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

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ABSTRACT

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.

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].

$$\sigma_f = \frac{E_s h_s^2}{6(1-\nu_s)h_f} K. \quad (1)$$

Here, σ_f represents the stress in the film, which is assumed to be uniform and biaxial in nature. E_s, h_s and ν_s 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].

$$\sigma_f h_f = \frac{E_s h_s^2}{6R}. \quad (2)$$

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_s with the biaxial modulus $E_s/(1-\upsilon_s)$ 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]

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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

$$\sigma_f h_f = \frac{h_s^2}{6(s_{11}^{Si} + s_{12}^{Si})R}. \tag{3}$$

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

$$\sigma_f h_f = \left(\frac{6}{4s_{11}^{Si} + 8s_{12}^{Si} + s_{44}^{Si}}\right)\frac{h_s^2}{6R}, \tag{4}$$

where s_{ij}^{Si} 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 $h_f \ll h_s$. 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,θ,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 θ 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].

$$\begin{pmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \\ \sigma_{\theta z} \\ \sigma_{rz} \\ \sigma_{r\theta} \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{pmatrix} \begin{pmatrix} \epsilon_{rr} \\ \epsilon_{\theta\theta} \\ \epsilon_{zz} \\ 2\epsilon_{\theta z} \\ 2\epsilon_{rz} \\ 2\epsilon_{r\theta} \end{pmatrix}, \tag{5}$$

where σ_{ij}: components of stress tensor, c_{ij}: elastic stiffness constants of Si and ϵ_{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 σ_{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

$$U(r,z) = \frac{1}{2}\sum(\sigma_i \epsilon_i), \tag{6}$$

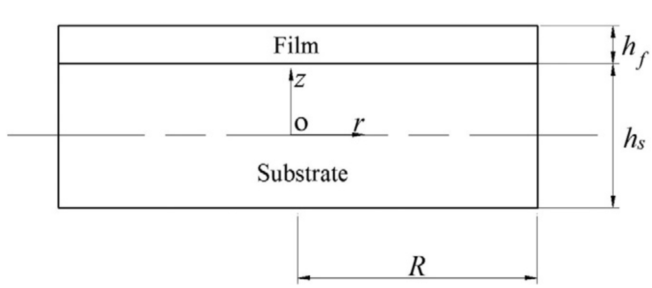

Fig. 1. Circular film deposited on a circular anisotropic substrate.