Elastic Bending of Semiconductor Wafer Revisited and Comments on Stoney's Equation

S. N. G. Chu*

Bell Laboratories, Lucent Technologies, Murray Hill, New Jersey 07974, USA

ABSTRACT

Since Stoney derived a simple relationship between the stress of a thin film and the curvature of its substrate for an electrolytically deposited metallic film on a thick substrate plate in 1909, the equation has been widely used by electrochemists to calculate stresses in electrolytically deposited films. Although the equation seems to work well for thin films with negligible thickness in comparison to the substrate, the underlying assumption in his derivation is found to be questionable. Various works have been published which calculate more precisely the stresses in the bending of a two-layer composite plate, where a thin layer on a thick substrate is an extreme case. However, there is some confusion in differentiating elastic bending due to internal stress from the externally applied moments (including our previous work). We re-examine the two bending conditions and point out that Stoney's equation was derived based on a neutral axis for zero bending moment which does not exist in the pure bending of a steel ruler on which his derivation was based. We also show that a single neutral axis for stresses does not exist in a two-layer system bent by internal stresses. Finally, we rederive the formula for the relationship between the wafer curvature and the lattice mismatch or differential thermal expansion for a binary composite plate using the proper bending moment calculation and examine the case of wafer bending of GaAs on Si substrate.

Introduction

Although elastic bending of semiconductor wafers or metal plates caused by deposited surface thin films can in general be treated by the methods of orthotropic elasticity in bending of laminated composite materials for construction and structural applications,[1-7] the simple relationship between the film stress and the bending curvature derived 88 years ago by Stoney[8] based on isotropic elasticity is still the most widely used by the electrochemist for electrolytically deposited films on a thick substrate and more recently, due to its simplicity, in the semiconductor industry for thin films on thick wafers. More refined calculation for wafer bending by surface layers has been done by many authors.[8-21] In principle, a precise expression for film stresses including the elastic anisotropy of the materials can be derived from the continuum theory of a laminated medium. However, unlike the thick plates used in the laminated composite, elastic anisotropy of most submicron thin films deposited on semiconductor substrates has not yet been studied in detail. On the other hand, the expressions derived based on the isotropic elasticity seem to work reasonably well. Commercial equipment is now available for characterizing film stresses based on the Stoney equation.[22] Large deviation does appear when the film thickness is non-negligible compared to the substrate. In refined calculations of a strained film on a substrate due to lattice mismatch or differential thermal expansion, confusion may arise in the bending moment calculation as to whether the bending moments of the indivdual beams are simply additive[9] and, in the case of bending by internal stresses such as due to differential thermal expansion or lattice mismatch, whether the total bending moment of the composite should be set to zero[10] under no externally applied moment. This also applies to the continuum theory of a laminated medium where a correct moment balance condition must be set in the beginning of the formulation. This study re-examines the two cases of simple bending of a two-layer composite beam or plate by an external moment and by internal stresses. It points out that the bending moments of individual beams are not additive for a composite beam with welded interfaces, and that the total bending moment cannot be zero as long as an elastic bending curvature exists. We further point out that a single neutral axis for stress exists only in the case of bending by an external moment and the Davidenkov's method[11] of moment calculation for a composite beam, which was previously used by us for calculating wafer bending by misfit stresses,[19] applies only to the case of bending by an external moment. The proper relationships between the bending curvature and the mismatch strain as well as the film stresses are, therefore, rederived and compared with the Stoney equation. The differences with our previous calculation are addressed. An example of GaAs on Si is used to demonstrate the effects of relative thickness and moduli on the bending curvature and stresses.

Bending of a Two-Phase Composite Beam with a Welded Interface

A classic example of bending of a two-phase composite elastic medium with a nonslippery or welded interface is the bending of a bimetallic strip. The elastic problem was first treated by Timoshenko in 1925.[9] However, in his calculation of the bending moment of the composite stripe, a linear superposition of the individual moments was used, but it is shown in the following that for a composite beam with a welded interface the bending moments are not additive.

Let us consider a composite beam of length ℓ and width w formed by two beams of thickness t_1 and t_2, respectively. For simplicity, we set $w = 1$. The two beams are welded together along the interface as shown in Fig. 1a. Let E_1 and E_2, ν_1 and ν_2, and α_1 and α_2, are the Young's moduli, Poisson's ratio, and thermal expansion coefficients of the beams, respectively. The simple beam bending formulation can be converted into a two-dimensional bending of a square plate by replacing E with $K = E/(1\text{-}\nu)$ for the biaxial stress case.

Bending of the Beam

A composite beam can be bent by an externally applied bending moment M, as shown in Fig. 1b, and/or by a moment generated from the internal stresses such as differential thermal expansion of the two beams upon heating as shown in Fig. 1c. In the latter case, since there is no externally applied moment to the beam, it tends to improperly set the total bending moment to zero even though the beam has a bending curvature.[10] Let us examine the case of bending of a bimetallic stripe due to differential thermal expansion (TEC) upon heating. Assuming $\alpha_2 > \alpha_1$, upon heating from room temperature to a higher temperature, beam 2 expands more than beam 1. Since it is constrained from full expansion by beam 1, it stretches beam 1 beyond its fully expanded length. Therefore beam 1 is under tension, and beam 2 is under compression. The expansion of beam 2 and the contraction of beam 1 produces a force-couple which bends the composite beam convexly upward. The confusion arises from the fact that beam 1 is under compression and beam 2 is under tension, the corresponding force-couple calculated from the stress fields results in a bending moment opposite to the curvature of the beam. This is because in the bending by internal stresses, it is the force of reaction which constitutes the bending of the structure as

* Electrochemical Society Fellow.

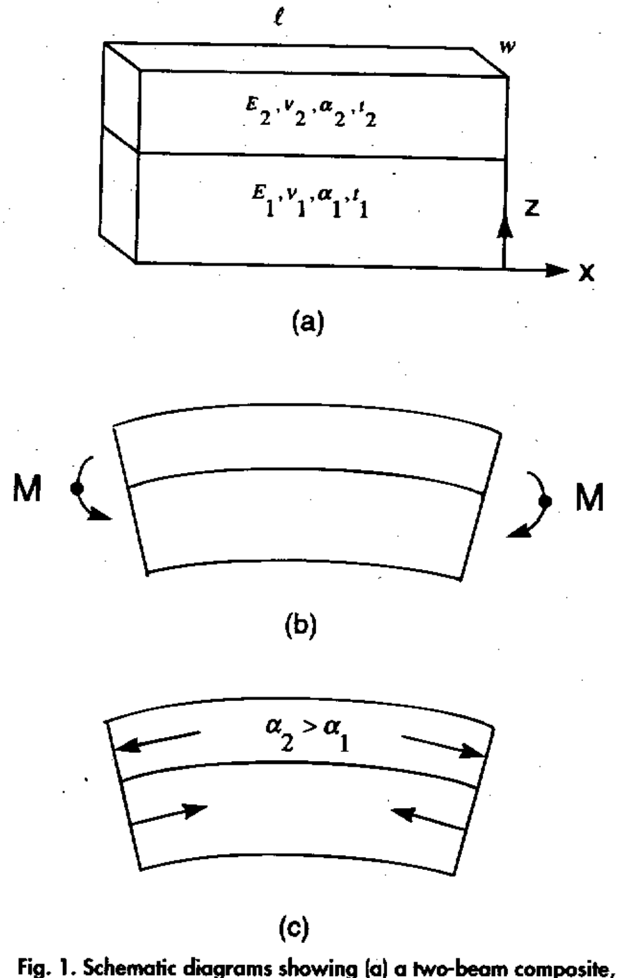

Fig. 1. Schematic diagrams showing (a) a two-beam composite, (b) bending by an external moment M, and (c) bending by internal stresses due to differential TEC upon heating.

opposed to the case of bending by external stresses where the force of action bends the structure. For a composite beam with three or more phases it is also possible to achieve a zero net bending moment upon heating. Then the corresponding curvature of bending will also be zero. Therefore as long as there is an elastic bending curvature, there will be a net bending moment whether it is due to internal or externally applied stresses. In a complex bending configuration, as shown in Fig. 2, where the bending curvature is a function of position, a neutral axis for bending, AB, is defined at the position where the bending curvature is zero. Obviously such a neutral axis does not exist in the simple bending configuration shown in Fig. 1 where the bending curvature is a nonzero constant.

Stoney Equation

Stoney considered the case of a thin metal film of thickness t deposited on a thick steel ruler of thickness d where the metal film was under tension and therefore the composite bent concave upward as shown in Fig. 3. Since t was negligible in comparison with d and both t and d were negligible in comparison with the radius of curvature r, he considered that the film was under tension only and the steel ruler was under simple bending with a constant radius of curvature r. The first equation in his paper on p. 174,[8] which is given in the original form here, set the condition for the position of a neutral axis b from the surface of the steel ruler by taking the moment for the steel ruler to zero

$$\int_d^0 \frac{E}{r}(b - x)x\,dx = 0 \quad \text{so that } b = 2d/3 \qquad [1]$$

where E is the Young's modulus of the steel ruler, and the width of the ruler is unity. As described previously, such a neutral axis does not exist in a simple bending with a constant radius of curvature r. (Note that the conventional definition of neutral axis for bending is the locus of zero stress in the plate where the stress field changes from tensile to compressive. Therefore instead of Eq. 1, the position b should be determined by $\int_d^0 E/r(b - x)dx = 0$ for pure bending which gives $b = d/2$.[23])

By using the value of $b = 2d/3$ as a neutral axis for stress in the force balance condition between the film and the steel ruler, he obtained a relationship between the stress in the film, P, and the bending curvature $1/r$ of the steel ruler in the second equation of his paper, which is again given in the original form

$$Pt = \int_d^0 \frac{E}{r}(b - r)dx \qquad [2]$$

$$= \frac{E}{r}\left(bd - \frac{d^2}{2}\right) = \frac{1}{6}E\frac{d^2}{r} \qquad [3]$$

where P is the uniaxial tension in the film, and E is the Young's modulus of the steel ruler.

Since the bending strain or stress of the film is neglected, substituting $P = E_f\Delta\epsilon$, into Eq. 3, where $\Delta\epsilon$ is the uniaxial strain in the film and E_f is the Young's modulus of the film one obtains the frequently used Stoney equation for calculating bending curvature from differential strain

$$\frac{1}{r} = \frac{6t}{d^2}\frac{E_f}{E}\Delta\epsilon \qquad [4]$$

where $\Delta\epsilon = \Delta\alpha\Delta T$, $\Delta\alpha = \alpha_2 - \alpha_1$, and $\Delta T = T - T_0$ for differential TEC. For a biaxial stress case, one can simply replace E by K.

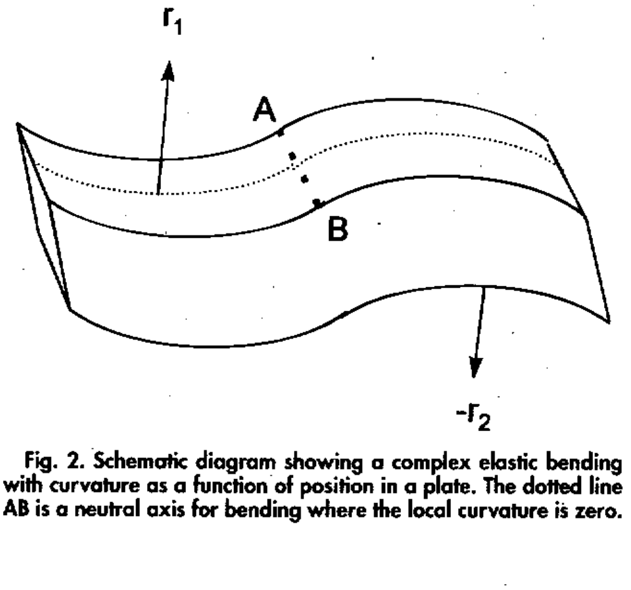

Fig. 2. Schematic diagram showing a complex elastic bending with curvature as a function of position in a plate. The dotted line AB is a neutral axis for bending where the local curvature is zero.

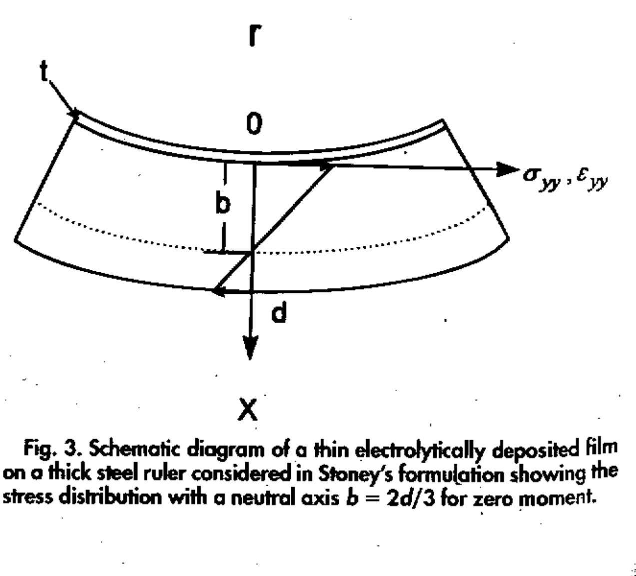

Fig. 3. Schematic diagram of a thin electrolytically deposited film on a thick steel ruler considered in Stoney's formulation showing the stress distribution with a neutral axis $b = 2d/3$ for zero moment.

Not only does the neutral axis set by Eq. 1 not exist for a simple bending configuration with a constant radius of curvature as illustrated in Fig. 3, but the use of such a neutral axis for bending moment as a neutral axis for the stress in Eq. 2, i.e., $E(b-x)/r$, is even more confusing. If the conventional definition of neutral axis for stress in a pure bending is used, i.e., $b = d/2$, [23] Eq. 2 yields $Pt = 0$. In other words the Stoney Eq. 3 or 4 would not have been derived.

Neutral Axis of the Bend Beam

In pure bending of a simple beam, the stress component σ_{xx} changes continuously from tensile on the convex side of the beam to compressive on the concave side of the beam. The crossover point defines the position of the neutral axis.[23] In the simple bending of a composite beam, each beam experiences both bending and uniaxial tension or compression. It is important to know the positions of the neutral axis in each beam in order to properly calculate the stress field and hence the bending moment. Davidenkov had treated the problem of elastic bending of a composite beam[11] under an applied moment by assuming a single neutral axis in the bent composite. The method was later used by us to calculate wafer bending of multilayer structures due to lattice mismatch.[19] It is shown below that a single neutral axis exists only in the case of bending by an externally applied moment but not for bending by internal stresses such as those due to misfit stresses or differential TEC.

Bending by externally applied moments.—Consider the case of bending of a composite beam by an applied bending moment M at the end of the beam as shown in Fig. 1b. The stress distribution across the thickness of the composite beam can be calculated by constructing the composite beam from two separated beams in two steps as described in Fig. 4. Specifically, the two individual beams with the same length ℓ are bent to the same final radius of curvature R by external bending moments M_1 and M_2 applied to the ends of the beams, respectively, as shown in Fig. 4a. Since both beams are under pure bending, the neutral axes are in the middle of each beam as indicated by the dotted line. Beam 2 is then stretched and beam 1 is compressed to match the interface at $z = t_1$. The two beams are then welded together into a composite beam as shown in Fig. 4b and c to produce the pure bending of a composite beam by an external moment M as shown in Fig. 1b. Since the final state is a pure bending, the forces applied to the two beams in Fig. 4b before the welding process should be added to zero. The equal and opposite force couple therefore creates an additional bending moment to the composite. Note also that the stretching of beam 1 moves the neutral downward and the compression of beam 2 moves the neutral axis upward as indicated by the arrows in Fig. 4b. The amount of movement is determined by the interface matching condition.

The corresponding stress fields in each beam, as shown in Fig. 4c, are given by

$$\sigma_{xx}^1 = E_1\left(\frac{z - \frac{t_1}{2}}{R} - \epsilon_1\right) \qquad [5]$$

and

$$\sigma_{xx}^2 = E_2\left(\frac{z - \frac{t_2}{2} - t_1}{R} + \epsilon_2\right) \qquad [6]$$

respectively, where the first term on the right is due to pure bending and the second term is due to uniaxial compression with a strain of $-\epsilon_1$ for beam 1 and uniaxial tension with a strain of ϵ_2 for beam 2. The shifting of the neutral axes, δ_1 and δ_2, from their pure bending positions in the middle of each beam can be found by setting $\sigma_{xx}^1 = \sigma_{xx}^2 = 0$, which gives $\delta_1 = \epsilon_1 R$ and $\delta_2 = \epsilon_2 R$. Let s be the separation between the two neutral axes, then

$$s = \frac{t_1 + t_2}{2} - (\delta_1 + \delta_2) = \frac{t_1 + t_2}{2} - R(\epsilon_1 + \epsilon_2) \qquad [7]$$

If the two neutral axes merge into one, $s = 0$. The amount of movement is determined by the uniaxial stresses in each beam to match the interface. The corresponding strain matching condition at the interface, $\epsilon_{xx}^1(t_1) = \epsilon_{xx}^2(t_1)$, gives

$$\frac{t_1}{2R} - \epsilon_1 = -\frac{t_2}{2R} + \epsilon_2 \qquad [8]$$

Substituting Eq. 8 into 7, indeed gives $s = 0$, which thus proves the existence of a single neutral axis in a composite

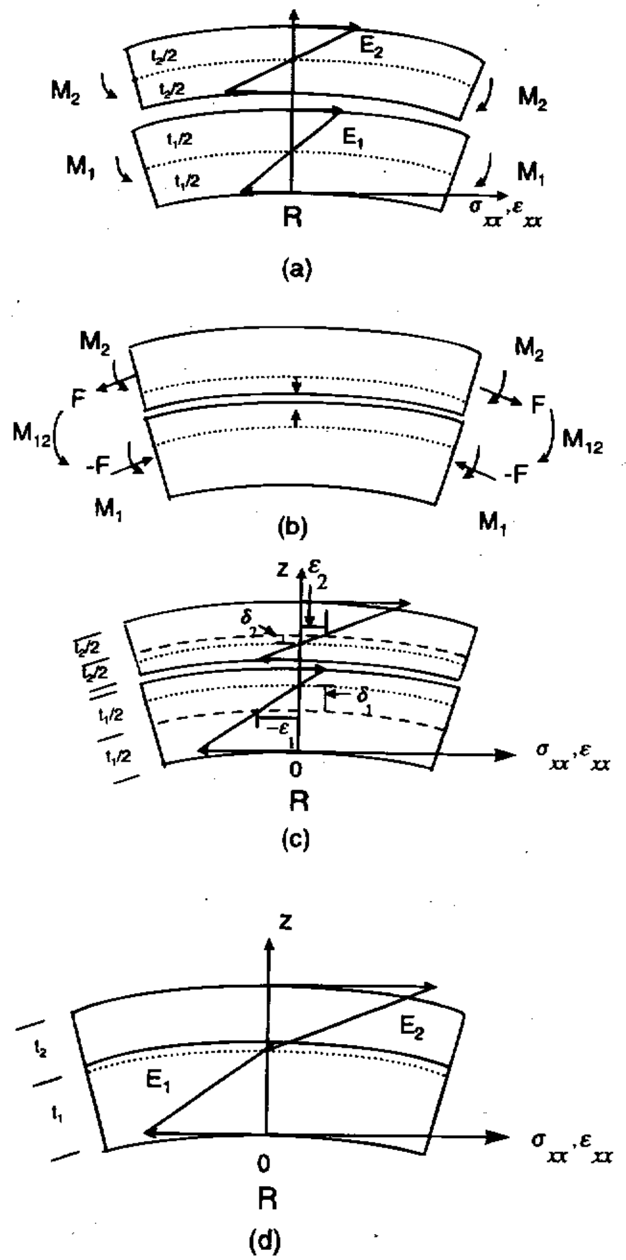

Fig. 4. Schematic diagrams of a two-step operation for constructing a composite beam bending by an external moment M showing (a) pure bending of two separated beams by external moments M_1 and M_2, respectively, to a final radius of curvature R and the positions of neutral axes for stress indicated by the dotted lines, (b) compressing beam 1 and stretching beam 2 by external forces to match the interface and the directions of shifting of the neutral axes as indicated by the arrows, (c) the corresponding stress distributions and the shifting of the neutral axes $\delta_{1,2}$ from the central axes of the beams by the applied uniaxial tensile and compressive stresses to the two beams, and (d) merging of the neutral axes into a single neutral axis after matching the boundary and welding of the two beams.

beam bent by an externally applied moment as shown in Fig. 4d. However, it is shown later that this is not the case for bending by internal stresses. Furthermore, because of the shifting of neutral axes in each of the beams, the bending moments of the individual beams are no longer additive in a composite beam.[9]

Nonadditivity of bending moments in a composite beam with a welded interface.—It is clear from Fig. 4b that in order to make a composite beam, additional stretch and compression are needed for the bent beams to match their interface. The force-couple generates an additional bending moment M_{12} besides the pure bending moments M_1 and M_2 for the individual beams. The total bending moment needed to achieve a radius of curvature R for a composite beam with a matching (welded) interface is therefore

$$M = M_1 + M_2 + M_{12} \qquad [9]$$

where $M_i = E_i I_i / R$, and $I_i = w t_i^3/12$ are the moments of inertia for the individual simple beams with width w and thickness t_i, for $i = 1, 2$, and

$$M_{12} = F\left(\frac{t_1 + t_2}{2}\right) \qquad [10]$$

where F is the magnitude of the tensile/compression forces given by the force balance condition

$$F = E_1 \epsilon_1 t_1 w = E_2 \epsilon_2 t_2 w \qquad [11]$$

where $w = 1$ in this calculation. Combining Eq. 11, 10, and 8, M_{12} becomes

$$M_{12} = \frac{E_1 E_2 t_1 t_2 (t_1 + t_2)^2}{4R(E_1 t_1 + E_2 t_2)} \qquad [12]$$

To test the validity of Eq. 9, we reduce the composite beam into a simple beam of thickness $t_1 + t_2$ by setting $E_1 = E_2 = E$. From Eq. 9 and 12, it is straightforward to show that

$$M = \frac{Ew(t_1 + t_2)^3}{12R} = \frac{EI}{R} \qquad [13]$$

which is the correct moment for pure bending of a simple beam. Therefore, for a composite beam with a welded interface, the bending moments of the individual beams are not additive in simple bending.

Bending by internal stresses.—Since there is no externally applied moment, it tends to falsely conclude that the net bending moment on the structure should be zero. The fact that elastic bending is created by a force-couple in an elastic medium does not depend on whether the force-couple is due to internal or external stresses. As long as there is an elastic bending, there is an associated bending moment. Let us examine in detail the case of bending due to internal stress. Consider the bending of a bimetallic strip upon heating as shown in Fig. 1c. Assuming $\alpha_2 > \alpha_1$, upon heating from the room temperature T_0 to a higher temperature T, beam 2 expands more than beam 1 and becomes longer than beam 1 by an amount $\Delta\alpha\Delta T\ell$, where $\Delta\alpha = \alpha_2 - \alpha_1$ and $\Delta T = T - T_0$. This causes the composite beam to bend convexly upward. To see how the neutral axes shift, we construct the bent composite beam again from two separated beams through a process similar to the case for external moment. In this case, since beam 2 is longer than beam 1, we first compress beam 2 and stretch beam 1 to match their lengths as shown in Fig. 5a, and then weld the two beams together. The applied forces are then removed so that beam 2 is free to expand and beam 1 is free to contract by the forces of the reaction as shown in Fig. 5b. In contrast to the previous case of bending by applied moment, here the force-couple of the reaction creates a bending moment which bends the composite. Even though the direction of the bending is the same as in the previous case, the uniaxial tension and compression states in the two beams are reversed due to internal stresses, i.e., beam 2 is under compression and beam 1 is under tension instead. As a result, the neutral axes in each beam move away from the other as shown in Fig. 5b. Therefore in a composite beam bent by internal stresses, a single neutral axis does not exist. This also applies to wafer bending by misfit stresses from lattice mismatched epi layers. It is now clear that in our previous treatment for the misfit stress in InGaAs/InP structures,[19] we incorrectly used Davidenkov method to calculate the stress field, which applies only to the case of bending by externally applied moment. We now rederive the relationship between the misfit strain and the wafer curvature below using two neutral axes.

Derivation of Relationship Between Differential Strain and Bending Curvature of a Two-Layer Composite Square Plate Due to Lattice Mismatch or Differential TEC

Although the direction of the bending moment calculated from the internal stresses is opposite to the bending curvature, the magnitude of the radius of curvature can be calculated from the stress field.

The stress fields in this case differs from that of Eq. 5 and 6 in the sign of the last term, they are

$$\sigma^1_{xx} = K_1\left(\frac{z - \frac{t_1}{2}}{R} + \epsilon_1\right) \qquad [14]$$

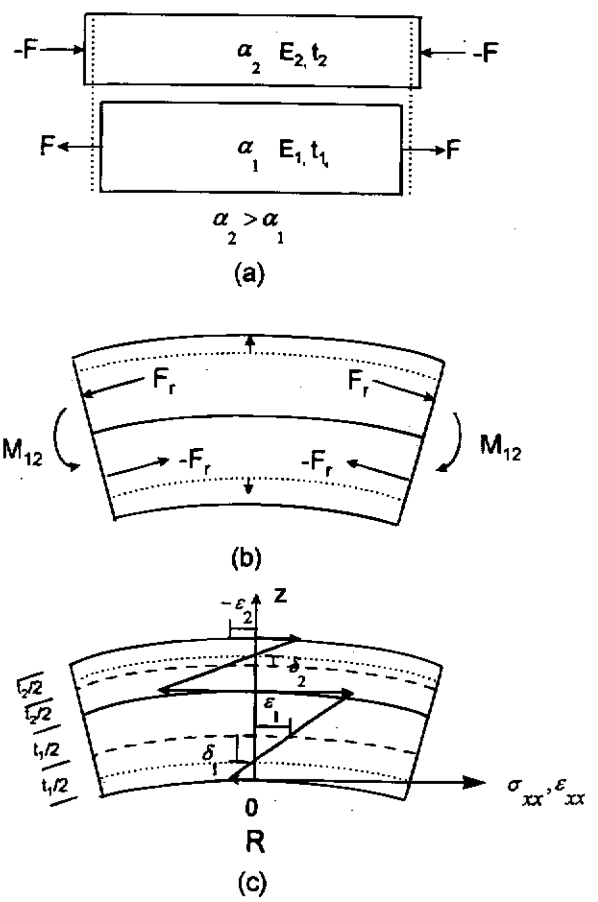

Fig. 5. Schematic diagrams of a two-step operation for constructing a composite beam bending by internal stresses due to differential TEC showing (a) stretching and compressing of the individual beams to match their lengths before welding, (b) bending of the composite beam after welding and removal of the external forces due to expansion and contraction of the beams by the forces of reaction and the moving apart of the neutral axes as indicated by the arrows, and (c) the stress distribution, the uniaxial tensile, and compressive strains and the shifting of the neutral axes.

and

$$\sigma_{xx}^2 = K_2\left(\frac{z - t_1 - \dfrac{t_2}{2}}{R} - \epsilon_2\right) \qquad [15]$$

respectively, for the two layers, as shown in Fig. 5c. Here we have replaced E_i by K_i for the biaxial stresses, where $i = 1$ and 2.

The corresponding forces on each layer are given by

$$F_1 = w\int_0^{t_1}\sigma_{xx}^1 dz = K_1\epsilon_1 t_1$$

and [16]

$$F_2 = w\int_{t_1}^{t_1+t_2}\sigma_{xx}^2 dz = -K_2\epsilon_2 t_2$$

respectively, where w is the width of the square plate.

The force balance requires, $F_1 + F_2 = 0$, which leads to $K_1\epsilon_1 t_1 w = K_2\epsilon_2 t_2 w = F$, where F is the magnitude of the forces. Let us consider again the case of differential TEC upon heating, with $\alpha_2 > \alpha_1$, and at a fixed temperature the boundary matching condition at $z = t_1$ is given by

$$\frac{t_1}{2R} + \epsilon_1 + \alpha_1\Delta T = -\frac{t_2}{2R} - \epsilon_2 + \alpha_2\Delta T \qquad [17]$$

Substituting $\epsilon_1 = F/K_1t_1w$ and $\epsilon_2 = F/K_2t_2w$ into Eq. 17, the magnitude of force F becomes,

$$F = K_2t_2w\left[\frac{\Delta\alpha\Delta T - \dfrac{t_1 + t_2}{2R}}{1 + \dfrac{K_2t_2}{K_1t_1}}\right] \qquad [18]$$

The bending moment in this case is generated by the forces of reaction F_r, which have the same magnitude as F but are in the opposite direction. The magnitude of the bending moment M is given by

$$M = |F_r|\left(\frac{t_1 + t_2}{2}\right) = K_2t_2w\left(\frac{t_1 + t_2}{2}\right)\left[\frac{\Delta\alpha\Delta T - \dfrac{t_1 + t_2}{2R}}{1 + \dfrac{K_2t_2}{K_1t_1}}\right] \qquad [19]$$

The value of M can also be calculated from the stress fields given by Eq. 14 and 15. It is straightforward to show that

$$M = w\int_0^{t_1}\sigma_{xx}^1 z dz + w\int_{t_1}^{t_1+t_2}\sigma_{xx}^2 z dz = \frac{K_1I_1 + K_2I_2}{R} - F\frac{t_1 + t_2}{2} \qquad [20]$$

where $I_i = wt_i^3/1, 2$, for $i = 1, 2$, and $-F(t_1 + t_2)/2$ is the interaction term.

Combining Eq. 18, 19, and 20, one obtains the following general relationship between the curvature and the differential strain $\Delta\epsilon$

$$\frac{1}{R} = \frac{\Delta\epsilon}{\dfrac{t_1}{2}\left[\dfrac{\left(1 + \dfrac{K_2I_2}{K_1I_1}\right)\left(1 + \dfrac{K_2t_2}{K_1t_1}\right)}{6\dfrac{K_2}{K_1}\dfrac{t_2}{t_1}\left(1 + \dfrac{t_2}{t_1}\right)} + \left(1 + \dfrac{t_2}{t_1}\right)\right]} \qquad [21]$$

where $\Delta\epsilon = \Delta\alpha\Delta T$ for TEC.

Equation 21 in general applies to a two-layer composite with differential strain $\Delta\epsilon$ of different origin. Therefore, for wafer bending by a lattice mismatched epi layer, one simply sets $\Delta\epsilon = \Delta a/a$ or $\Delta a/a - \rho b_{\text{II}}$ in the presence of misfit dislocations, where $\Delta a/a$, ρ, and b_{II} are the lattice misfit strain, linear density of misfit dislocations, and their Burgers vector parallel to the interface, respectively, to obtain the wafer curvature.

For most practical cases $t_2/t_1 < 0.01$, Eq. 21 reduces to the simple form

$$\frac{1}{R} = \frac{12\dfrac{K_2}{K_1}\dfrac{t_2}{t_1}}{t_1\left(1 + 6\dfrac{K_2}{K_1}\dfrac{t_2}{t_1}\right)}(\Delta\epsilon) \qquad [22]$$

Equation 22 differs from our previous formula for $1/R$ (Eq. 17 of Ref. 19) by a factor of $\sim 2\ K_2/K_1$. Note that in our previous formula, we set $K_2/K_1 = 1$ due to the unavailability of the Young's modulus and the Poisson's ratio for InGaAs. It is shown later that such a simplification can introduce significant deviation in lattice curvature.

Stress Fields

The expressions for the stress fields in each layer can be obtain by combining Eq. 14, 15, 18, 21, and $\epsilon_1 = F/K_1t_1w$ and $\epsilon_2 = F/K_2t_2w$. They are given in terms of R or $\Delta\epsilon$ as

$$\sigma_{xx}^1 = K_1\left[\left(z - \frac{t_1}{2}\right) + \frac{t_1\left(1 + \dfrac{K_2I_2}{K_1I_1}\right)}{12\left(1 + \dfrac{t_2}{t_1}\right)}\right]\frac{1}{R}$$

$$= K_1\left[\left(z - \frac{t_1}{2}\right) + \frac{t_1\left(1 + \dfrac{K_2I_2}{K_1I_1}\right)}{12\left(1 + \dfrac{t_2}{t_1}\right)}\right]\frac{\Delta\epsilon}{A} \qquad [23]$$

and

$$\sigma_{xx}^2 = K_2\left[\left(z - t_1 - \frac{t_2}{2}\right) - \frac{t_1\left(1 + \dfrac{K_2I_2}{K_1I_1}\right)}{12\dfrac{K_2t_2}{K_1t_1}\left(1 + \dfrac{t_2}{t_1}\right)}\right]\frac{1}{R}$$

$$= K_2\left[\left(z - t_1 - \frac{t_2}{2}\right) - \frac{t_1\left(1 + \dfrac{K_2I_2}{K_1I_1}\right)}{12\dfrac{K_2t_2}{K_1t_1}\left(1 + \dfrac{t_2}{t_1}\right)}\right]\frac{\Delta\epsilon}{A} \qquad [24]$$

for the substrate and layer, respectively, where

$$A = \frac{t_1}{2}\left[\frac{\left(1 + \dfrac{K_2I_2}{K_1I_1}\right)\left(1 + \dfrac{K_2t_2}{K_1t_1}\right)}{6\dfrac{K_2t_2}{K_1t_1}\left(1 + \dfrac{t_2}{t_1}\right)} + \left(1 + \frac{t_2}{t_1}\right)\right]$$

As shown in Fig. 5c, there is a discontinuity in the σ_{xx} at the interface, which is given by

$$\Delta\sigma_{xx}(t_1) = \sigma_{xx}^2(t_1) - \sigma_{xx}^1(t_1)$$

$$= -\frac{K_1t_1}{2}\left[\left(1 + \frac{K_2t_2}{K_1t_1}\right) + \frac{\left(1 + \dfrac{K_2I_2}{K_1I_1}\right)}{6\dfrac{t_2}{t_1}}\right]\frac{1}{R} \qquad [25]$$

This discontinuity in $\Delta\sigma_{xx}$ produces a maximum shear force at the interface. However, it is more realistic to think that the stress transition at the interface takes over a finite thickness instead of being atomically abrupt, then there will also be a neutral plane inside this transition region where the $\sigma_{xx} = 0$. In the extreme case where $t_2/t_1 << 1$, it is straightforward to show that $\Delta\sigma_{xx} \approx -K_2\ \Delta\epsilon$ and all the mismatch strain are distributed in the film as uniaxial compressive or tensile strain.

Discussion

To illustrate the dependence of bending curvature $1/R$ on various factors of the two-layer system described by Eq. 21, GaAs on Si is chosen because of the availability of their physical constants. The values used for the physical constants are $E_{GaAs} = 8.5 \times 10^{11}$ dyn/cm^2, $E_{Si} = 13.0 \times 10^{11}$ dyn/cm^2, $\nu_{GaAs} = 0.37$, $\nu_{Si} = 0.33$, $\alpha_{GaAs} = 5.9 \times 10^{-6}$/K, and $\alpha_{Si} = 2.5 \times 10^{-6}$/K. Figure 6 is a plot of the bending curvature $1/R$ vs. the film to substrate thickness ratio t_2/t_1 for a GaAs layer on a 100 μm thick Si substrate caused by differentiated thermal contraction between the GaAs and Si cooling from a growth temperature of 640°C to room temperature. Assuming no interfacial relaxation, $\Delta\epsilon$ due to differential TEC cooling from the growth temperate of 640 to 22°C is calculated to be 0.0021. Since GaAs shrinks faster than Si, the wafer bends concavely upward. For $t_2/t_1 << 1$, all the differential strain is accommodated by the film. Since the film is too thin to generate enough force to bend the thick substrate, the curvature is expected to be small as shown in Fig. 6. The bending curvature increases linearly with increasing film thickness, until it reaches a thickness such that elastically the film becomes the substrate and hence the curvature begins to decrease. This turn over characteristic in curvature is described by Eq. 21 and is revealed as a peak in Fig. 6 at $t_2/t_1 \sim 0.45$, i.e., ~45 μm for GaAs on a 100 μm thick Si substrate. Such turn over characteristics do not appear in the simplified equation, Eq. 22, which is plotted in Fig. 6 in a dash-dotted line. It can be seen that a significant deviation from the exact solution occurs only for $t_2/t_1 > 0.1$. Therefore for most practical cases, where $t_2/t_1 < 0.1$, Eq. 22 is accurate enough for calculating the lattice curvature. The Stoney equation, Eq. 4, is also plotted in a dotted line in Fig. 6 for comparison purposes. Since it applies only for small values of t_2/t_1, there is a factor of ~2 smaller in the curvature for $t_2/t_1 < 0.03$ in comparison with Eq. 21 and 22. Therefore the corresponding stress value calculated from Stoney's Eq. 3, will be a factor of two larger than that from Eq. 22. To further examine the effect of relative stiffness of the film to substrate on the bending, we plot the curvature vs. t_2/t_1 for K_2/K_1 ratio of 0.1, 1, and 10 in Fig. 7. For convenience, we use the same values for $\Delta\epsilon$ and t_1 as in Fig. 6. As expected, for the same layer thickness, the curvature increases with increasing K_2/K_1 ratio, i.e., the stiffer the film, the more the bending. Similarly, the turnover thickness of the film decreases with stiffer films. The dependence of curvature on K_2/K_1 is further plotted in Fig. 8 for a 1 μm GaAs on a 100 μm Si substrate to show the sensitivity of the curvature on K_2/K_1 (the K_2/K_1 value for this system is 0.69). The dash-dotted line is for the simplified equation Eq. 22. The slope of the solid curve decreases from ~2 m^{-1} for $K_2/K_1 <$ 1 to ~1 m^{-1} for $K_2/K_1 = 10$. Therefore, considerable error may result in the calculation of curvature by setting $K_2/K_1 = 1$ when the Young's moduli and Poisson's ratio for the system are not available. For example, for 1 μm GaAs on a 100 μm Si, Fig. 8 gives a value of curvature of 1.7 m^{-1} for $K_2/K_1 = 0.69$ as vs. 2.4 m^{-1} for $K_2/K_1 = 1$. Note that the value calculated from our previous formula, Eq. 17 of Ref. 12, is 1.2 m^{-1} for $K_2/K_1 = 1$. Unfortunately, the Young's modulus and the Poisson's ratio for InGaAs are not available at this moment to rationalize our previous data. It is clear, however, that the experimental value for K_2/K_1 is needed in order to accurately calculate the stress in the film from the measured curvature, assuming no interfacial relaxation.

Finally the stress along the central line $z = t_1 + t_2/2$ of the GaAs layer is plotted vs. t_2/t_1 in Fig. 9 using Eq. 24. For $t_2/t_1 < 0.02$, the stress σ_{xx} is nearly approaching the value of $K_2\Delta\epsilon$, which indicates that, within 5% error, the stress in the film can be considered as uniaxial stress calculated directly from $\Delta\epsilon$, this is similar to Stoney's formulation $P = E_f\Delta\epsilon$. Therefore, to calculate the stress in a thin film on a thick substrate, for example from differential TEC, Stoney's approximation works well. However, to calculate film stress from measured curvature, Stoney's equation is expected to deviate from the true stress by a factor of ~2, as shown in Fig. 6, despite of the fact that his formula was derived based on a neutral axis for bending moment which does not exist in the simple bending geometry. Within the uncertainty of the interfacial relaxation for most practical

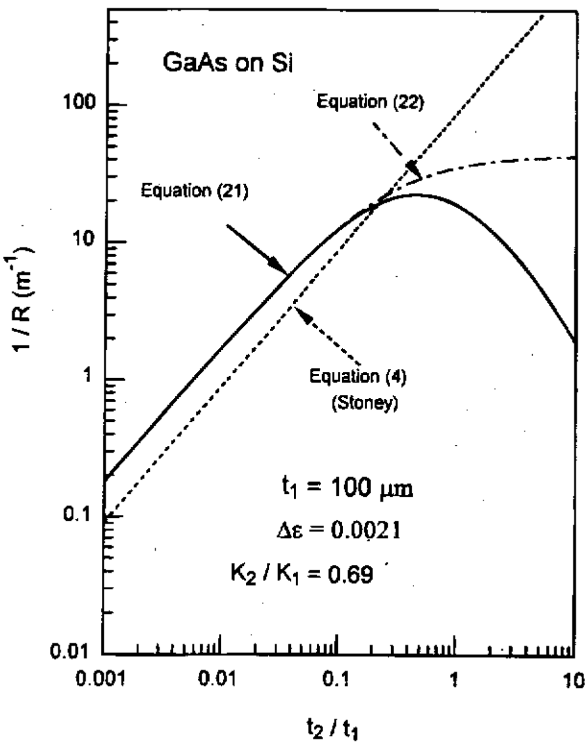

Fig. 6. Bending curvature vs. t_2/t_1 plot for GaAs on a 100 μm thick Si substrate showing the exact dependence, Eq. 21, the simplified equation Eq. 22, and the Stoney equation.

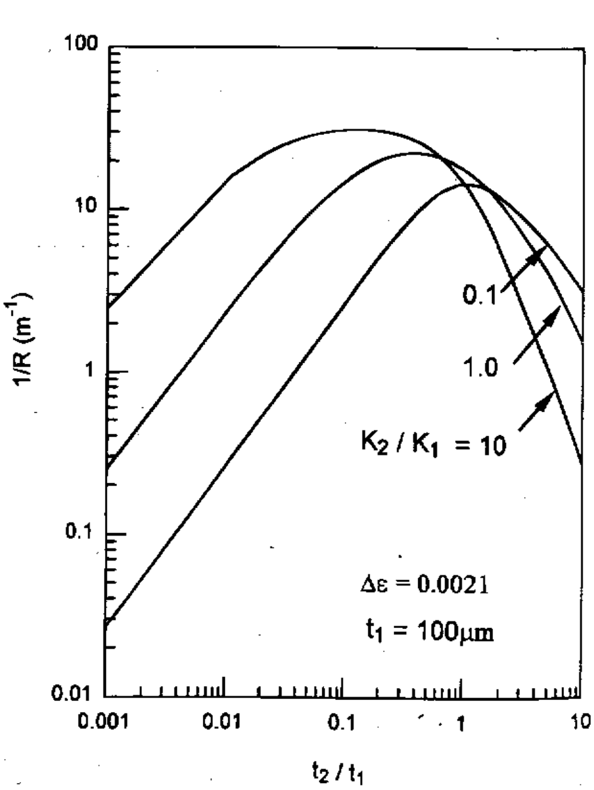

Fig. 7. Bending curvature vs. t_2/t_1 plot for GaAs on a 100 μm thick Si substrate for three different K_2/K_1 ratios showing increasing curvature and decreasing turnover thickness with increasing stiffness of the film.

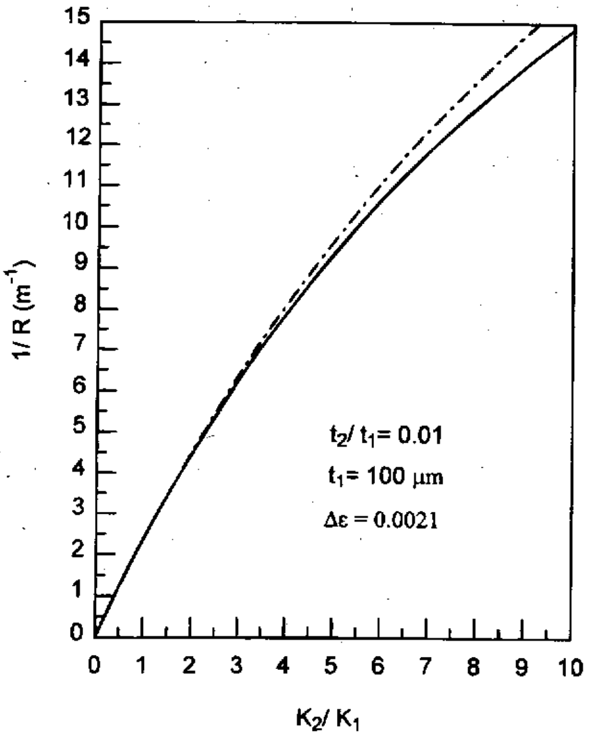

Fig. 8. Dependence of bending curvature on relative stiffness K_2/K_1 for a 1 μm GaAs film on a 100 μm thick Si substrate.

cases, a factor of two in stress is probably tolerable. This is why Stoney's equation has been around for many years.

Conclusions

We have revisited the general problem of elastic bending of a two-layer composite beam or plate. The same problem applies to the bending of wafers due to a lattice mismatched epitaxial layer or layer with different thermal expansion coefficients upon heating or cooling. We pointed out the difference between the bending of a two-layer composite by external moments and by internal stresses and have shown that a single neutral axis existed only in the case of bending by external moments. This finding indicated that our previous calculation in which we used a single neutral axis for wafer bending in a system which contained a misfit layer, needed to be rederived using two neutral axes. We have also shown that the bending moments in a composite structure with welded interfaces were nonadditive, an important condition often overseen in the formulation of this elastic problem, and the net bending moment in bending by internal stresses were nonzero for nonzero curvature. The improper neutral axis used by Stoney in deriving the Stoney equation was discussed in detail. Finally the bending curvature and the stresses in a two-layer composite were rederived and an example of wafer bending for GaAs on Si due to differential TEC in cooling from the growth temperature to room temperature was used to demonstrate the effects of the relative thickness and moduli of the film to the substrate on the bending curvature. The differences between our exact and simplified expressions for the bending curvature and the Stoney's equations as well as our previous formula were addressed.

Acknowledgments

The author wants to thank M. S. Hybertsen for the support and encouragement for this work. The valuable discussion with Dr. C. C. Chau of Dow Chemical Central Research and the critical reading of the manuscript by Professor Sanboh Lee of National Tsing Hua University are greatly acknowledged.

Manuscript submitted February 18, 1998; revised manuscript received June 15, 1998.

Bell Laboratories, Lucnt Technologies assisted in meeting the publication costs of this article.

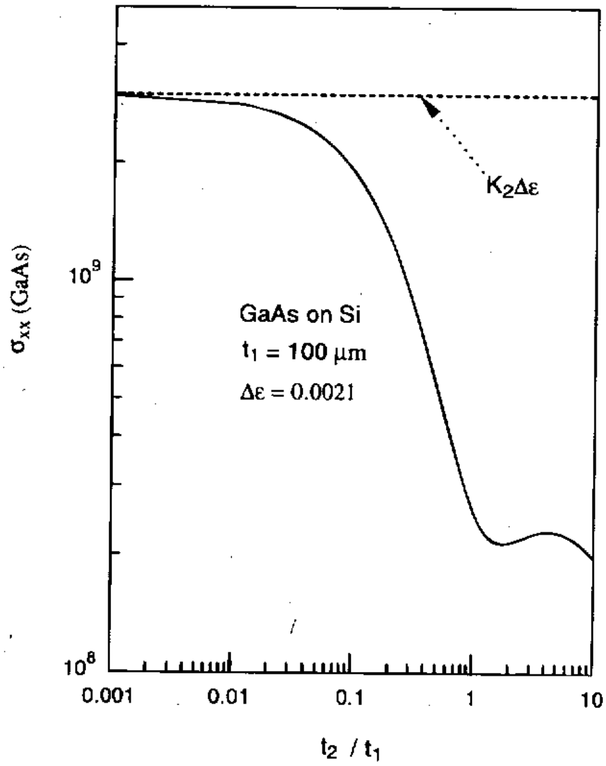

Fig. 9. Stress in the center of the GaAs film as a function of t_2/t_1 on a 100 μm thick Si substrate showing that the value approaches $K_2\Delta\varepsilon$ for $t_2/t_1 < 0.01$.

REFERENCES

1. E. Reissner and Y. Stavsky, *J. Appl. Mech.*, **28**, 402 (1968).
2. C. T. Sun, J. D. Achenbach, and G. Hermann, *J. Appl. Mech.*, **28**, 467 (1968).
3. N. J. Pagano, *J. Composite Mater.*, **3**, 398 (1969).
4. J. M. Whitney and N. J. Pagano, *J. Appl. Mech.*, **37**, 1031 (1970).
5. N. J. Pagano and R. B. Pipes, *J. Composite Mater.*, **5**, 50 (1971).
6. E. P. Chen and G. C. Sih, *J. Composite Mater.*, **5**, 12 (1971).
7. R. C. Wetherhold, in *Composites Engineering Handbook*, P. K. Mallick, Editor, Chap. 5, Marcel Dekker, Inc., New York (1997).
8. G. G. Stoney, *Proc. R. Soc., London*, **82**, 172 (1909).
9. S. Timoshenko, *J. Opt. Soc.*, **11**, 233 (1925).
10. A. Brenner and S. Senderoff, *J. Res. NBS*, **42**, 105 (1949).
11. N. N. Davidenkov, *Sov. Phys. Solid State*, **2**, 2595 (1961).
12. A. T. Vagramyan and Y. S. Petrova, *The Mechanical Properties of Electrolytic Deposits*, Consultant Bureau, New York (1962).
13. R. W. Hoffman, in *Physics of Thin Film*, Vol. 3, G. Hass and R. E. Thun, Editors, p. 211, Academic Press, New York (1966).
14. F. K. Reinhart and R. A. Logan, *J. Appl. Phys.*, **44**, 3171 (1973).
15. G. H. Olsen and M. Ettenberg, *J. Appl. Phys.*, **48**, 2543 (1977).
16. R. H. Saul, *J. Appl. Phys.*, **44**, 3171 (1977).
17. J. Vilms and D. Kerps, *J. Appl. Phys.*, **53**, 1536 (1982).
18. Z-C. Feng and H-D. Liu, *J. Appl. Phys.*, **54**, 83 (1983).
19. S. N. G. Chu, A. T. Macrander, K. E. Strege, and W. D. Johnston. Jr., *J. Appl. Phys.*, **57**, 249 (1985); *J. Appl. Phys.*, **60**, 1238 (1986).
20. I. C. Noyan and A. Segmuller, *J. Appl. Phys.*, **60**, 2980 (1986).
21. P. M. Marcus, *Phys. Rev. B*, **53**, 2481 (1996).
22. *FLX-Series Thin Film Stress Measurement Systems*, KLA-Tencor Co., San Jose, CA (1995).
23. *An Introduction to Mechanics of Solids*, 2nd ed., S. H. Crandall, N. C. Dahl, and T. Lardner, Editors, p. 421, McGraw-Hill, New York (1972).