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Non-uniform, axisymmetric misfit strain: in thin films bonded on plate substrates/substrate systems: 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 non-uniform, but axisymmetric misfit strain distributions in the thin film, we derived 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 derived relations between the polar components of the film stress and those of system curvatures which allow for the experimental inference of such stresses from full-field curvature measurements in the presence of arbitrary radial non-uniformities. These relations also feature a "non-local" dependence on curvatures making a full-field measurement a necessity. Finally, it is shown that the interfacial shear tractions between the film and the substrate are proportional to the radial gradients of the first curvature invariant and can also be inferred experimentally.

Keywords Non-uniform misfit strain · Non-uniform wafer curvatures · Stress-curvature relations · Non-local effects · Interfacial shears

1 Introduction

Substrates formed of suitable solid-state materials may be used as platforms to support various thin film structures.

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Integrated electronic circuits, integrated optical devices and optoelectronic circuits, micro-electro-mechanical systems (MEMS) 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, and rapid deposition by evaporation or sputtering. 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 these steps include stress-induced film cracking and film/substrate delamination resulting from 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.

Stress changes in thin films following discrete process steps 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 known [2]. Various formulations have been developed for this purpose and most of these are essentially extensions of Stoney's approximate plate analysis [3].

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

as follows:

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

In the above the subscripts “*f*” and “*s*” denote the thin film and substrate, respectively, and *E* and *ν* are the Young’s modulus and Poisson’s ratio. Equation (1) is called the Stoney formula, and it has been extensively used in the literature to infer film stress changes from experimental measurement of system curvature changes [2].

Stoney’s formula was derived for an isotropic “thin” solid film of uniform thickness deposited on a much “thicker” plate substrate based on a number of assumptions. Stoney’s assumptions include the following: (1) Both the film thickness *h_f* and the substrate thickness *h_s* are uniform and *h_f* ≪ *h_s* ≪ *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 compo-

nents are spatially constant over the plate system’s surface, a situation which is often violated in practice.

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. To the best knowledge of the authors, no analytical formulation capable of dealing with non-uniform stress and deformation states has been existence.

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 [2]. Related analyses treating discontinuous films in the form of bare periodic lines [4] or composite films with periodic line structures (e.g., bare or encapsulated periodic lines) have also been derived [5–7]. These latter analyses have also removed the assumption of 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 [8–11]. 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 which have also been observed experimentally [12,13]. These bifurcations are transformations from an initially equi-biaxial to a subsequently biaxial curvature state that may be induced by an increase

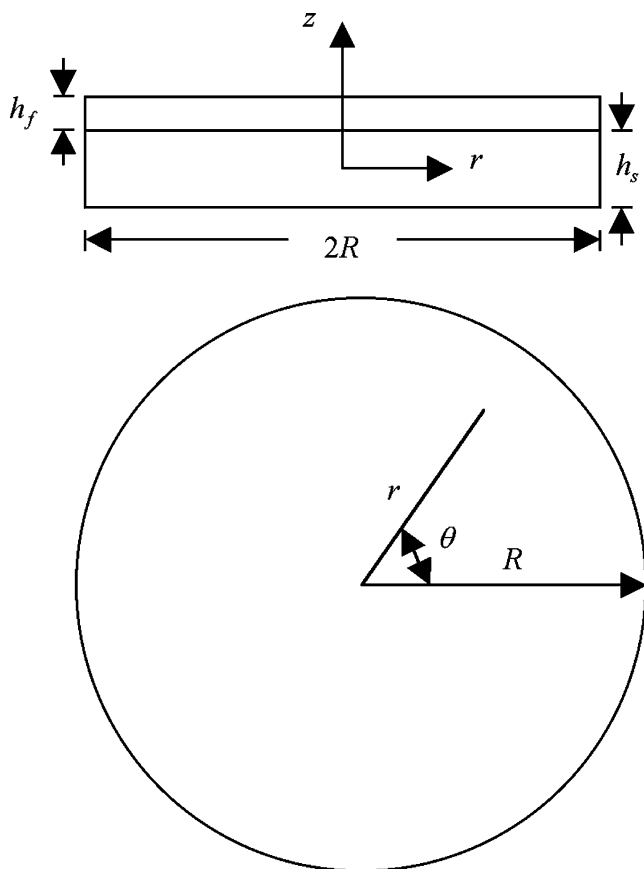


Fig. 1 A schematic diagram of the thin film/substrate system, showing the cylindrical coordinates (*r*, *θ*, *z*)

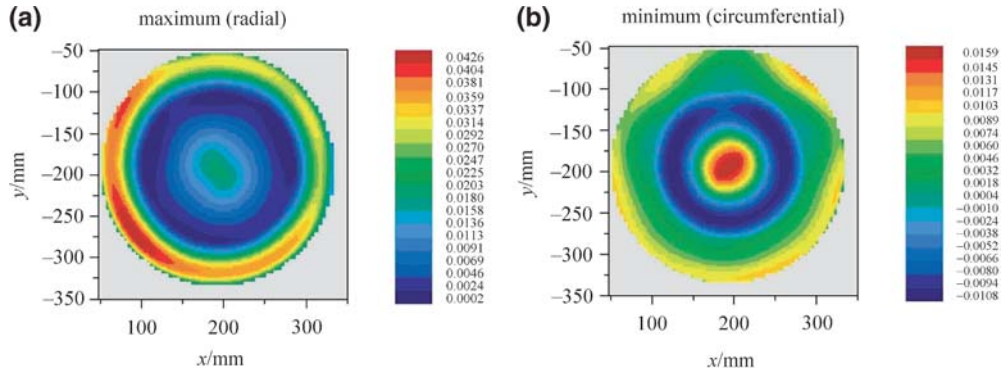


Fig. 2 Maximum and minimum principal curvatures of a thin film/substrate system

in film stress beyond a critical level. This critical level is intimately related to the systems aspect ratio, i.e., the ratio of in-plane to thickness dimension and the elastic stiffness. These analyses also retain the assumption of spatial curvature and stress uniformity across the system. However, they allow for deformations to evolve from an initially spherical shape to an energetically favored shape (e.g., ellipsoidal, cylindrical or saddle shapes) which features three different, still spatially constant, curvature components [12,13].

None of the above-discussed extensions of Stoney's methodology has relaxed the most restrictive of Stoney's original assumption of spatial uniformity which does not allow either film stress or curvature components to vary across the plate surface. This crucial assumption is often violated in practice since film stresses and the associated system curvatures are non-uniformly distributed over the plate area. Radially symmetric or axisymmetric variations in particular are often present in film/substrate systems. This is part due to the circular wafer geometry and part due to the axisymmetric geometries of most processing equipment used to manufacture such wafers.

An example of axisymmetric radial curvature distribution is given in Fig. 2. Figures 2(a) and 2(b) show the maximum and the minimum curvature distributions (principal curvature maps) of a large, industrial 300 mm wafer composed of a $1\mu\text{m}$ thick low-k dielectric film deposited on a $730\mu\text{m}$ Si substrate. This wafer was subjected to thermal anneal and the curvatures shown correspond to curvature changes (after-before) following cooling from 400°C . The principal curvatures have been obtained by means of CGS interferometry [14], a technique capable of performing full-field, real-time measurements of all three independent Cartesian components (κ_{xx} , κ_{yy} and $\kappa_{xy} = \kappa_{yx}$) of the curvature tensor over the entire wafer. Following optical measurement of the Cartesian components, the principal curvatures κ_1 and κ_2 were obtained [13] by using

$$\kappa_{1,2} = \frac{\kappa_{xx} + \kappa_{yy}}{2} \pm \left\{ \left(\frac{\kappa_{xx} - \kappa_{yy}}{2} \right)^2 + \kappa_{xy}^2 \right\}^{1/2}. \quad (2)$$

The wafer shape was not *a priori* assumed to be radially symmetric. However, the resulting principal curvature maps clearly show that this would be an accurate approximation in

this case. The axisymmetry of these maps as well as the clear presence of large scale curvature non-uniformities, along the radial direction, provides strong motivation for this study. This non-uniformity is in clear violation of Stoney's 6th assumption. Furthermore the two maps in Fig. 2 are clearly different. This is also in clear violation of Stoney's 5th assumption which requires equi-biaxiality of curvature. To clarify the last statement one should recall that once radial symmetry is established the only two surviving components of curvature are $\kappa_{rr}(r) = \frac{d^2w(r)}{dr^2}$ and $\kappa_{\theta\theta}(r) = \frac{1}{r} \frac{dw}{dr}$, where $z = w(r)$ is the equation of the radial wafer shape. With respect to the polar system of Fig. 1, κ_{rr} and $\kappa_{\theta\theta}$ are the radial and circumferential curvature components, respectively, and are also equal to the maximum and minimum principal curvatures. The remaining independent curvature component (twist) vanishes along radial lines [13]. Indeed in this case $\kappa_{rr}(r) \neq \kappa_{\theta\theta}(r) \forall R > r > 0$, clearly indicating that Stoney's assumption of equi-biaxiality is violated.

The main purpose of the present paper is to remove the two restrictive assumptions of the Stoney analysis relating to spatial uniformity and equi-biaxiality. This is done here only in relation to axisymmetric variations. To do so we consider the case of a thin film/substrate system subjected to arbitrary, radially symmetric misfit strain fields $\varepsilon_m(r)$ in the thin film whose presence will create a radially symmetric stress and curvature field as well as arbitrarily large stress and curvature gradients. Here the misfit strain refers to the intrinsic strain in thin film that is not associated with the stress. Our goal is to relate film stresses and system curvatures to the misfit strain distribution and to ultimately derive a relation between the film stresses and the system curvatures that would allow for the accurate experimental inference of film stress from full-field and real-time curvature measurements.

2 Governing equations

A thin film deposited on a substrate is subject to axisymmetric misfit strain distribution $\varepsilon_m(r)$, where r is the radial coordinate (Fig. 1). The thin film and substrate are circular in the lateral direction and have a radius R .

The thin-film thickness h_f is much less than the substrate thickness h_s , and both are much less than R , i.e., $h_f \ll h_s \ll R$. The Young's modulus and Poisson's ratio of the film and substrate are denoted by E_f, ν_f, E_s , and ν_s , respectively. The deformation is axisymmetric and is therefore independent of the polar angle θ , where (r, θ, z) are cylindrical coordinates with the origin at the center of the substrate (Fig. 1).

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 $u_f = u_f(r)$ denote the displacement in the radial (r) direction. The strains in the thin film are $\varepsilon_{rr} = \frac{du_f}{dr}$ and $\varepsilon_{\theta\theta} = \frac{u_f}{r}$. The stresses in the thin film can be obtained from the linear elastic constitutive model as

$$\begin{aligned}\sigma_{rr} &= \frac{E_f}{1-\nu_f^2} \left[\frac{du_f}{dr} + \nu_f \frac{u_f}{r} - (1+\nu_f)\varepsilon_m \right], \\ \sigma_{\theta\theta} &= \frac{E_f}{1-\nu_f^2} \left[\nu_f \frac{du_f}{dr} + \frac{u_f}{r} - (1+\nu_f)\varepsilon_m \right].\end{aligned}\quad (3)$$

The membrane forces in the thin film are

$$N_r^{(f)} = h_f \sigma_{rr}, \quad N_\theta^{(f)} = h_f \sigma_{\theta\theta}.\quad (4)$$

It is recalled that, for uniform misfit strain $\varepsilon_m(r) = \text{constant}$, the normal and shear stresses across the thin film/substrate interface vanish except near the free edge $r = R$, i.e., $\sigma_{zz} = \sigma_{rz} = 0$ at $z = \frac{h_s}{2}$ and $r < R$. For non-uniform misfit strain $\varepsilon_m = \varepsilon_m(r)$ as in the present study, the shear stress traction may not vanish anymore, and this shear stress σ_{rz} is denoted by $\tau(r)$ as shown in Fig. 3. 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 equation for the thin film, accounting for the effect of interface shear stress traction $\tau(r)$, becomes

$$\frac{dN_r^{(f)}}{dr} + \frac{N_r^{(f)} - N_\theta^{(f)}}{r} - \tau = 0.\quad (5)$$

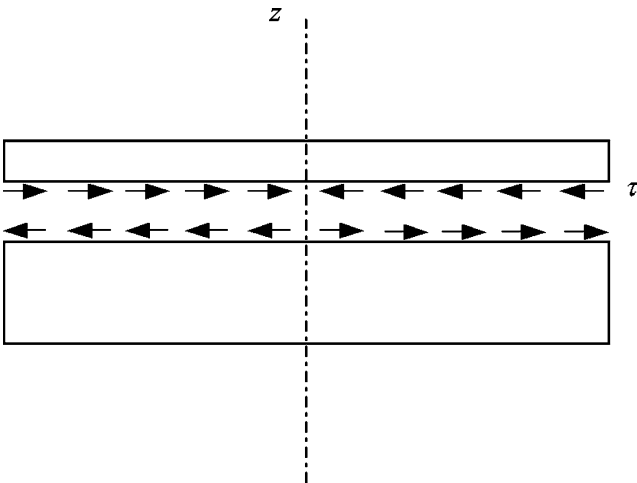


Fig. 3 A schematic diagram of the non-uniform shear traction distribution at the interface between the film and the substrate

The substitution of Eqs. (3) and (4) into (5) yields the following governing equation for u_f (and τ)

$$\frac{d^2 u_f}{dr^2} + \frac{1}{r} \frac{du_f}{dr} - \frac{u_f}{r^2} = \frac{1-\nu_f^2}{E_f h_f} \tau + (1+\nu_f) \frac{d\varepsilon_m}{dr}.\quad (6)$$

Let u_s denote the displacement in the radial (r) direction at the neutral axis ($z = 0$) of the substrate, and w the displacement in the normal (z) direction. It is important to consider w since the substrate can be subject to bending and is modeled as a plate. The strains in the substrate are given by

$$\varepsilon_{rr} = \frac{du_s}{dr} - z \frac{d^2 w}{dr^2}, \quad \varepsilon_{\theta\theta} = \frac{u_s}{r} - z \frac{1}{r} \frac{dw}{dr}.\quad (7)$$

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

$$\begin{aligned}\sigma_{rr} &= \frac{E_s}{1-\nu_s^2} \left[\frac{du_s}{dr} + \nu_s \frac{u_s}{r} - z \left(\frac{d^2 w}{dr^2} + \frac{\nu_s}{r} \frac{dw}{dr} \right) \right], \\ \sigma_{\theta\theta} &= \frac{E_s}{1-\nu_s^2} \left[\nu_s \frac{du_s}{dr} + \frac{u_s}{r} - z \left(\nu_s \frac{d^2 w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right) \right].\end{aligned}\quad (8)$$

The forces and bending moments in the substrate are

$$\begin{aligned}N_r^{(s)} &= \int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} \sigma_{rr} dz = \frac{E_s h_s}{1-\nu_s^2} \left[\frac{du_s}{dr} + \nu_s \frac{u_s}{r} \right], \\ N_\theta^{(s)} &= \int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} \sigma_{\theta\theta} dz = \frac{E_s h_s}{1-\nu_s^2} \left[\nu_s \frac{du_s}{dr} + \frac{u_s}{r} \right], \\ M_r &= - \int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} z \sigma_{rr} dz = \frac{E_s h_s^3}{12(1-\nu_s^2)} \left(\frac{d^2 w}{dr^2} + \frac{\nu_s}{r} \frac{dw}{dr} \right), \\ M_\theta &= - \int_{-\frac{h_s}{2}}^{\frac{h_s}{2}} z \sigma_{\theta\theta} dz = \frac{E_s h_s^3}{12(1-\nu_s^2)} \left(\nu_s \frac{d^2 w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right).\end{aligned}\quad (9)$$

The shear stress τ at the thin film/substrate interface is equivalent to the distributed axial force $\tau(r)$ and bending moment $\frac{h_s}{2} \tau(r)$ applied at the neutral axis ($z = 0$) of the substrate. The in-plane force equilibrium equation of the substrate then becomes

$$\frac{dN_r^{(s)}}{dr} + \frac{N_r^{(s)} - N_\theta^{(s)}}{r} + \tau = 0.\quad (11)$$

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

$$\frac{dM_r}{dr} + \frac{M_r - M_\theta}{r} + Q - \frac{h_s}{2} \tau = 0,\quad (12)$$

$$\frac{dQ}{dr} + \frac{Q}{r} = 0,\quad (13)$$

where Q is the shear force normal to the neutral axis. The substitution of Eq. (9) into Eq. (11) yields the following governing equation for u_s (and τ)

$$\frac{d^2 u_s}{dr^2} + \frac{1}{r} \frac{du_s}{dr} - \frac{u_s}{r^2} = - \frac{1-\nu_s^2}{E_s h_s} \tau.\quad (14)$$

Equation (13), together with the requirement of finite Q at the center $r = 0$, gives $Q = 0$ in the entire substrate. Its

substitution into Eq. (12), in conjunction with Eq. (10), gives the following governing equation for w (and τ)

$$\frac{d^3w}{dr^3} + \frac{1}{r} \frac{d^2w}{dr^2} - \frac{1}{r^2} \frac{dw}{dr} = \frac{6(1-\nu_s^2)}{E_s h_s^2} \tau. \quad (15)$$

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

$$u_f = u_s - \frac{h_s}{2} \frac{dw}{dr}. \quad (16)$$

Equations (6) and (14)–(16) constitute four ordinary differential equations for u_f , u_s , w and τ .

We can eliminate u_f , u_s and w from these four equations to obtain the shear stress at the thin film/substrate interface in terms of the misfit strain as

$$\tau = -\frac{(1+\nu_f)}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} \frac{d\varepsilon_m}{dr}, \quad (17)$$

which is a remarkable result that holds regardless of boundary conditions at the edge $r = R$. Therefore, the interface shear stress is proportional to the gradient of misfit strain. For uniform misfit strain $\varepsilon_m(r) = \text{constant}$, the interface shear stress vanishes, i.e., $\tau = 0$.

The substitution of the above solution for shear stress τ into Eqs. (15) and (14) yields ordinary differential equations for displacements w and u_s in the substrate. Their general solutions are

$$\frac{dw}{dr} = -\frac{6(1-\nu_s^2)}{E_s h_s^2} \frac{1+\nu_f}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} \times \frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{B_1}{2} r, \quad (18)$$

$$u_s = \frac{1-\nu_s^2}{E_s h_s} \frac{1+\nu_f}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} \times \frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{B_2}{2} r, \quad (19)$$

where B_1 and B_2 are constants to be determined by boundary conditions to be given in the next section. We have imposed the conditions that w and u_s are bounded at the center of the substrate $r = 0$. The displacement u_f in the thin film can be obtained from interface continuity condition in Eq. (16) as

$$u_f = \frac{4(1-\nu_s^2)}{E_s h_s} \frac{(1+\nu_f)}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} \frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \left(\frac{B_2}{2} - \frac{h_s B_1}{4} \right) r. \quad (20)$$

The force $N_r^{(f)}$ in the thin film, which is needed for boundary conditions in the next section, is obtained from Eq. (4) as

$$N_r^{(f)} = \frac{E_f h_f}{1-\nu_f^2} \left\{ -(1+\nu_f) \frac{\frac{1-\nu_f^2}{E_f h_f} \varepsilon_m}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} - 4(1-\nu_f^2) \frac{\frac{1-\nu_s^2}{E_s h_s}}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} \frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1+\nu_f}{2} \left(B_2 - \frac{h_s}{2} B_1 \right) \right\}. \quad (21)$$

The force $N_r^{(s)}$ and moment M_r in the substrate, which are also needed for boundary conditions in the next section, are obtained from Eqs. (9) and (10) as

$$N_r^{(s)} = \frac{E_s h_s}{1-\nu_s^2} \left\{ (1+\nu_f) \frac{\frac{1-\nu_s^2}{E_s h_s} \varepsilon_m}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} - (1-\nu_s)(1+\nu_f) \frac{\frac{1-\nu_s^2}{E_s h_s}}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} \frac{1}{r^2} \times \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1+\nu_s}{2} B_2 \right\}, \quad (22)$$

$$M_r = \frac{h_s}{2} \left\{ -\frac{(1+\nu_f)\varepsilon_m}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} + \frac{(1-\nu_s)(1+\nu_f)}{\frac{1-\nu_f^2}{E_f h_f} + 4\frac{1-\nu_s^2}{E_s h_s}} \frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{E_s h_s^2}{12(1-\nu_s)} B_1 \right\}. \quad (23)$$

It is interesting to observe that, in the limit of $h_f/h_s \ll 1$, the displacements in Eqs. (18)–(20) become

$$\frac{dw}{dr} = -6 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s^2}{E_s h_s^2} \frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{B_1}{2} r + O\left(\frac{h_f^2}{h_s^2}\right), \quad (24)$$

$$u_s = \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s^2}{E_s h_s} \frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{B_2}{2} r + O\left(\frac{h_f^2}{h_s^2}\right), \quad (25)$$

$$u_f = 4 \frac{E_f h_f}{1-\nu_f} \frac{1-\nu_s^2}{E_s h_s} \frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \left(\frac{B_2}{2} - \frac{h_s B_1}{4} \right) r + O\left(\frac{h_f^2}{h_s^2}\right). \quad (26)$$

3 Boundary conditions

The first boundary condition at the free edge $r = R$ requires that the net force vanishes,

$$N_r^{(f)} + N_r^{(s)} = 0 \quad \text{at } r = R. \quad (27)$$

The second boundary condition at the free edge $r = R$ is vanishing of net moment, i.e.,

$$M_r - \frac{h_s}{2} N_r^{(f)} = 0 \quad \text{at } r = R. \quad (28)$$

The above two equations in conjunction with Eqs. (21)–(23), give

$$\frac{B_2}{2} = \frac{E_f h_f}{1 - \nu_f} \frac{(1 - \nu_s)^2}{E_s h_s} \frac{1}{R^2} \int_0^R \eta \varepsilon_m(\eta) d\eta + O\left(\frac{h_f^2}{h_s^2}\right) \quad (29)$$

$$\frac{B_1}{2} = -6 \frac{E_f h_f}{1 - \nu_f} \frac{(1 - \nu_s)^2}{E_s h_s^2} \frac{1}{R^2} \int_0^R \eta \varepsilon_m(\eta) d\eta + O\left(\frac{h_f^2}{h_s^2}\right). \quad (30)$$

under the limit $\varepsilon = h_f/h_s \ll 1$.

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

$$\Pi = 2\pi \int_0^R r dr \int_{-\frac{h_s}{2}}^{\frac{h_s}{2} + h_f} U dz, \quad (31)$$

where U is the strain energy density which gives $\frac{\partial U}{\partial \varepsilon_{rr}} = \sigma_{rr}$ and $\frac{\partial U}{\partial \varepsilon_{\theta\theta}} = \sigma_{\theta\theta}$. For constitutive relations in Eqs. (3) and (8), we obtain

$$U = \frac{E}{2(1 - \nu^2)} \left[\varepsilon_{rr}^2 + \varepsilon_{\theta\theta}^2 + 2\nu \varepsilon_{rr} \varepsilon_{\theta\theta} - 2(1 + \nu) \varepsilon_m (\varepsilon_{rr} + \varepsilon_{\theta\theta}) \right], \quad (32)$$

where E and ν take their corresponding values in the thin film (i.e., E_f and ν_f for $h_s/2 + h_f \geq z \geq h_s/2$) and in the substrate (i.e., E_s and ν_s for $h_s/2 \geq z \geq -h_s/2$), and ε_m is zero in the substrate. For the displacement field in Section 2 and the associated strain field, the potential energy Π in Eq. (31) becomes a quadratic function of parameters B_1 and B_2 . The principle of minimal potential energy requires

$$\frac{\partial \Pi}{\partial B_1} = 0 \quad \text{and} \quad \frac{\partial \Pi}{\partial B_2} = 0. \quad (33)$$

It can be shown that, as expected in the limit $h_f/h_s \ll 1$, the above two equations are equivalent to the vanishing of net force in Eq. (27) and net moment in Eq. (28). The displacements in Eqs. (24)–(26) now become

$$\frac{dw}{dr} = -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \left[\frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1 - \nu_s}{1 + \nu_s} \frac{r}{R^2} \int_0^R \eta \varepsilon_m(\eta) d\eta \right], \quad (34)$$

$$u_f = 4u_s = 4 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s} \left[\frac{1}{r} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1 - \nu_s}{1 + \nu_s} \frac{r}{R^2} \int_0^R \eta \varepsilon_m(\eta) d\eta \right] \quad (35)$$

for $h_f/h_s \ll 1$.

4 Stresses and curvatures in thin film and substrate

The substrate curvatures can be obtained from the displacement w as

$$\begin{aligned} \kappa_{rr} &= \frac{d^2 w}{dr^2} = -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \left[\varepsilon_m - \frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1 - \nu_s}{1 + \nu_s} \frac{1}{R^2} \int_0^R \eta \varepsilon_m(\eta) d\eta \right], \\ \kappa_{\theta\theta} &= \frac{1}{r} \frac{dw}{dr} = -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \left[\frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta + \frac{1 - \nu_s}{1 + \nu_s} \frac{1}{R^2} \int_0^R \eta \varepsilon_m(\eta) d\eta \right]. \end{aligned} \quad (36)$$

The sum of these two curvatures is

$$\kappa_{rr} + \kappa_{\theta\theta} = -12 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s}{E_s h_s^2} \left[\bar{\varepsilon}_m + \frac{1 + \nu_s}{2} (\varepsilon_m - \bar{\varepsilon}_m) \right], \quad (37)$$

or equivalently

$$\kappa_{rr} + \kappa_{\theta\theta} = -12 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s}{E_s h_s^2} \left[\varepsilon_m - \frac{1 - \nu_s}{2} (\varepsilon_m - \bar{\varepsilon}_m) \right], \quad (38)$$

where $\bar{\varepsilon}_m = \frac{2}{R^2} \int_0^R \eta \varepsilon_m(\eta) d\eta = \frac{\iint \varepsilon_m dA}{\pi R^2}$ is the average misfit strain in the thin film. The first term on the right hand side of Eq. (37) corresponds to a uniform (average) misfit strain, while the second term gives the deviation from the uniform misfit strain. Such a deviation is proportional to the difference between the local misfit strain ε_m and the average misfit strain $\bar{\varepsilon}_m$. Similarly, the first term on the right hand side of Eq. (38) corresponds to the local misfit strain ε_m , while the second term gives the deviation from the local misfit strain and is also proportional to $\varepsilon_m - \bar{\varepsilon}_m$.

The difference between two curvatures in Eq. (36) is

$$\kappa_{rr} - \kappa_{\theta\theta} = -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} \left[\varepsilon_m - \frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta \right] \quad (39)$$

The forces in the substrate are obtained from Eq. (9) as

$$\begin{aligned} N_r^{(s)} &= \frac{E_f h_f}{1 - \nu_f} \left\{ \varepsilon_m - \frac{1 - \nu_s}{2} \times \left[\frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta - \bar{\varepsilon}_m \right] \right\}, \\ N_\theta^{(s)} &= \frac{E_f h_f}{1 - \nu_f} \left\{ \nu_s \varepsilon_m + \frac{1 - \nu_s}{2} \times \left[\frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta + \bar{\varepsilon}_m \right] \right\} \end{aligned} \quad (40)$$

for $h_f/h_s \ll 1$. The bending moments in the substrate are obtained from Eq. (10) as

$$\begin{aligned} M_r &= \frac{E_f h_f h_s}{1 - \nu_f} \frac{h_s}{2} \left\{ -\varepsilon_m + \frac{1 - \nu_s}{2} \right. \\ &\quad \times \left[\frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta - \bar{\varepsilon}_m \right] \left. \right\}, \\ M_\theta &= \frac{E_f h_f h_s}{1 - \nu_f} \frac{h_s}{2} \left\{ -\nu_s \varepsilon_m - \frac{1 - \nu_s}{2} \right. \\ &\quad \times \left[\frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta + \bar{\varepsilon}_m \right] \left. \right\} \end{aligned} \quad (41)$$

for $h_f/h_s \ll 1$. The stresses in the substrate are related to the forces and moments by

$$\begin{aligned} \sigma_{rr}^{(s)} &= \frac{N_r^{(s)}}{h_s} - \frac{12M_r}{h_s^3} z, \\ \sigma_{\theta\theta}^{(s)} &= \frac{N_\theta^{(s)}}{h_s} - \frac{12M_\theta}{h_s^3} z. \end{aligned} \quad (42)$$

The stresses in the thin film are obtained from Eq. (3),

$$\begin{aligned} \sigma_{rr}^{(f)} &= \frac{E_f}{1 - \nu_f} \left\{ -\varepsilon_m + 4 \frac{E_f h_f}{1 - \nu_f^2} \frac{1 - \nu_s^2}{E_s h_s} \right. \\ &\quad \times \left[\varepsilon_m - (1 - \nu_f) \frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta \right. \\ &\quad \left. \left. + \frac{1 + \nu_f}{2} \frac{1 - \nu_s}{1 + \nu_s} \bar{\varepsilon}_m \right] \right\} + O\left(\frac{h_f^2}{h_s^2}\right), \\ \sigma_{\theta\theta}^{(f)} &= \frac{E_f}{1 - \nu_f} \left\{ -\varepsilon_m + 4 \frac{E_f h_f}{1 - \nu_f^2} \frac{1 - \nu_s^2}{E_s h_s} \right. \\ &\quad \times \left[\nu_f \varepsilon_m + (1 - \nu_f) \frac{1}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta \right. \\ &\quad \left. \left. + \frac{1 + \nu_f}{2} \frac{1 - \nu_s}{1 + \nu_s} \bar{\varepsilon}_m \right] \right\} + O\left(\frac{h_f^2}{h_s^2}\right), \end{aligned} \quad (43)$$

where we have kept the terms that are up to the order of $O(\frac{h_f}{h_s})$ in order to illustrate the difference between these two stresses. The sum and difference of these stresses have the following simple expressions:

$$\begin{aligned} \sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)} &= \frac{E_f}{1 - \nu_f} (-2\varepsilon_m) + O\left(\frac{h_f}{h_s}\right), \\ \sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} &= 4E_f \frac{E_f h_f}{1 - \nu_f^2} \frac{1 - \nu_s^2}{E_s h_s} \\ &\quad \times \left[\varepsilon_m - \frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta \right] + O\left(\frac{h_f^2}{h_s^2}\right) \end{aligned} \quad (44)$$

It is noted that $\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)}$ is in general expected to be smaller than $\sigma_{rr}^{(f)} + \sigma_{\theta\theta}^{(f)}$ for $h_f/h_s \ll 1$. This issue will be discussed again in the next section in relation to the dependence of this stress difference to the difference between polar curvature components.

For uniform misfit strain $\varepsilon_m = \text{constant}$, the curvatures in the substrate obtained from Eqs. (37)–(39) become

$$\kappa = \kappa_{rr} = \kappa_{\theta\theta} = -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s}{E_s h_s^2} \varepsilon_m. \quad (45)$$

The stresses in the thin film obtained from Eq. (44) become

$$\sigma = \sigma_{rr}^{(f)} = \sigma_{\theta\theta}^{(f)} = \frac{E_f}{1 - \nu_f} (-\varepsilon_m). \quad (46)$$

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 $\sigma = \frac{E_s h_s^2}{6(1 - \nu_s) h_f} \kappa$. This is the relation obtained by Stoney (see Eq. (1)) and it has been used to estimate the thin-film stress σ from the substrate curvature κ , if the misfit strain, stress and curvature are all constants, and if the plate system shape is spherical. In the following, we extend such a relation for non-uniform misfit strain distribution.

5 Extension of Stoney formula for non-uniform misfit strain distribution

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

It is shown that both $\kappa_{rr} - \kappa_{\theta\theta}$ in Eq. (39) and $\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)}$ in Eq. (44) are proportional to $\varepsilon_m(r) - \frac{2}{r^2} \int_0^r \eta \varepsilon_m(\eta) d\eta$. Therefore, elimination of misfit strain gives the difference $\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)}$ in thin-film stresses directly proportional to the difference $\kappa_{rr} - \kappa_{\theta\theta}$ in substrate curvatures,

$$\sigma_{rr}^{(f)} - \sigma_{\theta\theta}^{(f)} = -\frac{2E_f h_s}{3(1 + \nu_f)} (\kappa_{rr} - \kappa_{\theta\theta}). \quad (47)$$

The above relation clearly shows that the radial and circumferential stress components will be equal only if the equivalent curvature components are also equal (unlike what was stated in Stoney's 5th and 6th assumptions this is not true in general as can be clearly seen from Fig. 2). In this experimental example, the two polar components of curvature displayed are radially varying but are clearly unequal.

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

$$\begin{aligned} \overline{\kappa_{rr} + \kappa_{\theta\theta}} &= \frac{1}{\pi R^2} \iint_A (\kappa_{rr} + \kappa_{\theta\theta}) \eta d\eta d\theta \\ &= \frac{2}{R^2} \int_0^R \eta (\kappa_{rr} + \kappa_{\theta\theta}) d\eta. \end{aligned} \quad (48)$$

It can be related to the average misfit strain $\bar{\varepsilon}_m$ by averaging both sides of Eq. (38), i.e.,

$$\overline{\kappa_{rr} + \kappa_{\theta\theta}} = 12 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s}{E_s h_s^2} (-\bar{\varepsilon}_m). \quad (49)$$

The deviation from the average curvature, $\overline{\kappa_{rr} + \kappa_{\theta\theta} - \kappa_{rr} + \kappa_{\theta\theta}}$, can be related to the deviation from the average misfit strain $\varepsilon_m - \bar{\varepsilon}_m$ as

$$\overline{\kappa_{rr} + \kappa_{\theta\theta} - \kappa_{rr} + \kappa_{\theta\theta}} = -6 \frac{E_f h_f}{1 - \nu_f} \frac{1 - \nu_s^2}{E_s h_s^2} (\varepsilon_m - \bar{\varepsilon}_m). \quad (50)$$

The elimination of misfit strain $\varepsilon_m - \bar{\varepsilon}_m$ and average misfit strain $\bar{\varepsilon}_m$ from Eqs. (49), (50) and (44) gives the sum of thin-film stresses in terms of curvature as

$$\sigma_{rr} + \sigma_{\theta\theta} = \frac{E_s h_s^2}{6(1 - \nu_s) h_f} \left\{ \kappa_{rr} + \kappa_{\theta\theta} + \frac{1 - \nu_s}{1 + \nu_s} [\kappa_{rr} + \kappa_{\theta\theta} - \overline{\kappa_{rr} + \kappa_{\theta\theta}}] \right\}. \quad (51)$$

The above equation, together with Eq. (47), provide direct relations between thin-film stresses and substrate curvatures. It is important to note that stresses at a point in the thin film depend not only on curvatures at the same point (local dependence), but also on the average curvature in the entire substrate (non-local dependence).

The interface stress $\tau(r)$ given in Eq. (17) can also be directly related to substrate curvatures via

$$\tau = \frac{E_s h_s^2}{6(1 - \nu_s^2)} \frac{d}{dr} (\kappa_{rr} + \kappa_{\theta\theta}). \quad (52)$$

This provides a remarkably simple way to estimate the interface shear stress from radial gradients of the two non-zero substrate curvatures.

Since interfacial shear stresses are responsible for promoting system failures through delamination of the thin film from the substrate, Eq. (52) has particular significance. It shows that such stresses are proportional to the radial gradient of $\kappa_{rr} + \kappa_{\theta\theta}$ and not to its magnitude as might have been expected of a local, Stoney-like formulation. The implementation value of Eq. (52) is that it provides an easy way of inferring these special interfacial shear stresses once the full-field curvature information is available. As a result, the methodology also provides a way to evaluate the risk of and to mitigate such important forms of failure. It should be noted that for the special case of spatially constant curvatures, this interfacial shear stress τ vanishes as is the case for all Stoney-like formulations described in the introduction.

Finally it should be noted that Eq. (51) also reduces to Stoney's result for the case of spatial curvature uniformity. Indeed for this case, Eq. (51) reduces to

$$\sigma_{rr} + \sigma_{\theta\theta} = \frac{E_s h_s^2}{6(1 - \nu_s) h_f} (\kappa_{rr} + \kappa_{\theta\theta}). \quad (53)$$

If in addition the curvature state is equi-biaxial ($\kappa_{rr} = \kappa_{\theta\theta}$), as assumed by Stoney, Eq. (1) is recovered while relation (47) furnishes $\sigma_{rr} = \sigma_{\theta\theta}$ (stress equi-biaxiality) as a special case.

dependence of the stresses on the 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 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 both κ_{rr} and $\kappa_{\theta\theta}$) from the entire plate surface.

Regarding the curvature-misfit strain (Eqs. (36)–(39)) and stress-misfit strain (Eqs. (43)–(45)) relations the following points are noteworthy. These relations also generally feature a dependence of local misfit strain $\varepsilon_m(r)$ 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., $\sigma_{rr}^{(f)} \neq \sigma_{\theta\theta}^{(f)}$ and $\kappa_{rr} \neq \kappa_{\theta\theta}$) in the presence of misfit strain non-uniformities. Only if $\varepsilon_m = \text{constant}$ these states become equi-biaxial, the "non-local" contributions vanish and Stoney's original results are recovered as a special case and a highly unlikely scenario as clearly demonstrated from Fig. 2.

Finally it should be noted that the existence of radial non-uniformities also results in the establishment of shear stresses along the film/substrate interface. These stresses are in general proportional to the radial derivatives of the first curvature invariant $\kappa_{rr} + \kappa_{\theta\theta}$ (Eq. (52)). In terms of misfit strain these interfacial shear stresses are also proportional to the radial gradient of the misfit strain distribution $\varepsilon_m(r)$. 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.

6 Discussion and conclusions

Unlike Stoney's original analysis and its extensions discussed in the introduction, the present analysis shows that the depen-

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