An Approximate Analysis of Stresses in Multilayered Elastic Thin Films

E. Suhir
AT&T Bell Laboratories,
Murray Hill, NJ 07974
Mem. ASME

The analysis contains an engineering method for the approximate evaluation of thermally induced stresses in single and multilayered heteroepitaxial structures fabricated on thick substrates, with consideration of the finite size of the structure. The examined stresses include normal stresses, acting in the film layers themselves and responsible for their ultimate and fatigue strength, as well as interfacial stresses, responsible for film blistering and peeling. The developed formulas are simple, easy-to-use, and clearly indicate how material and structural characteristics affect the magnitude and the distribution of stresses and deflections. Some recommendations for smaller stresses in film structures are presented. The obtained results can be utilized as a guidance for physical design of multilayered heteroepitaxial structures in microelectronics.

Introduction

The first theoretical formula for the evaluation of stresses, arising in a thin film prepared on a thick substrate, was suggested by G. G. Stoney (1909), and is still widely utilized for stress calculation from the measured deformation of the substrate. This formula can be written down as follows:

$$\sigma_f = E_s^0 \frac{h_s^2}{6\rho h_f}, \qquad (1)$$

where σ_f is the stress in the film, $E_s^0 = E_s/1-\nu_s$ is the generalized Young's modulus for the substrate material, E_s and ν_s are elastic constants of this material, h_s and h_f are thicknesses of the substrate and the film, respectively, and ρ is the radius of curvature.

The formula (1) can be obtained on the basis of the following elementary considerations. The bending moment, which a film, experiencing stress σ_f, applies to the substrate, is $M_f = \sigma_f h_f\,(h_s/2)$. On the other hand, this moment is related to the moment of inertia $I_s = h_s^3/12$ of the substrate cross-sectional area of unit width by the formula $M_f = E_s^0\,(I/\rho) = (E_s^0 h_s^3)/(12\rho)$, where the generalized Young's modulus E_s^0 is used to account for the two-dimensional stress condition. The above two formulas for the bending moment result in the equation (1).

Stoney's formula has to be used, as long as the elastic constants of the film material and its thermal expansion mismatch with the substrate are unavailable. Otherwise the formula

$$\sigma_f = E_f^0 \Delta\alpha\Delta t, \quad \Delta\alpha = \alpha_f - \alpha_s, \qquad (2)$$

should be utilized. This formula follows from the fact, that the strain $\epsilon_s = \alpha_s \Delta t + F/E_s^0 h_s$ in the substrate must be equal to the strain $\epsilon_f = \alpha_f \Delta t - F/E_f^0 h_f$ in the film. The force F, arising between the film and the substrate, can be found on the basis of the strain compatibility condition and is as follows: $F \cong E_f^0 h_f \Delta\alpha\Delta t$. Then the stress in the film is expressed by the formula (2), which, unlike Stoney's formula (1), reflects the role of the actual factors, affecting the stress in the film, while formula (1) can be even misleading, if used for the purpose of optimal structural design.

The formulas for the curvature and the maximum bow can be easily obtained from (1) and (2):

$$\frac{1}{\rho} = 6\,\frac{E_f^0}{E_s^0}\,\frac{h_f}{h_s^2}\,\Delta\alpha\Delta t, \quad w_0 = 3\,\frac{E_f^0}{E_s^0}\left(\frac{\ell}{h_s}\right)^2 h_f \Delta\alpha\Delta t, \qquad (3)$$

where ℓ is half the film length. The existing methods of stress calculations for multilayered heteroepitaxial structures (Reinhart and Logan, 1973; Röll, 1976; Olsen and Ettenberg, 1977; Vilms and Kerps, 1982) are based on the formulas (1)-(3). Since these methods deal with the stresses in the film layered themselves, they can be used only for an indirect judgement of the level of the interfacial stresses, responsible for film blistering and peeling.

Therefore the major objective of the analysis below is to develop an engineering method for an approximate evaluation of the interfacial stresses in single and multilayered heteroepitaxial structures, fabricated on thick substrates, and to find out how the material and structural characteristics affect these stresses. This would enable one to decide what could be done in order to reduce the interfacial stresses if necessary. The suggested approach, based on the concept of the interface

Contributed by the Applied Mechanics Division for presentation at the Winter Annual Meeting, Chicago, IL, November 28 to December 2, 1988, of the American Society of Mechanical Engineers.

Discussion on this paper should be addressed to the Editorial Department, ASME, United Engineering Center, 345 East 47th Street, New York, N.Y. 10017, and will be accepted until two months after final publication of the paper itself in the JOURNAL OF APPLIED MECHANICS. Manuscript received by ASME Applied Mechanics Division, February 23, 1987; final revision, September 24, 1987.

Paper No. 88-WA/APM-14.

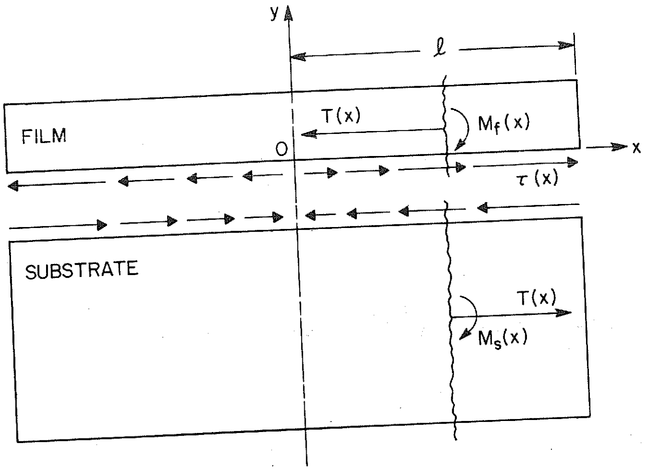

Fig. 1 Stress analysis model

compliance (Suhir, 1986), makes it possible to determine the magnitude and the distribution of the shearing and peeling stresses in the interfaces, as well as the normal stresses in the layers, with consideration of the finite size of the structure. It should be noted that the developed approach is equally applicable to other areas of physics and material science where thermal or lattice-mismatched stresses occur (Luryi and Suhir, 1986). It can also be used in those areas of engineering where lap shear joints subjected to external or thermally induced loading are utilized (Suhir, 1986).

Theory

1 Single-Layered Structure. Examine first the simplest case of a single layer structure fabricated at an elevated temperature and subsequently cooled (Fig. 1). The longitudinal displacements $u_f(x)$ and $u_s(x)$ of the lower extreme fiber of the film and the upper extreme fiber of the substrate, respectively, can be expressed by the formulas:

$$\left.\begin{aligned} u_f(x) &= \alpha_f \Delta t x - \lambda_f \int_0^x T(\xi)d\xi + \kappa_f \tau(x) + \frac{1}{2} h_f \int_0^x \frac{d\xi}{\rho(\xi)} \\ u_s(x) &= \alpha_s \Delta t x + \lambda_s \int_0^x T(\xi)d\xi - \kappa_s \tau(x) - \frac{1}{2} h_s \int_0^x \frac{d\xi}{\rho(\xi)} \end{aligned}\right\}, \quad (4)$$

where $\tau(x)$ is the shearing stress in the interface,

$$T(x) = \int_{-\ell}^{x} \tau(\xi)d\xi \quad (5)$$

is the shearing force per unit film width for the given cross section x, ℓ is half the film length, $\rho(x)$ is the radius of curvature, α_f and α_s are thermal expansion coefficients for the film and the substrate materials, $\lambda_f = (E_f^0 h_f)^{-1}$ and $\lambda_s = (E_s^0 h_s)^{-1}$ are coefficients of axial compliance for the film and the substrate, $E_f^0 = E_f/(1-\nu_f)$ and $E_s^0 = E_s/(1-\nu_s)$ are generalized Young moduli of the materials, h_f and h_s are the thicknesses of the film and the substrate,

$$\kappa_f = 2/3\,(1+\nu_f)/(1-\nu_f)\; h_f/E_f^0$$

and

$$\kappa_s = 2/3\,(1+\nu_s)/(1-\nu_s)\; h_s/E_s^0$$

are coefficients of interfacial compliance (Suhir, 1986), E_f and E_s are Young moduli, ν_f and ν_s are Poisson ratios for the film and the substrate materials, and Δt is the temperature differential. The origin O of the rectangular coordinates x, y is in the middle of the structure on the interface.

The first terms in equations (4) are unrestricted thermal contractions. The second terms are due to the forces (5) and are calculated under an assumption that these forces are uniformly distributed over the film and the substrate thicknesses. The third terms account for the additional displacements due to the actual (nonuniform) distribution of the above forces, and are calculated under an assumption that the corresponding corrections are directly proportional to the shearing stress in the given cross section and are not affected by the stresses in other cross sections. The last terms are due to bending.

The equation of equilibrium for a portion of the film-substrate structure is as follows:

$$\frac{h_f + h_s}{2} T(x) = M_f(x) + M_s(x), \quad (6)$$

where

$$M_f(x) = \frac{E_f^0 h_f^3}{12\rho(x)}, \quad M_s(x) = \frac{E_s^0 h_s^3}{12\rho(x)} \quad (7)$$

are bending moments acting over the cross sections of the film and the substrate. From the equations (6) and (7) we have:

$$\frac{1}{\rho(x)} = 6\frac{h_f + h_s}{E_f^0 h_f^3 + E_s^0 h_s^3} T(x) \cong 6\frac{T(x)}{E_s^0 h_s^2}. \quad (8)$$

After substituting (8) in (4) and using the condition $u_f(x) = u_s(x)$ of the displacement compatibility, we obtain the following basic equation for the unknown shearing stress function $\tau(x)$:

$$\tau(x) - k^2 \int_0^x T(\xi)d\xi = -\frac{\Delta\alpha\Delta t}{\kappa} x, \quad (9)$$

where

$$\left.\begin{aligned} &k = \sqrt{\frac{\lambda}{\kappa}}, \quad \lambda = \lambda_f + \lambda_s + \frac{(h_f + h_s)^2}{E_f^0 h_f^3 + E_s^0 h_s^3} \cong \lambda_f = \frac{1}{E_f^0 h_f}, \\ &\kappa = \kappa_f + \kappa_s = \frac{2}{3}\left(\frac{1+\nu_f}{1-\nu_f}\frac{h_f}{E_f^0} + \frac{1+\nu_s}{1-\nu_s}\frac{h_s}{E_s^0}\right), \\ &\Delta\alpha = \alpha_f - \alpha_s \end{aligned}\right\}. \quad (10)$$

The equation (9) has the following solution:

$$\tau(x) = -E_f^0 h_f \chi_1(x)\Delta\alpha\Delta t, \quad (11)$$

where the function $\chi_1(x) = k\,(\sinh kx)/(\cosh k\ell)$ characterizes the distribution of the shearing stress along the film. The maximum shearing stress is at the end of the film:

$$\tau_{\max} = \tau(\ell) = -kE_f^0 h_f \Delta\alpha\Delta t \tanh k\ell. \quad (12)$$

The solution (11) satisfies the condition $\tau(0) = 0$ of symmetry and the boundary condition $T(\ell) = 0$.

Calculations show that for the structures in question the k values are very great. Therefore, formulas (11) and (12) can be simplified as follows:

$$\tau(x) = \tau_{\max} e^{-k(\ell - x)}, \quad \tau_{\max} = -kE_f^0 h_f \Delta\alpha\Delta t. \quad (13)$$

As is evident from these formulas, the maximum shearing stress is independent from the film size, and the stresses drop exponentially with the decrease in x, i.e., they concentrate near the film ends. The length of the zone of high stresses can be defined, for instance, as such a length, for which the stresses decrease by, say, 95 percent of their maximum values at the edges. This results in the following formula for the length of the zone of appreciable shearing stresses: $\ell_i = -(\ln 0.05/k) \cong 3/k$.

After substituting equation (11) in (5) we find:

$$T(x) = E_f^0 h_f \chi_0(x)\Delta\alpha\Delta t, \quad (14)$$

where the function $\chi_0(x) = 1 - (\cosh kx)/(\cosh k\ell)$ and the characterizes the distribution of the forces $T(x)$ and the

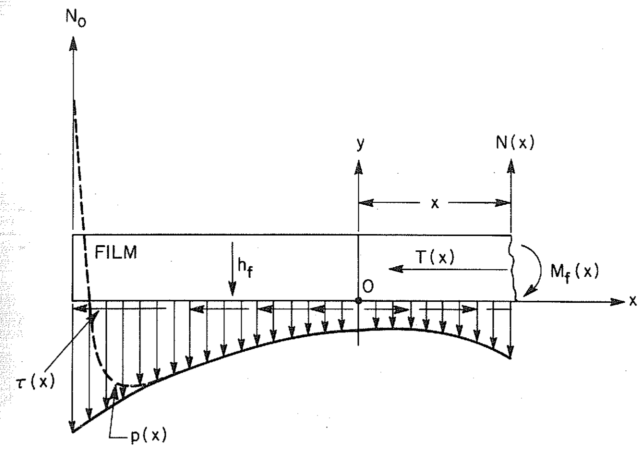

Fig. 2 Peeling stresses

resulting normal stresses along the film. Note, that $\chi_1(x) = -(d\chi_0(x))/(dx)$.

By substituting the equation (14) in (8) we obtain the following formula for the curvature:

$$\frac{1}{\rho(x)} = 6\,\frac{E_f^0 h_f}{E_s^0 h_s^2}\,\chi_0(x)\Delta\alpha\Delta t. \tag{15}$$

Then the formulas (7) yield:

$$\left.\begin{aligned} M_f(x) &= \frac{(E_f^0)^2 h_f^4}{2E_s^0 h_s^2}\,\chi_0(x)\Delta\alpha\Delta t, \\ M_s(x) &= \frac{E_f^0 h_f h_s}{2}\,\chi_0(x)\Delta\alpha\Delta t. \end{aligned}\right\} \tag{16}$$

Since the thickness of the film is small, the bending moment $M_f(x)$ is also small, and therefore the stresses in the film are due to the forces $T(x)$ only:

$$\sigma_f(x) = \frac{T(x)}{h_f} = E_f^0 \chi_0(x)\Delta\alpha\Delta t. \tag{17}$$

For great k values, the function $\chi_0(x)$ can be calculated by the formula $\chi_0(x) = 1 - e^{-k(\ell - x)}$. As evident from this formula, for small enough x values, i.e., for the cross-sections sufficiently remote from the film ends, the factor $\chi_0(x)$ is close to unity, and the stresses in the film are independent from the location of the given cross-section along the film length. Near the ends, where the x coordinate is on the same order as half the film length ℓ, the stresses rapidly drop and turn to zero at the edges.

Stresses in the substrate, unlike the stresses in the film, are due both to the force $T(x)$ and the bending moment $M_s(x)$. The total stresses are maximum at the interface and can be evaluated as follows:

$$\sigma_s(x) = -\frac{T(x)}{h_s} - 6\,\frac{M_s(x)}{h_s^2} = -4E_f^0\,\frac{h_f}{h_s}\,\chi_0(x)\Delta\alpha\Delta t. \tag{18}$$

The deflection function can be found from the equation (15), since for small curvatures $1/(\rho(x)) \cong (d^2w(x))/(dx^2)$. For sufficiently great k values this formula results in the following equation for the maximum bow:

$$w_0 = 3\,\frac{E_f^0}{E_s^0}\left(\frac{\ell}{h_s}\right)^2 h_f\Delta\alpha\Delta t. \tag{19}$$

The expected distribution of the transverse normal (peeling) stresses is schematically shown in Fig. 2 by the dotted line. To simplify the analysis, however, we replace the stresses, directed upward and distributed over small areas near the edges, by concentrated forces N_0 applied at the edges. These forces, as well as the distributed peeling stress $p(x)$, can be found on the basis of the following equation of equilibrium for the portion of the film:

$$(x+\ell)N_0 - \int_{-\ell}^{x}\int_{-\ell}^{\xi} p(\xi')d\xi' d\xi' = M_f(x) - \frac{h_f}{2}\,T(x) \cong -\frac{h_f}{2}\,T(x).$$

Using the equation (14) we obtain:

$$N(x) = \int_{-\ell}^{x} p(\xi)d\xi = N_0 - \frac{1}{2}\,E_f^0 h_f^2 \chi_1(x)\Delta\alpha\Delta t = N_0 + \frac{1}{2}\,h_f\tau(x), \tag{20}$$

$$p(x) = \frac{dN(x)}{dx} = -\frac{1}{2}\,E_f^0 h_f^2 \Delta\alpha\Delta t\,\frac{d\chi_1(x)}{dx} = \frac{1}{2}\,E_f^0 h_f^2 \chi_2(x)\Delta\alpha\Delta t, \tag{21}$$

where the function $\chi_2(x) = -(d\chi_1(x))/(dx) = -k^2$ (cosh kx)/(cosh $k\ell$) characterizes the longitudinal distribution of the peeling stress. Since the equilibrium condition requires that $N(\ell) = 0$, then

$$N_0 = -\frac{1}{2}\,h_f\tau_{\max} = \frac{1}{2}\,kE_f^0 h_f^2 \Delta\alpha\Delta t. \tag{22}$$

The distributed peeling stress $p(x)$ is maximum at the end cross sections:

$$p_{\max} = p(\ell) = -\frac{1}{2}\,E_f^0(kh_f)^2\Delta\alpha\Delta t = \frac{1}{2}\,kh_f\tau_{\max}. \tag{23}$$

For great k values the formula (21) can be simplified as follows:

$$p(x) = p_{\max}e^{-k(\ell - x)}. \tag{24}$$

Hence, the distribution of the peeling stresses in this case is similar to the distribution of the shearing stress.

It is noteworthy, that while the normal stress in a thin film is independent from the film thickness, the interfacial stresses increase with an increase in the thickness of the film. Therefore, there is an incentive to reduce, for smaller interfacial stresses, the film thickness in the zone of high stresses by slanting the film edges. In addition, the interfacial stresses, unlike the stresses in the film, depend on the parameter k of the interfacial compliance, which, in its turn, depends on the thickness and the Young's modulus of the substrate. The stress in the film itself, however, is independent from the thickness and the Young modulus of the substrate, as long as these parameters are substantially greater than the thickness and the Young modulus of the film.

2 Multilayered Structure. Examine now a multilayered heteroepitaxial structure (Fig. 3). We assume, for instance, that the coefficients α_i ($i = 0, 1, 2, \ldots, m$ with $i = 0$ referring to substrate) of linear thermal expansion of the layers increase with an increase in the number i, and that the entire structure is subjected to uniform cooling.

The analysis, carried out for a single-layered structure, has indicated that the formula for the shearing force $T(x)$ in the film can be obtained by multiplying the force $T = E_f^0 h_f \Delta\alpha\Delta t$, calculated under an assumption that it is constant along the film, by the factor $\chi_0(x)$, which considers the longitudinal distribution of this force. The interfacial stresses can be then evaluated by the formulas

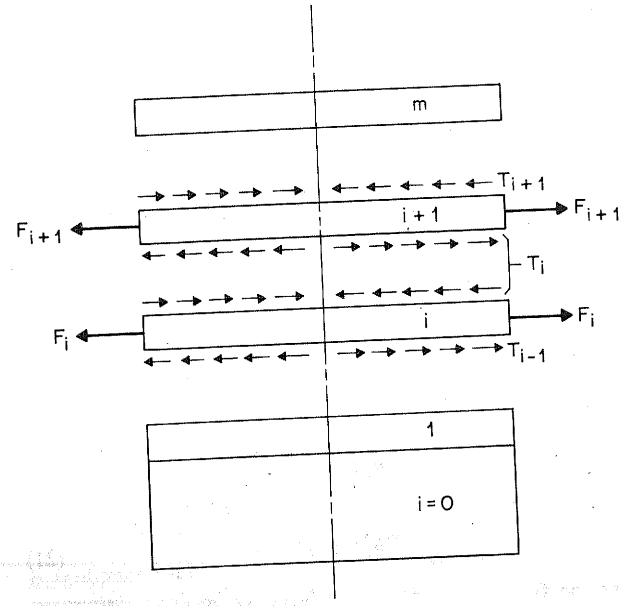

Fig. 3 Multilayered structure

$$\tau(x)=T\frac{d\chi_0(x)}{dx}=-T\chi_1(x),\quad N_0=-\frac{1}{2}h_t\tau_{\max},$$

$$p(x)=-\frac{1}{2}h_fT\chi_2(x). \tag{25}$$

This enables one to simplify the analysis for a multilayered structure and to avoid forming and solving a system of integral equations of the type (9). Therefore, the analysis below is based on the strain compatibility conditions rather than on the conditions of the compatibility of displacements. The longitudinal strains e_{i-1}^{+} and e_i^{-} of the upper extreme fiber of the $(i-1)$-*st* layer and the lower extreme fiber of the *i*th layer, respectively, can be expressed as follows:

$$e_{i-1}^{+}=\alpha_{i-1}\Delta t-\lambda_{i-1}F_{i-1}+\frac{h_{i-1}}{2\rho},\quad e_i^{-}=\alpha_i\Delta t-\lambda_iF_i-\frac{h_i}{2\rho},$$
$$i=0,1,2,\ldots,m. \tag{26}$$

Here α_i is the coefficient of thermal expansion for the *i*th layer material, $\lambda_i=(E_i^0h_i)^{-1}$ is the axial compliance of this layer, F_i is the force acting in the *i*th layer, ρ is the radius of curvature, and Δt is the temperature differential. Using the condition $e_{i-1}^{+}=e_i^{-}$ of strain compatibility, we obtain:

$$\lambda_iF_i-\lambda_{i-1}F_{i-1}+\frac{h_i+h_{i-1}}{2\rho}=(\alpha_i-\alpha_{i-1})\Delta t,$$
$$i=0,1,2,\ldots,m. \tag{27}$$

After summarizing these equations from $i=0$ to i we have:

$$F_i=\frac{1}{\lambda_i}\left(\lambda_0F_0+\Delta\alpha_i\Delta t-\frac{a_i}{\rho}\right),\quad i=0,1,2,\ldots,m, \tag{28}$$

where $\Delta\alpha_i=\alpha_i-\alpha_0$ is the thermal expansion mismatch between the *i*th layer and the substrate materials, and

$$a_i=\sum_{j=0}^{i}h_j-\frac{h_0+h_i}{2}. \tag{29}$$

By summarizing all the equations (28) and considering the obvious equilibrium condition $\sum_{i=0}^{m}F_i=0$, we find:

$$\lambda_0F_0=-s\Delta t+\frac{s_1}{\rho}, \tag{30}$$

where

$$s=\frac{\sum_{i=0}^{m}\Delta\alpha_i/\lambda_i}{\sum_{i=0}^{m}1/\lambda_i},\quad s_1=\frac{\sum_{i=0}^{m}a_i/\lambda_i}{\sum_{i=0}^{m}1/\lambda_i}. \tag{31}$$

For a multilayered structure on a thick substrate ($h_0\gg\sum_{i=0}^{m}h_i$) the formula (29) yields: $a_i\cong h_0/2$. In this case $s_1=h_0/2$ and $s\cong 0$. Then the equation (30) results in the formula: $\lambda_0F_0\cong h_0/2\rho$, and the equation (28) yields:

$$F_i=\frac{\Delta\alpha_i\Delta t}{\lambda_i}=E_i^0h_i\Delta\alpha_i\Delta t,\quad i=1,2,\ldots,m. \tag{32}$$

The corresponding stresses in the film layers are as follows:

$$\sigma_i=\frac{F_i}{h_i}=E_i^0\Delta\alpha_i\Delta t,\quad i=1,2,\ldots,m. \tag{33}$$

The shearing force acting in the *i*th interface, i.e., in the interface between the *i*th and the $(i+1)$-*st* layers, is

$$T_i=\sum_{j=i}^{m}F_j=\Delta t\sum_{j=i}^{m}E_j^0h_j\Delta\alpha_j,\quad i=0,1,2,\ldots,m-1. \tag{34}$$

We present the k^2 value in the formulas (10) for the case of a multilayered structure in the following approximate way:

$$k^2=\frac{\sum_{i=0}^{m}\lambda_i}{\sum_{i=0}^{m}\kappa_i}\cong\frac{3}{4}\,\frac{\sum_{i=0}^{m}\lambda_i}{\sum_{i=0}^{m}h_i^2\lambda_i}, \tag{35}$$

where the interfacial compliances κ_i of the layers can be assessed, assuming $\nu_1=1/3$, by the formula:

$$\kappa_i=\frac{2}{3}\,\frac{1+\nu_i}{1-\nu_i}\,\frac{h_i}{E_i^0}\cong\frac{4}{3}\,\frac{h_i}{E_i^0}=\frac{4}{3}h_i^2\lambda_i. \tag{36}$$

The distributed stresses in the *i*th interface can be calculated on the basis of the formulas (25) as follows:

$$\left.\begin{aligned}\tau_i(x)&=-T_i\chi_1(x)=-kT_i\frac{\sinh kx}{\cosh k\ell},\\ p_i(x)&=-\frac{1}{2}T_i\chi_2(x)\sum_{j=i+1}^{m}h_j\\ &=-\frac{1}{2}k^2T_i\frac{\cosh kx}{\cosh k\ell}\sum_{j=i+1}^{m}h_i.\end{aligned}\right\} \tag{37}$$

The maximum values of the interfacial forces occur at the end cross sections:

$$\left.\begin{aligned}\tau_{i,\max}&\cong-kT_i=-k\Delta t\sum_{j=i}^{m}E_j^0h_j\Delta\alpha_j,\\ N_i&=-\frac{1}{2}\tau_{i,\max}\sum_{j=i+1}^{m}h_j\\ p_{i,\max}&=-\frac{1}{2}k^2T_i\sum_{j=i+1}^{m}h_j\\ &=-\frac{1}{2}k^2\Delta t\sum_{j=i+1}^{m}h_j\sum_{j=i}^{m}E_j^0h_j\Delta\alpha_j,\end{aligned}\right\} \tag{38}$$

$$i=0,1,2,\ldots,m-1$$

If the layers are applied at different temperatures, the above formulas for the $\tau_{i,\max}$ and $p_{i,\max}$ could be written as follows:

$$\left.\begin{aligned}
\tau_{i,\max} &= -k\sum_{j=i}^{m} E_j^0 h_j \Delta\alpha_j \Delta t_j = -k\sum_{j=i}^{m}\sigma_j h_j,\\
p_{i,\max} &= -\frac{1}{2}k^2 \sum_{j=i+1}^{m} h_j \sum_{j=i}^{m} E_j^0 \mathrm{k}_j \Delta\alpha_j \Delta t_j\\
&= \frac{1}{2}k\tau_{i,\max}\sum_{j=i+1}^{m} h_j,\\
i &= 0, 1, 2, \ldots, m-1,
\end{aligned}\right\} \tag{39}$$

where Δt_i is the temperature change for the ith layer, i.e., the difference between the application temperature of the material and the given temperature. On the interface with the substrate ($i=0$) we have:

$$\left.\begin{aligned}
\tau_{0,\max} &= -k\sum_{i=0}^{m} E_i^0 h_i \Delta\alpha_i \Delta t_i,\\
N_0 &= -\frac{1}{2}\tau_{0,\max}\sum_{i=1}^{m} h_i,\\
p_{0,\max} &= \frac{1}{2}k\tau_{0,\max}\sum_{i=1}^{m} h_i.
\end{aligned}\right\} \tag{40}$$

The maximum bow can be calculated by the formula:

$$w_0 = \frac{3}{E_s^0}\left(\frac{\ell}{h_s}\right)^2 \sum_{i=1}^{m}\sigma_i h_i. \tag{41}$$

Numerical Example

The numerical example is executed for a hypothetical multilayered structure, where a 0.25 μm thick SiO_2 layer, 1.5 μm thick Al layer, and 5 μm thick polymide layer are applied on a 0.51 mm thick Si substrate. The stresses and maximum bow are evaluated for the room temperature conditions (t = 20°C). Calculations are performed in Table 1. The half length of the structure, affecting the maximum bow, is ℓ = 25.4 mm. The obtained results indicate that the thermally induced stresses are rather great and could possibly result in insufficient ultimate and fatigue strength.

Obviously, in order to be able to make a final conclusion regarding the cohesive and the adhesive strength of the materials, one has to know not only the actual stresses, but also the allowable (design) stress values. The latters are, unfortunately, not available for many materials utilized in multilayered structures. For this reason, until an appropriate strength data is available, our analysis, dealing only with the left part of the strength condition "actual stress ≤ design stress," can be used for the prediction of the stress level and could, of course, be utilized as a guidance for structural design of low stress multilayered structures.

Discussion

We now consider how the results of the above analysis might help our understanding of the thermally induced stresses in multilayered structures. In addition to normal stresses acting in the film layers themselves, there are shearing and transverse normal (peeling) stresses, acting in the interfaces. While the stresses in the layers themselves are responsible for the strength of the film materials, the interfacial stresses are responsible for blistering and peeling.

The normal stresses in the film layers are practically uniformly distributed along the film. Only at the very ends of the structure these stresses rapidly drop to zero. The interfacial stresses, on the contrary, concentrate near the edges at the distances on the same order of magnitude as the thickness of the multilayered structure. Since thin films do not experience bending stresses, the normal stresses in thin films are independent from the layer thicknesses. If, in addition, the substrate is thick, compared to the total thickness of the heteroepitaxial structure, then the normal stresses in the given film layer become independent from the mechanical properties of the other film layers and are characterized by the generalized Young modulus of the given layer, temperature differential, and the thermal expansion mismatch between this layer and the substrate materials. The corresponding normal stresses in the layers can be calculated by formula (33).

The maximum interfacial stresses arising in the ith layer of a multilayered heteroepitaxial structure, fabricated on a thick substrate, can be evaluated by formulas (37). These stresses increase with an increase in the normal stress level and in the thicknesses of the layers, located on the "free surface" of the structure. The interfacial stresses increase with an increase in the interfacial stiffness. This effect is accounted for by the factor k, which is affected by the stiffness of all the heteroepitaxial layers.

Thus, if there is a need to reduce the stress level, one should use materials with small Young moduli and small thermal expansion mismatch with the substrate. In the case of interfacial stresses, in addition to the above measure, smaller stresses

Table 1 Stresses in Multilayered Structures (Calculation Sheet)

						Stresses in films, σ_i, PA		Maximum shearing: Stiffness factor k, 1/m			Maximum shearing stresses, τ_i, PA		Maximum peeling stresses, p_i, PA		Pelling force N_0, N/m
Component number, i	Material	Thickness, h_i, m	Generalized Young modulus, E_i^0, PA	Coefficient of thermal expansion, α_i, 1/°C	Temperature differential, Δt_i, °C	Film stress factor, $f_i = E_i^0\Delta\alpha_i$, PA/°C	Stresses, $\sigma_i = f_i\Delta t_i$, PA	Axial compliance $\lambda_i = (E_i^0 h_i)^{-1}$, m/N	Interfacial compliance $\varkappa_i = 4/3\, h_i^2\lambda_i$, m³/N	Shearing stress factor, $\sigma_i h_i$, N/m	$S_i' = \sum_{j=i} \sigma_i h_i$, N/m	Stresses, $\tau_i = kS_i'$, PA	$S_i'' = \sum_{j=i+1} h_j$, m	Stresses, $p_i = 1/2\, k\tau_i S_i''$, PA	$N_0 = -1/2\,\tau_i S_i''$, N/m
0	Si	0.508×10^{-3}	1.80×10^{7}	3.2×10^{-6}	0	0	0	1.094×10^{-4}	3.764×10^{-11}	0	0.044	569	6.75×10^{-6}	248	0.0019
1	SiO_2	2.50×10^{-7}	1.60×10^{7}	0.9×10^{-6}	980	-36.81	-36074	0.250	0.208×10^{-13}	-0.0090	0.0134	1733	6.50×10^{-6}	728	0.0056
2	Aℓ	1.50×10^{-6}	1.08×10^{7}	23.6×10^{-6}	0	219.54	0	0.0617	1.850×10^{-13}	0	0.0134	1733	5.00×10^{-6}	560	0.0043
3	POLY	5.00×10^{-6}	0.276×10^{6}	38.0×10^{-6}	280	9.60	2688	0.725	241.6×10^{-13}	0.0134					
							Σ	1.0368	6.201×10^{-11}	0.0044	Maximum bow factor $f_b = \frac{3}{E_0^0}\left(\frac{\ell}{h_0}\right)^2 = 4.167 \times 10^{-4}$ m²/N				
								$k = \sqrt{\frac{1.0368}{6.201 \times 10^{-11}}} = 1.293 \times 10^{5}$ 1/m			Maximum bow $W_0 = f_b \sum_{i=1}^{m} \sigma_i h_i = 0.183 \times 10^{-5}$ m				

Table 2 Summary of stress characteristics

STRESSES	NORMAL	SHEAR	PEELING
	IN THE FILMS	IN THE INTERFACES	
RESPONSIBLE FOR:	STRENGTH OF THE FILMS	BLISTERING AND PEELING (INTERFACIAL STRENGTH)	
DISTRIBUTION	UNIFORMLY DISTRIBUTED OVER THE FILM LENGTH	CONCENTRATE NEAR THE FILM ENDS AT DISTANCES ON THE ORDER OF THE FILM THICKNESS	
CALCULATION FORMULAS	$\sigma_i = E_i^0 \Delta\alpha_i \Delta t$ $E_i^0 = \frac{E_i}{1 - \nu_i}$ $\Delta\alpha_i = \alpha_i - \alpha_s$	$\tau_i = k_i \sum_{j=i+1}^{m} h_j \sigma_j$ $k_i^2 = \frac{3}{4} \frac{\sum_{j=0}^{i+1} \lambda_j}{\sum_{j=0}^{i+1} h_j^2 \lambda_j}$	$P_i = \frac{1}{2} k_i \tau_i \sum_{j=i+1}^{m} h_j$ $N_i = -\frac{1}{2} \tau_i \sum_{j=i+1} h_j$ $\lambda_i = \frac{1}{E_i^0 h_i}$
DEPEND ON:	YOUNG MODULUS; THERMAL EXPANSION MISM. w/SUBSTRATE; TEMP. DIFFERENTIAL	NORMAL STRESSES AND THICKNESS OF THE GIVEN LAYER STRUCTURAL STIFFNESS (FACTOR k)	SHEAR STRESSES AND THICKNESSES OF THE GIVEN LAYER
CAN BE REDUCED BY:	USING SOFTER MATERIALS, HAVING SMALLER THERMAL MISMATCH WITH THE SUBSTRATE	REDUCING THE NORMAL STRESSES IN THE LAYERS ABOVE THE GIVEN LAYER, SLOPING THE ENDS OF THE LAYERS, REDUCING STRUCTURAL STIFFNESS (FACTOR k)	

could be obtained by a proper slanting of the layer ends and by increasing the structural compliance (resulting in smaller values of the stiffness factor k). The summary of the results is given in Table 2. Note, that the developed theory is equally applicable to heteroepitaxial lattice mismatched structures. In this case the thermal mismatch strain $\Delta\alpha\Delta t$ should be substituted by the lattice mismatch strain f (Luryi and Suhir, 1986).

Conclusion

An approximate engineering theory of stresses in multilayered thin film structure fabricated on a thick substrate is developed. The obtained formulas are simple, easy-to-use, and clearly indicate the role of the major factors affecting the stresses. The results of analysis can be utilized for guidance in the physical design of multilayered heteroepitaxial structures in microelectronics.

Acknowledgment

The author thanks H. J. Levinstein, W. J. Bertram, C. J. Bartlett, and J. M. Segelken for useful discussions, and L. B. Freund for indicating his unpublished work, where an approach, similar to ours, was taken.

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