}^{(\mathrm{f})}$ $(=-\sigma_{\theta\theta}^{(\mathrm{f})})$ and shear stress $\sigma_{r\theta}^{(\mathrm{f})}$ for $n=2$ and 3. The spatial variation of stresses is clearly observed. On the contrary, the Stoney formula (1.1) gives a vanishing stress state.

7. Discussion and conclusions

Unlike Stoney's original analysis and its extensions discussed in the introduction, the present analysis, together with Huang and Rosakis [14] and Huang et al.[15] for the special case of axisymmetry, show that the dependence of film stresses on substrate curvatures is not generally "local". Here the stress components at a point on the film will, in general, depend on both the local value of the curvature components (at the same point) and on the value of curvatures of all other points on the plate system (non-local dependence). The more pronounced the curvature non-uniformities are, the more important such non-local effects become in accurately determining film stresses from curvature measurements. This demonstrates that analyses methods based on Stoney's approach and its various extensions cannot handle the non-locality of the stress/curvature dependence and may result in substantial stress prediction errors if

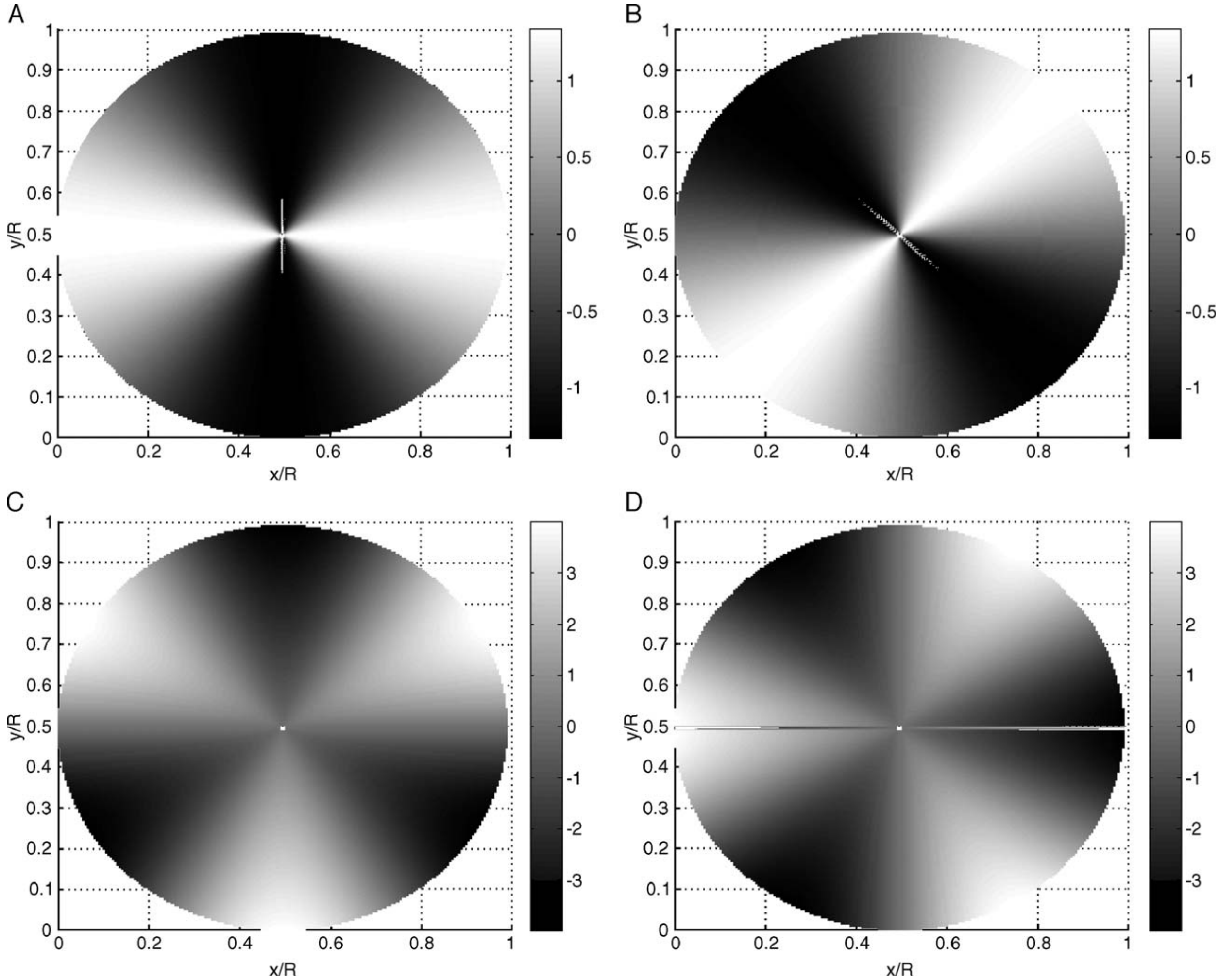

Fig. 2. Contour plots of dimensionless stress components $\left(\hat{\sigma}_{ij}^{\mathrm{f}}=\frac{\sigma_{ij}^{(\mathrm{f})}(1+\nu_{\mathrm{f}})R^2}{E_{\mathrm{f}}h_{\mathrm{s}}w_0}, i,j=r,\theta\right)$ for the displacement profile in Eq. (6.1). (a) $n=2$, $\hat{\sigma}_{rr}^{(\mathrm{f})}$; (b) $n=2$, $\hat{\sigma}_{r\theta}^{(\mathrm{f})}$; (c) $n=3$, $\hat{\sigma}_{rr}^{(\mathrm{f})}$; (d) $n=3$, $\hat{\sigma}_{r\theta}^{(\mathrm{f})}$;.

such analyses are applied locally in cases where spatial variations of system curvatures and stresses are present.

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. This is because the stress state at a point depends on curvature contributions (from κ_{rr}, $\kappa_{\theta\theta}$ and $\kappa_{r\theta}$) from the entire plate surface.

Regarding the curvature-misfit strain [Eqs. (4.2)–(4.4)] and stress-misfit strain [Eqs. (4.5)–(4.7)] relations the following points are noteworthy. These relations also generally feature a dependence of local misfit strain $\varepsilon^m(r,\theta)$ which is “Stoney-like” as well as a “non-local” contribution from the misfit strain of other points on the plate system. Furthermore the stress and curvature states are always non-equibiaxial (i.e., $\sigma_{rr}^{(\mathrm{f})} \neq \sigma_{\theta\theta}^{(\mathrm{f})}$ and $\kappa_{rr} \neq \kappa_{\theta\theta}$) in the presence of misfit strain non-uniformities. Only if $\varepsilon^m=$constant these states become equi-biaxial, the “non-local” contributions vanish and Stoney’s original results are recovered as a special case.

Finally it should be noted that the existence of non-uniformities also results in the establishment of shear stresses along the film/substrate interface. These stresses are in general related to the derivatives of the first curvature invariant $\kappa_{rr}+\kappa_{\theta\theta}$ [Eqs. (5.11) and (5.12)]. In terms of misfit strain these interfacial shear stresses are also related to the gradients of the misfit strain distribution $\varepsilon^m(r,\theta)$. The occurrence of such stresses is ultimately related to spatial non-uniformities and as a result such stresses vanish for the special case of uniform $\kappa_{rr}+\kappa_{\theta\theta}$ or ε^m considered by Stoney and its various extensions. Since film delamination is a commonly encountered form of failure during wafer manufacturing, the ability to estimate the level and distribution of such stresses from wafer-level metrology might prove to be invaluable in enhancing the reliability of such systems.

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