Extending Stoney's equation to thin, elastically anisotropic substrates and bilayer films

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The Stoney equation has been a powerful tool for the thin film community to measure the residual stresses induced in a film through the measurement of curvature of a film–substrate system. Two of the main assumptions of the original Stoney equation are that the substrate is much thicker than the film and its material is isotropic in nature. However, in majority of the cases where the film stress is measured from the system curvature, Si wafers are used as substrates, which are anisotropic in nature. The anisotropic substrate problem was solved by Nix [1] for thick substrates. In this paper, a modified version of the Stoney equation is derived for configurations with thin anisotropic substrates, specifically for the cases of Si(001) and Si(111) wafers. The same methodology is then used to extend the Stoney formula to systems with bilayer films on thin substrates.

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1. Introduction

In a thin film configuration, the film is often stressed to conform to the substrate, commonly due to epitaxial effects, difference in thermal expansion coefficients between the film and the substrate materials, or phase transformations accompanied with volume changes. This stress causes the system to assume a curvature. The equation that relates this curvature to the stress in the film is referred to as the Stoney equation [2].

\[
\sigma_f = \frac{E_f h_f^2}{6(1-\nu_f)} h_f K. \tag{1}
\]

Here, \(\sigma_f\) represents the stress in the film, which is assumed to be uniform and biaxial in nature. \(E_f\), \(h_f\) and \(\nu_f\) are the Young's modulus of elasticity, thickness and the Poisson's ratio, respectively of the isotropic and linear elastic substrate material. Furthermore, \(h_f\) represents the thickness of the film and \(K\) is the curvature of the film–substrate system. The system is assumed to deform spherically with a uniform curvature. It is important to realize that Eq. (1) is obtained by making several assumptions. These have been highlighted in works by Freund et al. [3], Freund [4]. Some of the limitations for using Eq. (1) are as listed below.

1. The thickness of the film–substrate system is much smaller in comparison to its lateral dimensions.
2. The thickness of the film is negligible in comparison to the thickness of the substrate.
3. The substrate material is homogeneous, isotropic and linear elastic.
4. The film material is isotropic as well.
5. The system deforms spherically with a uniform curvature.
6. The stress state in the plane of the film is isotropic or equibiaxial with equal stresses along any two mutually perpendicular directions in the plane.
7. All strains and rotations are infinitesimal.

1.1. Evolution of the Stoney equation

The very first form of the Stoney formula was proposed in 1909 by Stoney [5].

\[
\sigma_f h_f = \frac{E_f h_f^2}{6K}. \tag{2}
\]

While deriving this expression, Stoney considered the stress state in the film to be uniaxial because the length of the film is usually much larger in comparison to its width. It was realized later that an equibiaxial stress state in the film is more meaningful because, even though the length of the system dominates its width, the width is still considerably large in comparison to its thickness. To incorporate this change, one simply needs to replace \(E_f\) with the biaxial modulus \(E_f/(1-\nu_f)\) of the substrate material in Eq. (2), which then results in Eq. (1).

Brenner and Senderoff [6] have relaxed the thin film assumption (\(h_f \ll h_s\)) and derived the stress–curvature relationship. But this paper still incorporates a uniaxial film stress state and not a biaxial state. Following this, it was not until 1977 that Thornton and Hoffman [7]
derived a relation for the non-uniform curvature of a glass slide caused due to a non-uniform stress in the film, by relaxing another important assumption of the traditional Stoney equation, that the stress in the film must be uniform.

The first appearance of the Stoney equation as given in Eq. (1) is in a paper by Flinn et al. [2]. Two years later, Nix [1] proposed results for configurations which use single crystal silicon wafers as substrates. Freund et al. [3] extended the Stoney equation for systems with thin and elastically isotropic substrates or those undergoing large deformations. Results of this paper show significant differences from the traditional Stoney equation. Janssen et al. [8] have derived the Stoney equation for the case of a thick anisotropic substrate using a force and moment equilibrium approach assuming spherical deformation. For Si(001) wafers, the stress–curvature relation is given by

$$\sigma_{fj} h_f = \frac{h_f^2}{6(c_{11} + c_{12})R}$$  \hspace{1cm} (3)

For Si(111) wafers, the stress–curvature relation is given by

$$\sigma_{fj} h_f = \left( \frac{6}{4c_{11} + 8c_{12}} + \frac{6}{s_{00}^*} \right) \frac{h_f^2}{6R^2}$$  \hspace{1cm} (4)

where $s_{00}^*$ are elements of the compliance matrix of Si.

1.2. Scope of the paper

In this paper, a modified version of the Stoney equation is derived considering the substrate to be thin and made of single crystal silicon wafers (specifically Si(001) and Si(111)). These equations are derived from the equilibrium requirement that the potential energy of the system must be stationary. The results are compared with Eqs. (3) and (4) on incorporating back the thin film assumption that $h_f \approx h_s$. The same methodology is then applied to configurations with a bilayered film whose thickness is comparable to that of the substrate, and a relation for the curvature of the system is derived.

2. Mathematical formulation and derivation

In this paper, discussion is based on a circular geometry of the substrate and film, for the ease of analytical development. It is to be noted that the results will be identical for other shapes of the system as well, in the small deformation regime. In the linear elastic deformation regime, the curvature of the configuration is spherical with a nearly uniform curvature throughout the substrate [9]. In this work, the film material is considered to be homogeneous and isotropic with a uniform distribution of stress through the thickness of the film material.

Fig. 1 shows the cross sectional view of the film–substrate configuration. The radius of the circular system is $R$ while $h_f$ and $h_s$ represent the thicknesses of the film and substrate, respectively. A cylindrical polar coordinate system ($r,h,z$) is chosen with the origin lying at the intersection of the mid-plane of the substrate and the axis of symmetry of the system. The deformation in the system is measured using this coordinate system.

2.1. Modified Stoney equation for thin Si(001) wafer substrate

The most commonly used substrate for curvature measurements through the stress curvature relationships is made from Si(001) wafer. In this wafer, the [001] direction is perpendicular to the plane of the wafer. This direction coincides with the $z$-axis of the deformation coordinate system. Furthermore, the $r$ and $\theta$ directions of the coordinate axes of the deformation can be represented by two mutually orthogonal axes in the plane of the single crystal wafer. Hence, in this case the axes of deformation also coincide with the crystallographic axes of the Si(001) wafer. The stiffness matrix that relates the stress and strain tensors, has only three distinct components for cubic crystals, which can be written as [8].

$$\begin{pmatrix}
\sigma_{rr} & \sigma_{r\theta} \\
\sigma_{\theta r} & \sigma_{\theta \theta} \\
\sigma_{zz} & \sigma_{z\theta}
\end{pmatrix} =
\begin{pmatrix}
c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\
c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\
0 & 0 & c_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{44}
\end{pmatrix}
\begin{pmatrix}
\epsilon_{rr} \\
\epsilon_{r\theta} \\
\epsilon_{\theta r} \\
\epsilon_{\theta \theta} \\
\epsilon_{z\theta} \\
\epsilon_{z\theta}
\end{pmatrix},$$  \hspace{1cm} (5)

where $\sigma_{ij}$, $\epsilon_{ij}$ components of stress tensor, $c_{ij}$ elastic stiffness constants of Si and $\epsilon_{ij}$ components of strain tensor.

In this work, we consider a radially symmetric deformation because of circular substrate geometry and uniformity in film stress. The axially symmetric deformation coupled with the assumption that the out of plane stresses are negligible leaves only $\sigma_{rr}$ and $\sigma_{\theta \theta}$ as the non zero stress components in the film and the substrate. The elastic strain energy density is given by

$$U(r,z) = \frac{1}{2} \sum (\alpha_{ij} \varepsilon_{ij}),$$  \hspace{1cm} (6)

![Fig. 1. Circular film deposited on a circular anisotropic substrate.](image-url)
where $\sigma_r, \epsilon_r$ (i goes from 1 to 6) represent the corresponding components in the stress and strain tensors, respectively, as given in Eq. (5). In the current discussion, $\sigma_r$, i.e. $\sigma_z$, is zero.

Hence, in the substrate material, from Eq. (5)

$$\sigma_{zz} = C_{11}\epsilon_{rr} + C_{12}\epsilon_{tt} + C_{13}\epsilon_{tt} = 0 \Rightarrow \epsilon_{zz} = -\frac{C_{12}}{C_{11}} (\epsilon_{tt} + \epsilon_{ww}) \Rightarrow \sigma_{tt} = \left( \frac{C_{11}^2-C_{12}^2}{C_{11}} \right) \epsilon_{rr} + \left( \frac{C_{11}C_{12}-C_{12}^2}{C_{11}} \right) \epsilon_{ww},$$

$$\Rightarrow \sigma_{tt} = \left( \frac{C_{11}C_{12}-C_{12}^2}{C_{11}} \right) \epsilon_{rr} + \left( \frac{C_{11}^2-C_{12}^2}{C_{11}} \right) \epsilon_{ww}.$$  

Due to the assumptions mentioned earlier along with the nature of deformation, Eq. (6) becomes

$$U(r, z) = \frac{1}{2} (\sigma_{rr}\epsilon_{rr} + \sigma_{ww}\epsilon_{ww}).$$

Using Eqs. (7) and (8), the elastic strain energy density in the substrate material takes the form

$$U^f(r, z) = \frac{1}{2} \left[ \left( \frac{C_{11}^2-C_{12}^2}{C_{11}} \right) \epsilon_{rr}^2 + \epsilon_{ww}^2 \right] + 2 \left( \frac{C_{11}C_{12}-C_{12}^2}{C_{11}} \right) \epsilon_{rr}\epsilon_{ww}.$$  

Let $u(r)$ and $w(r)$ represent the radial and transverse displacements of the points on the substrate mid-plane, respectively. Then for small deformations, the strain components can be written in terms of the substrate mid-plane displacement components as [3]

$$\epsilon_r(r, z) = u(r) - z\omega(r), \quad \epsilon_{ww}(r, z) = w(r) + z\omega(r).$$

In Eq. (11), all derivatives of the displacements are considered with respect to the radial coordinate, $r$. $\epsilon_m$ represents the misfit strain in the system. If the misfit is due to heteroepitaxy, then it can be represented as $(a_l - a_i)/a_i$, where $a_l$ and $a_i$ are the lattice parameters of the film and substrate materials, respectively. It is also very likely to occur because of differences in thermal expansion coefficients between the substrate and the film materials ($\alpha_s$ and $\alpha_l$ respectively), in which case $\epsilon_m$ is given by $(\alpha_s - \alpha_l)\Delta T$. It is assumed that the misfit strain is completely accommodated in the film itself and is zero throughout the substrate material [3].

For small deformations in the system where the configuration assumes a uniform spherical shape with curvature $K$ and an extensional strain of the substrate mid-plane $\epsilon_0$, the displacement components are given by

$$u(r) = \epsilon_0 r, \quad w(r) = \frac{Kr^2}{2}.$$  

Substituting Eq. (12) in Eq. (11) results in

$$\epsilon_r = \epsilon_{ww} = \epsilon_0 - Kz + \epsilon_m.$$  

Using Eq. (13), Eq. (10) reduces to

$$U^f(r, z) = \frac{2}{r} \left[ \left( \frac{C_{11}^2-C_{12}^2}{C_{11}} \right) \epsilon_{rr}^2 + \epsilon_{ww}^2 \right] + 2 \left( \frac{C_{11}C_{12}-C_{12}^2}{C_{11}} \right) \epsilon_{rr}\epsilon_{ww}.$$  

Assuming the film material to be elastically isotropic, the strain energy density in the film, $U^f(r, z)$ for the plane stress case can be written as

$$U^f(r, z) = \frac{1}{2} \left[ E_f \left( \frac{\epsilon_{rr}^2}{1-\nu_f^2} + \epsilon_{ww}^2 + 2\nu_f \epsilon_{rr}\epsilon_{ww} \right) \right].$$

where $E_f$ and $\nu_f$ denote the Young’s modulus of elasticity and the Poisson’s ratio of the film material, respectively. Substituting Eq. (13) in Eq. (15) results in

$$U^f(r, z) = \frac{E_f}{1-\nu_f} \left[ \epsilon_{rr}^2 + \epsilon_{ww}^2 + 2\nu_f \epsilon_{rr}\epsilon_{ww} \right].$$

where $E_f$ and $\nu_f$ denote the Young’s modulus of elasticity and the Poisson’s ratio of the film material. Comparing Eqs. (16) and (14), $1/(s_{11} + s_{12})$ represents an equivalent biaxial modulus for the Si(001) wafer material. A similar observation was made by Janssen et al. [8] while deriving Eq. (3). Hence, Eq. (14) can be written as

$$U^f(r, z) = \epsilon_{rr}^2 M_f,$$

where $M_f$ is the biaxial modulus of the film material. Comparing Eqs. (16) and (14), $1/(s_{11} + s_{12})$ represents an equivalent biaxial modulus for the Si(001) wafer material. A similar observation was made by Janssen et al. [8] while deriving Eq. (3). Hence, Eq. (14) can be written as

$$U^f(r, z) = \epsilon_{rr}^2 M_f.$$  

The total potential energy of the system in terms of $\epsilon_0$ and $K$ is given by [3]

$$V(\epsilon_0, K) = 2\pi \int_0^R \left[ \frac{d}{2} U^f(r, z) dz \right] + 2\pi \int_0^R \frac{h_f/2}{h_s/2} U^f(r, z) r dz = V^f(\epsilon_0, K) + V^l(\epsilon_0, K).$$
The equilibrium condition requires the potential energy to be stationary and hence \( \partial V / \partial K = 0 \) and \( \partial V / \partial \epsilon_0 = 0 \). The potential energy of the substrate can be written as

\[
V'(\epsilon_0, K) = 2\pi \int_{-h/2}^{h/2} M_f (\epsilon_0 - K z)^2 \ r \ dr dz = M_f \pi R^2 \left[ \frac{K^2 h_0^2}{12} + \epsilon_0^2 h_0 \right].
\]  

(19)

Note that in the above integral, \( \epsilon_r \) is replaced by \( (13) \) with \( \epsilon_m = 0 \) for the substrate.

The potential energy of the film can be written as

\[
V'(\epsilon_0, K) = 2\pi \int_{-h/2}^{h/2} M_f (\epsilon_0 - K z + \epsilon_m)^2 \ r \ dr dz = M_f \pi R^2 \left[ \frac{K^2 h_0^2}{12} \left( 4 h^3 + 6 h^2 + 3 h \right) + (\epsilon_0 + \epsilon_m)^2 \ h - (\epsilon_0 + \epsilon_m) K h_0^2 \left( h^2 + h \right) \right],
\]  

(20)

where \( h = h_f/h_0 \).

The first condition for stationary potential energy leads to

\[
\frac{\partial V}{\partial \epsilon_0} + \frac{\partial V}{\partial \epsilon_m} = 0 \Rightarrow M_f \pi R^2 (2 \epsilon_0 h_0) + M_f \pi R^2 \left[ 2(\epsilon_0 + \epsilon_m) h h - K h_0^2 \left( h^2 + h \right) \right] = 0.
\]  

(21)

Let \( M_f/M \) be represented by \( m \) so that Eq. (21) can be written as

\[
\epsilon_0 = \frac{K m h_0 \left( h^2 + h \right) - 2 \epsilon_m h m}{2(1 + h m)}.
\]  

(22)

The second condition for stationary potential energy results in

\[
\frac{\partial V}{\partial K} = \frac{\partial V}{\partial \epsilon_m} = 0 \Rightarrow M_f \pi R^2 \left( \frac{K h_0^2}{6} \right) + M_f \pi R^2 \left[ \frac{K h_0^2}{6} \left( 4 h^3 + 6 h^2 + 3 h \right) - \epsilon_0 (\epsilon_0 + \epsilon_m) \left( h^2 + h \right) \right] = 0.
\]  

(23)

Substituting Eq. (22) in Eq. (23) and further simplifying results in

\[
K = \left( \frac{6 \epsilon_m h m}{h_0} \right) \left[ \frac{1 + h}{1 + h m (4 + 6 h + 4 h^2) + h^2 m^2} \right].
\]  

(24)

For the film to conform perfectly onto the substrate, strain compatibility should be satisfied as given by

\[
\epsilon_f^{\text{elastic}} - \epsilon_m = \epsilon_f^{\text{elastic}} (z = h_f/2),
\]  

(25)

where

\[
\epsilon_f^{\text{elastic}} = \left( \frac{1 - v_f}{E_f} \right) \sigma_f,
\]  

(26)

\[
\epsilon_f^{\text{elastic}} (z = h_f/2) = (s_{11} + s_{12}) \left( -\frac{4h_f}{h_0} \right) \sigma_f.
\]  

(27)

Substituting Eqs. (26) and (27) in Eq. (25)

\[
\sigma_f = \epsilon_m M_f \left( \frac{1 - v_f}{E_f} + (s_{11} + s_{12}) \frac{4h_f}{h_0} \right) \frac{1 + h m (4 + 6 h + 4 h^2) + h^2 m^2}{1 + h m (4 + 6 h + 4 h^2) + h^2 m^2} \Rightarrow \epsilon_m = \frac{\sigma_f (1 + 4 h m)}{M_f}.
\]  

(28)

Substituting Eq. (28) in Eq. (24)

\[
K = \left( \frac{6 h_f \sigma_f (1 + 4 h m)}{M_f} \right) \left[ \frac{1 + h}{1 + h m (4 + 6 h + 4 h^2) + h^2 m^2} \right] = \left( \frac{6 h_f \sigma_f (1 + 4 h m)}{M_f} \right) \left[ \frac{(1 + h)(1 + 4 h m)}{1 + h m (4 + 6 h + 4 h^2) + h^2 m^2} \right] \frac{(1 + h)(1 + 4 h m)}{1 + h m (4 + 6 h + 4 h^2) + h^2 m^2}.
\]  

(29)
From Eq. (3), it is clear that the term in parentheses in the above equation is the curvature according to the Stoney equation derived for Si(001) wafer substrates by Janssen et al. [8]. Therefore, Eq. (29) can be rewritten as

\[ K = K_{\text{st}}^{\text{Si(001)}} \left( \frac{(1 + h)(1 + 4hm)}{1 + hm(4 + 6h + 4h^2) + h^4m^4} \right). \]  

(30)

By substituting back the thin film assumption that \( h << h_0 \), i.e. \( h \rightarrow 0 \) in this equation, the curvature of the system approaches \( K_{\text{st}}^{\text{Si(001)}} \). Eq. (30) has an additional term multiplied in the numerator \( (1 + 4hm) \) when compared with the equation presented by Freund et al. [3]. This term accounts for the cases when the biaxial moduli of the film and substrate materials are comparable. Furthermore, Eq. (24) was also derived by Murray and Saenger [10] through a force and moment equilibrium approach.

2.2. Modified Stoney equation for thin Si(111) wafer substrate

In the previous case, the deformation of the Si(001) wafer took place in the frame of the wafer which is the same as the frame of the crystal in which the constitutive equation is written. For Si(111) wafer, the [111] direction is perpendicular to the plane of the wafer. The deformation of the substrate takes place in the frame of the wafer while the constitutive equation is written in the frame of the Si crystal, which in this case do not match. In order to formulate the elastic deformation of the Si(111) wafer, the axes representing the constitutive equation are rotated to coincide with the coordinate system used to describe the deformation in the wafer. For this, an approach similar to that followed by Janssen et al. [8] is used.

Let \( \mathbf{x}_1 = 1/\sqrt{2}(1 \quad 1 \quad 0) \), \( \mathbf{x}_2 = 1/\sqrt{6}(1 \quad 1 \quad -2)^T \) and \( \mathbf{x}_3 = 1/\sqrt{3}(1 \quad 1 \quad 1)^T \) be the orthonormal basis to describe the deformation of the wafer. Here, \( \mathbf{x}_3 \) represents a unit vector perpendicular to the plane of the wafer while \( \mathbf{x}_1 \) and \( \mathbf{x}_2 \) represent two randomly chosen mutually orthonormal vectors in the plane of the wafer. Let \( \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 \) where \( \mathbf{x}_1 = (1 \quad 0 \quad 0)^T \), \( \mathbf{x}_2 = (0 \quad 1 \quad 0)^T \), and \( \mathbf{x}_3 = (0 \quad 0 \quad 1)^T \), represent the orthonormal basis that form the coordinate system of the crystal. In order to describe the elastic response of the substrate, the coordinate system represented by \( (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \) is to be rotated to match the coordinate system represented by \( (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \). The transformation matrix associated with this transformation is given by

\[ \mathbf{T} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{6} & 1/\sqrt{3} \\ -1/\sqrt{2} & 1/\sqrt{6} & 1/\sqrt{3} \\ 0 & -2/\sqrt{6} & 1/\sqrt{3} \end{pmatrix}, \]

(31)

and the inverse of this transformation matrix is the same as its transpose, i.e. \( \mathbf{T}^{-1} = \mathbf{T}^T \).

The stress and strain tensors in the rotated frame are given by \( \mathbf{\sigma} = \mathbf{T}^T \mathbf{\sigma} \mathbf{T} \) and \( \mathbf{\epsilon} = \mathbf{T}^T \mathbf{\epsilon} \mathbf{T} \), respectively. Due to orthogonality of the transformation matrix, the transformed compliance matrix takes the form \( \mathbf{S} = \mathbf{T}^T \mathbf{S} \mathbf{T} \), which can be represented as

\[ \mathbf{S} = \mathbf{T}^T \mathbf{S} \mathbf{T} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}, \]

(32)

where

\[ \mathbf{A} = \begin{pmatrix} \frac{s_{11}}{6} + \frac{s_{12}}{3} + \frac{s_{44}}{4} & \frac{s_{11}}{6} + \frac{s_{12}}{3} + \frac{s_{44}}{4} & \frac{s_{11}}{6} + \frac{s_{12}}{3} - \frac{s_{44}}{6} \\ \frac{s_{11}}{6} + \frac{s_{12}}{3} + \frac{s_{44}}{4} & \frac{s_{11}}{6} + \frac{s_{12}}{3} + \frac{s_{44}}{4} & \frac{s_{11}}{6} + \frac{s_{12}}{3} - \frac{s_{44}}{6} \\ \frac{s_{11}}{6} + \frac{s_{12}}{3} + \frac{s_{44}}{4} & \frac{s_{11}}{6} + \frac{s_{12}}{3} + \frac{s_{44}}{4} & \frac{s_{11}}{6} + \frac{s_{12}}{3} - \frac{s_{44}}{6} \end{pmatrix}, \]

\[ \mathbf{B} = \begin{pmatrix} \frac{\sqrt{2}s_{11}}{3} - \frac{\sqrt{2}s_{12}}{3} - \frac{\sqrt{2}s_{44}}{6} & 0 & 0 \\ \frac{\sqrt{2}s_{11}}{3} - \frac{\sqrt{2}s_{12}}{3} - \frac{\sqrt{2}s_{44}}{6} & 0 & 0 \\ \frac{\sqrt{2}s_{11}}{3} - \frac{\sqrt{2}s_{12}}{3} - \frac{\sqrt{2}s_{44}}{6} & 0 & 0 \end{pmatrix}, \]

\[ \mathbf{C} = \begin{pmatrix} \sqrt{2}\left(\frac{s_{11}}{3} - \frac{s_{12}}{3} - \frac{s_{44}}{6}\right) & \sqrt{2}\left(\frac{s_{11}}{3} - \frac{s_{12}}{3} + \frac{s_{44}}{6}\right) & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \]

\[ \mathbf{D} = \begin{pmatrix} \frac{4}{3}(s_{11} - s_{12} + s_{44}) & 0 & 0 \\ 0 & \left(\frac{4}{3}(s_{11} - s_{12} + s_{44})\right) & \left(\frac{\sqrt{2}}{3}(2s_{11} - 2s_{12} - s_{44})\right) \\ 0 & \left(\frac{\sqrt{2}}{3}(2s_{11} - 2s_{12} - s_{44})\right) & \frac{2}{3}(s_{11} - s_{12} + s_{44}) \end{pmatrix}. \]
From Eq. (32)

\[ \epsilon_{rr} = \left( \frac{s_{11}}{2} + \frac{s_{12}}{2} + \frac{s_{44}}{4} \right) \sigma_{rr} + \left( \frac{s_{11}}{6} + \frac{s_{12}}{6} - \frac{s_{44}}{12} \right) \sigma_{\theta \theta} = A\sigma_{rr} + B\sigma_{\theta \theta}, \]  

(33)

\[ \epsilon_{\theta \theta} = \left( \frac{s_{11}}{6} + \frac{s_{12}}{6} - \frac{s_{44}}{12} \right) \sigma_{rr} + \left( \frac{s_{11}}{2} + \frac{s_{12}}{2} + \frac{s_{44}}{4} \right) \sigma_{\theta \theta} = B\sigma_{rr} + A\sigma_{\theta \theta}. \]  

(34)

Solving Eqs. (33) and (34) leads to

\[ \sigma_{rr} = \frac{1}{A^2 - B^2} (A\epsilon_{rr} - B\epsilon_{\theta \theta}), \]  

(35)

\[ \sigma_{\theta \theta} = \frac{1}{A^2 - B^2} (A\epsilon_{\theta \theta} - B\epsilon_{rr}). \]  

(36)

From Eqs. (6) and (13)

\[ U^f(r, z) = \frac{1}{A^2 + B^2} \epsilon_{rr}^2 = \left( \frac{6}{4s_{11} + 8s_{12} + s_{44}} \right) \epsilon_{rr}^2 = M_r \epsilon_{rr}^2, \]  

(37)

where \( M_r \) represents the equivalent biaxial modulus for the Si(111) wafer. On following the same approach as before, the curvature of the substrate in this case turns out to be

\[ K = \left( \frac{6s_{11}h_f}{h_i^2} \times \frac{4s_{11} + 8s_{12} + s_{44}}{6} \right) \left[ \frac{(1 + h)(1 + 4hm)}{1 + hm(4 + 6h + 4h^2) + h^4m^2} \right]. \]  

(38)

From Eq. (4) it is clear that the term in the parentheses in the above equation is the curvature according to the Stoney equation derived for Si(111) wafer substrates by Janssen et al. [8]. Therefore, the above equation takes the same form as Eq. (30), i.e.,

\[ K = K^f_{Si(111)} \left[ \frac{(1 + h)(1 + 4hm)}{1 + hm(4 + 6h + 4h^2) + h^4m^2} \right]. \]  

(39)

### 2.3. Configurations with bilayered films and thin substrates

Fig. 2 shows the configuration of a bilayer film deposited on a substrate. In Fig. 2, \( h_f \) represents the substrate thickness, and \( h_1 \) and \( h_2 \) represent the thicknesses of each layer in the bilayered film, respectively. The current discussion is limited to the case where both films are of equal thickness, \( h_f \). Let the biaxial modulus of the substrate be \( M_s \) and those of the two layers in the film be \( M_{f1} \) and \( M_{f2} \), respectively. The mismatch strains in layer 1 and layer 2 of the film are represented by \( \epsilon_{m1} \) and \( \epsilon_{m2} \), respectively. All other assumptions regarding the stresses in the system remain the same as in the previous sections.

The total potential energy of the system is given as

\[ V(\epsilon_0, K) = V^1(\epsilon_0, K) + V^2(\epsilon_0, K) + V^f(\epsilon_0, K), \]  

(40)

where

\[ V^f(\epsilon_0, K) = 2\pi \int_{0}^{R} \int_{h_f/2}^{h_f/2} U^f(r, z) r dr dz. \]  

(41)

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**Fig. 2.** Bilayered film deposited on a circular substrate.
Furthermore, \( K_{th} = \frac{1}{2} M f \) whereas Eq.(51) can be used even when the layers are anisotropic. A proper substitution of the biaxial modulii in place of \( K_{th} \) results in Eq.(24).

From Eq.(20)

Using Eqs. (19), (45) and (46), the first condition for stationary potential energy results in

The second condition for stationary potential energy leads to

Substituting Eq. (48) in Eq. (49)

Simplification of Eq. (50) results in

It is worth noting that Eq. (51) can be used irrespective of the in-plane geometry of the system, in the small deformation regime. The mathematical model for the curvature of a rectangular multilayer system undergoing small deformations was derived by Nikishkov [11]. The equation derived by Nikishkov is equivalent to Eq. (51), on considering three layers. However, the formula derived by Nikishkov considers elastically isotropic layers, whereas Eq. (51) can be used even when the layers are anisotropic. A proper substitution of the biaxial modulii in place of \( M_f \) and \( M_s \) is sufficient. For a special case where the layers of the film are made of the same material and share a common mismatch strain, \( m_1 \) and \( m_2 \) are replaced with \( m \) in (51). Furthermore, \( \epsilon_m \) and \( \epsilon_m \) are replaced with \( \epsilon_m \). Also, \( h \) must be replaced by \( H/2 \) where \( H \) is the ratio of total film thickness to the thickness of the substrate. On making these changes Eq. (51) reduces to Eq. (24)
3. Discussion

Curvature relations represented by Eqs. (30) and (39) reduce to the Stoney equations derived for the cases of Si(001) and Si(111) by Janssen et al. [8], when the thin film assumption that \( h_f \ll h_s \) is incorporated. When the biaxial modulii of the substrate and film materials are the same (\( m = 1 \)), then Eqs. (30) and (39) result in

\[
\frac{K}{K_{st}} = \frac{(1 + 4h)}{(1 + h)^2}
\]

Considering a thickness ratio of 0.1, the deviation from the Stoney equation for this case would be approximately 5% with respect to the derived formulae. Whereas this deviation is overestimated by the expression derived by Freund et al. [3] as 30% (for isotropic substrates), as the expression for \( K_{st} \) in the paper does not account for the case when the biaxial modulii of the film and substrate materials are comparable. It is to be noted that if the mismatch strain is large enough, then the system would assume a stable non-axisymmetric (ellipsoidal) shape rather than a spherical shape [9]. The variation of curvature with respect to the conventional Stoney equation is shown in Fig. 3, where the value of \( K/K_{st} \) is indicated against each contour. The region between curves A and B depicts the area, where using the Stoney equation would result in a deviation within 10%, from the equations derived.

4. Conclusions

Stress curvature relations have been derived for configurations with thin and anisotropic substrates (Eqs. (30) and (39)) using the equilibrium condition of stationary potential energy. The same method has been extended to derive a formula for the curvature of a system with a bilayered film and a thin substrate, due to thin film elastic mismatch (Eq. (51)). These equations can also be used when the film material is also anisotropic. Depending on the material, an equivalent biaxial modulus is to be substituted in place of \( M_f \). The formulae derived for thin Si(001) and Si(111) wafer substrates reduce to existing results [8] in the limit of thick substrates.

References