# On the determination of film stress from substrate bending: STONEY´s formula and its limits

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## Abstract

The paper examines the problem of film stress applying a correct three dimensional model. The results are compared with two different forms of Stoney´s equation existing in the Literature and being widely used in the determination of stresses in thin films.

It is shown theoretically that only one of the forms is based on an adequate model and yields accurate results whereas the other causes errors of about 30-40 % for typical substrate materials. In addition limits for the applicability of the correct Stoney equation are given.

## Introduction

Internal stress in a film on a plate-like substrate causes the film-substrate compound to warp until mechanical equilibrium is reached, i.e. until both net force and bending moment are zero. A plate-like form of the substrate means that the substrate thickness, $h_s$, is constant and small in comparison to its lateral dimensions. From the curvature of the elastically deformed coated substrate the average film stress, $\sigma^f$, can be calculated. This method is very popular since the curvature of the bent substrate can easily be measured and no information on the elastic parameters of the film material is necessary. As substrate material often silicon is used since its mechanical properties are well defined and well known. If necessary, small beams (cantilevers) can be made of single-crystal silicon using micromechanical technology (e.g. Elwenspoek and Jansen 1998) which allows to apply the method also to very thin films. When the thickness of the film, $h_f$, is small compared to that of the substrate, a simple formula holds which was first published by STONEY 1909:

$$\sigma_{zz}^{f} \approx -E_s \frac{h_s^2}{6h_f}\frac{1}{R}, \tag{1}$$

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with R - radius of curvature and $E_s$ - YOUNG´s modulus of the substrate. In its original form, the STONEY formula is valid only for a narrow coated beam. The index “zz” denotes the stress component in direction of the length side of the beam which we chose to be along the z-axis.

When measuring thin films deposited on plate-like substrates, the corresponding biaxial deformation has to be taken into account (see, for instance Ohring 1992) by using the biaxial modulus, $E_{b,s}$, of the substrate rather than the YOUNG´s modulus alone:

$$E_s \rightarrow E_{b,s} = E_s / (1 - \nu_s) \qquad (2)$$

with $\nu_s$ - POISSON´s ratio of the substrate. This corresponds to the cap or bowl-like deformation of a circular substrate under the influence of intrinsic film stress. Since many solid materials have POISSON´s ratios between 0.2 and 0.3, using the biaxial modulus instead of $E_s$ yields a modification in the calculated $\sigma_f$ values by 25 to 43 %.

For practical reasons, instead of a circular substrate often an elongated rectangular substrate is used, either as a "macroscopic" strip having a length in the centimetre range, or as a micromechanical cantilever typically few 100 µm in length. It was argued by Berry 1988 that such a substrate rather curls into an approximately cylindrical shape instead of bowl or cap-like deformation. Therefore, in STONEY´s formula $E_s$ should be replaced in this case by the plate modulus, $E_{p,s}$, rather than by the bipolar modulus of the substrate:

$$E_s \rightarrow E_{p,s} = E_s / (1 - \nu_s^2). \qquad (3)$$

In the meantime, this apparently plausible argumentation was repeatedly followed in the literature (see, for instance Ljungcrantz et al. 1993 or Berry and Pritchet 1990). Considering transverse contraction in this manner modifies $\sigma^f$ only by 4 to 9 % when typical $\nu_s$ values between 0.2 and 0.3 are assumed.

The aim of this paper is to examine the argumentation given in Berry 1988.

## *Theoretical Part*

**General Preliminaries**

Let's consider a coated plate of arbitrary symmetry. The curvature R of this plate in the direction of x may be described exactly by (see figure 1):

$$\frac{1}{R} = \frac{d\varphi}{ds} = \frac{(\arctan(w'))'dx}{\sqrt{dx^2 + dw^2}} = \frac{w''dx}{\left(1 + w'^2\right)^{3/2} dx} \cong w'' . \qquad (4)$$

Here, w means the displacement in z-direction. s and $\varphi$ are the length and the angle of the arc, which follows the deformation curve of the plate. The latter approximation is valid for small deformations which is equivalent to small w'.

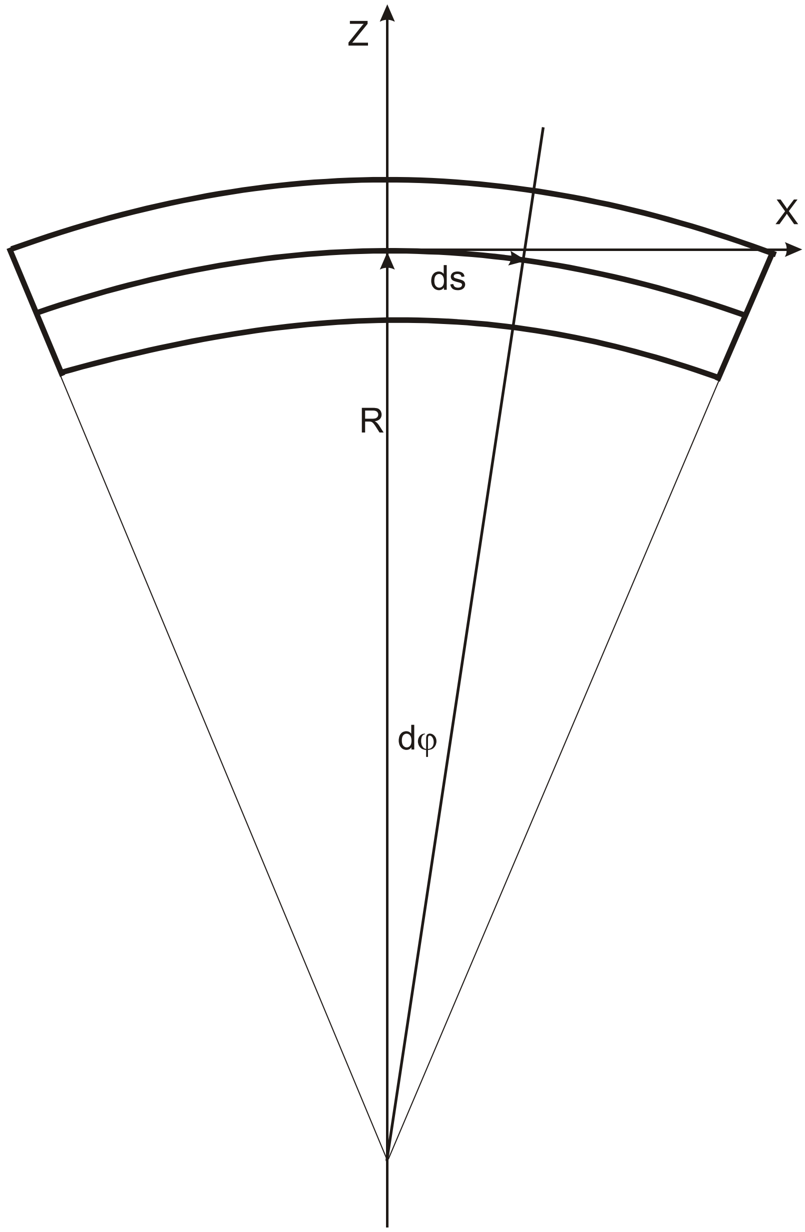


**Fig. 1:** **To the calculation Radius of curvature, R, of the plate.**

The basic relations between the deformations $u_{ij}$ and stress components $\sigma_{ij}$ (i, j = x, y, z) in the isotropic linear elastic case may be written as (e.g. Landau and Lifschitz 1989)

$$\sigma_{jk} = \frac{E}{1+\nu}\left(u_{jk} + \frac{\nu}{1-2\nu} u_{ll}\delta_{jk}\right). \qquad (5)$$

**The coated rectangular substrate**

We use the ordinary plate approximation (see e.g. the book of Landau and Lifschitz 1989 p. 48) assuming that the z-dimension of the plate is very small compared to the others and we can neglect all stress components in this direction:

$$\sigma_{xz} = \sigma_{yz} = \sigma_{zz} = 0. \qquad (6)$$

With the origin of the z-axis laying at the substrate bottom we can give the following equations for the normal deformations

$$u_{xx} = -(z-\alpha)\frac{\partial^2 w}{\partial x^2}; \quad u_{yy} = -(z-\alpha)\frac{\partial^2 w}{\partial y^2}; \quad u_{zz} = \frac{(z-\alpha)\nu}{1-\nu}\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}\right), \tag{7}$$

with z = α being the position of the neutral surface within the compound. This yields with equation (5):

$$\sigma_{xx} = \frac{E}{(1+\nu)(1-2\nu)}\left[(1-\nu)u_{xx} + \nu\left(u_{yy} + u_{zz}\right)\right]$$

$$\sigma_{yy} = \frac{E}{(1+\nu)(1-2\nu)}\left[(1-\nu)u_{yy} + \nu\left(u_{xx} + u_{zz}\right)\right].$$

After few simplifications we get:

$$\sigma_{xx} = -\frac{Ez}{1-\nu^2}\left[\frac{\partial^2 w}{\partial x^2} + \nu\frac{\partial^2 w}{\partial y^2}\right],$$

$$\sigma_{yy} = -\frac{Ez}{1-\nu^2}\left[\frac{\partial^2 w}{\partial y^2} + \nu\frac{\partial^2 w}{\partial x^2}\right].$$

According to the original Stoney evaluation we assume a constant stress over the coating thickness and a linear z dependent stress distribution in the substrate. In the case of a rectangular substrate the problem is asymmetric. Therefore, in order to stay on a general level, we will consider for the moment different film stress values in the x and y directions, $\sigma_{xx}^{f}$ and $\sigma_{yy}^{f}$, respectively. Using the formula above one obtains from the conditions of the force and torque freedom of the whole compound:

Force freedom:

$$F_x = 0 = \int_0^{h_{tot}} \sigma_{xx}(z)dz = \int_0^{h_s} \frac{E_s}{1-\nu_s^2}\left[\frac{\partial^2 w}{\partial x^2} + \nu_s\frac{\partial^2 w}{\partial y^2}\right](z-\alpha)dz + \int_{h_s}^{h_{tot}} \sigma_{xx}^{f} dz, \tag{8}$$

$$F_y = 0 = \int_0^{h_{tot}} \sigma_{yy}(z)dz = \int_0^{h_s} \frac{E_s}{1-\nu_s^2}\left[\frac{\partial^2 w}{\partial y^2} + \nu_s\frac{\partial^2 w}{\partial x^2}\right](z-\alpha)dz + \int_{h_s}^{h_{tot}} \sigma_{yy}^{f} dz. \tag{9}$$

Torque freedom:

$$M_x = 0 = \int_0^{h_{tot}} \sigma_{xx}(z)(z-\alpha)dz = \int_0^{h_s} \frac{E_s}{1-\nu_s^2}\left[\frac{\partial^2 w}{\partial x^2} + \nu_s\frac{\partial^2 w}{\partial y^2}\right](z-\alpha)^2 dz + \int_{h_s}^{h_{tot}} \sigma_{xx}^{f}(z-\alpha)dz, \tag{10}$$

$$M_y = 0 = \int_0^{h_{tot}} \sigma_{yy}(z)(z-\alpha)dz = \int_0^{h_s} \frac{E_s}{1-\nu_s^2}\left[\frac{\partial^2 w}{\partial y^2} + \nu_s\frac{\partial^2 w}{\partial x^2}\right](z-\alpha)^2 dz + \int_{h_s}^{h_{tot}} \sigma_{yy}^{f}(z-\alpha)dz. \tag{11}$$

The origin for the z-axis was again laid at the substrate bottom and $h_{tot}$ stands for the compound thickness being a sum of the substrate thickness, $h_s$, and the thickness of the film, $h_f$. From these four equations we first evaluate the position of the neutral surface within the compound as[2]:

$$\alpha = \frac{h_s\left(3h_f + 2h_s\right)}{6\left(h_f + h_s\right)}, \tag{12}$$

In addition we can give a relation between the normal stresses within the film and the resulting curvature of the compound:

$$\sigma_{xx}^f = -\frac{E_s h_s^3}{6\left(1-\nu_s^2\right)h_f\left(h_f+h_s\right)}\left(\frac{\partial^2 w}{\partial x^2} + \nu_s \frac{\partial^2 w}{\partial y^2}\right) \cong -\frac{E_s h_s^3}{6\left(1-\nu_s^2\right)h_f\left(h_f+h_s\right)}\left(\frac{1}{R_x} + \nu_s \frac{1}{R_y}\right), \tag{13}$$

$$\sigma_{yy}^f = -\frac{E_s h_s^3}{6\left(1-\nu_s^2\right)h_f\left(h_f+h_s\right)}\left(\frac{\partial^2 w}{\partial y^2} + \nu_s \frac{\partial^2 w}{\partial x^2}\right) \cong -\frac{E_s h_s^3}{6\left(1-\nu_s^2\right)h_f\left(h_f+h_s\right)}\left(\frac{1}{R_y} + \nu_s \frac{1}{R_x}\right), \tag{14}$$

where $R_x$ and $R_y$ denote the radius of curvature for the main axis directions x and y. Rearranging yields:

$$\frac{\partial^2 w}{\partial x^2} = \frac{\sigma_{xx}^f - \nu_s \sigma_{yy}^f}{N\left(\nu_s^2 - 1\right)}; \quad \frac{\partial^2 w}{\partial y^2} = \frac{\sigma_{yy}^f - \nu_s \sigma_{xx}^f}{N\left(\nu_s^2 - 1\right)}, \tag{15}$$

$$\text{with } N \equiv \frac{E_s h_s^3}{6\left(1-\nu_s^2\right)h_f\left(h_f+h_s\right)}, \tag{16}$$

Assuming a homogeneous deposition process, the biaxial film stress should be isotropic and homogeneous, i. e.[3] $\sigma_{xx}^f = \sigma_{yy}^f = \sigma_{rr}^f$ at any single point and $\sigma_{rr}^f$ being constant everywhere on the surface. This obviously holds in the case of a relatively thick substrate compared to the film thickness, because there the bending of the compound caused by the film stress and thus the reduction of this stress can only be relatively small. Applying the results of this section we can give a formula for the ratio of the film stress reduced due to bending, $\sigma_b^f$, and the film stress $\sigma_{rr}^f$ corresponding to equations (13) and (14) as a first perturbation of the $\sigma_{rr}^f$=constant case:

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[2] A more general consideration for various forms of plate deformation using the calculus of the free energy is given in Schwarzer 2002.

[3] This directly follows in the case $\sigma_{xy}^f = 0$ and $\sigma_{xx}^f = \sigma_{yy}^f$, because we have the general transformation rule

$$\sigma_{rr}^f = \cos^2\varphi\, \sigma_{xx}^f + \sin 2\varphi\, \sigma_{xy}^f + \sin^2\varphi\, \sigma_{yy}^f.$$

$$\frac{\sigma_b^f}{\sigma_{rr}^f}=\frac{1-\nu_s}{E_s}\frac{E_f}{1-\nu_f}\frac{h_f\left(6h_f^2+9h_f h_s+4h_s^2\right)}{h_s^3}, \tag{17}$$

which yields very low values for typical $h_f/h_s$ ratios usually being well below 0.01. The reader may find a more comprehensive consideration which distinguishes between the effect of thermal and lattice mismatch caused stresses in Schwarzer 2002.

For a rectangular substrate the above equations (13) and (14) can be used to find the displacement w(x,y) applying a Fourier series approach. We obtain the result (for the evaluation see appendix A):

$$w=-\frac{4\sigma_{rr}^f}{N\pi^3\left(1+\nu_s\right)}\left[\sum_{j=1}^{\infty}\frac{a^2}{j^3}\sin\left[\frac{j\pi x}{a}\right]+\sum_{k=1}^{\infty}\frac{b^2}{k^3}\sin\left[\frac{k\pi y}{b}\right]\right]\quad ;\quad \left(j,k=1,3,5,...\right). \tag{18}$$

From that, one can prove directly that the assumption of a homogeneous and isotropic stress distribution within the film leads also for a rectangular substrate to a bowl or cap-like deformation of the compound:

$$\frac{\partial^2 w}{\partial y^2}=\frac{\partial^2 w}{\partial x^2}\quad\xrightarrow{\simeq}\quad\frac{1}{R_y}=\frac{1}{R_x}. \tag{19}$$

The value of the biaxial stress is given by:

$$\sigma_{rr}^f\cong-\frac{E_s h_s^3}{6\left(1-\nu_s\right)h_f\left(h_f+h_s\right)}\frac{1}{R_r}, \tag{20}$$

For $h_f << h_s$ the well known equation for the thin biaxially stressed substrate is received

$$\sigma_{rr}^f\simeq-\frac{E_s h_s^2}{6\left(1-\nu_s\right)h_f}\frac{1}{R_r}, \tag{21}$$

which is usually referred to as "Stoney´s formula".

It should be pointed out here that this result is independent of the concrete aspect ratio a/b of the rectangular substrate as long as the conditions for the plate approximation (6) are valid. This, however, is determined by the ratio of the substrate thickness to the smaller edge, b, of the rectangular plate (with b < a). If $h_s << b$ is not maintained, as for instance in the case of a very small cantilever, a certain deviation of the true stress value from that obtained from eq. (20) (general case) or eq. (21) (for $h_f << h_s$) occurs. From three dimensional calculations applying the Fourier approach for an internally stressed rectangular thick bi-layer plate given in appendix B we can extract the limits of the Stoney equation (21) concerning the ratios $(h_f+h_s)/b$ and a/b. At first, however, we need to determine the number of terms in our Fourier series in order to fulfil the condition of a sufficiently homogenous film stress. As an example we use the parameters given in table 1. Figure 2 shows the resulting stress distribution along the x-axis (y=0, co-ordinate origin at x=y=0) with 99 terms for an assumed average film stress of $\sigma_{xx}^{f} = \sigma = 1GPa$ at z=$h_f$/2.

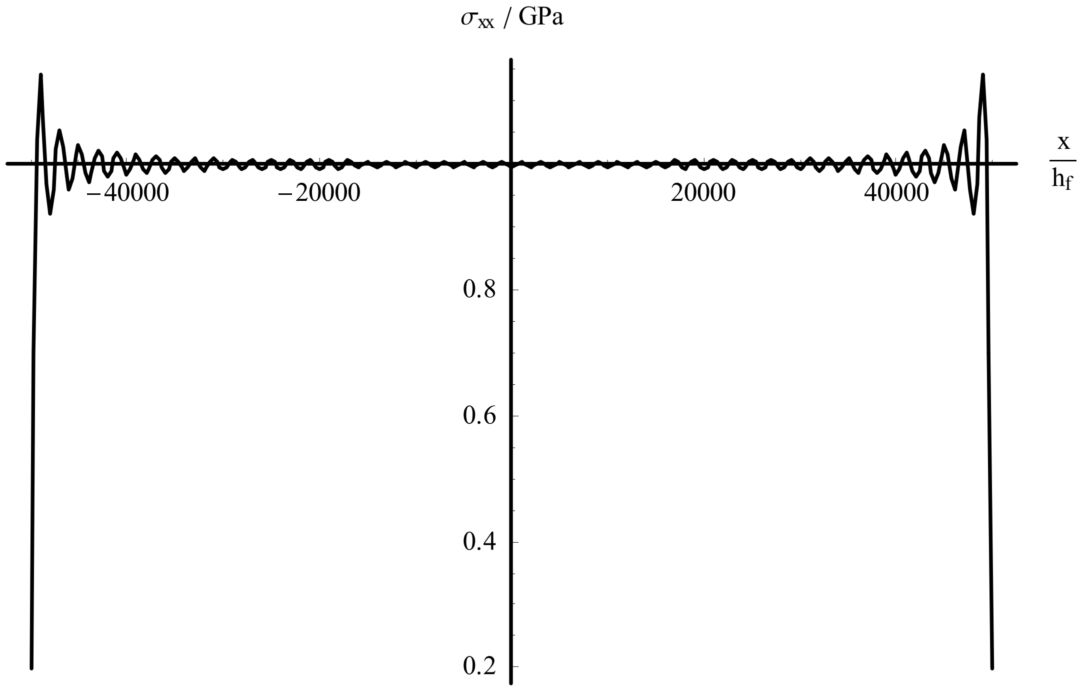


**Fig. 2:** **Film stress along the x-axis as evaluated applying the three dimensional approach given in appendix B with 99 terms.**

We see that the approach also provides a rather constant stress distribution along the normal axis (here z) within the film (Fig. 3) and a linearly dependent stress in the substrate (Fig. 4).

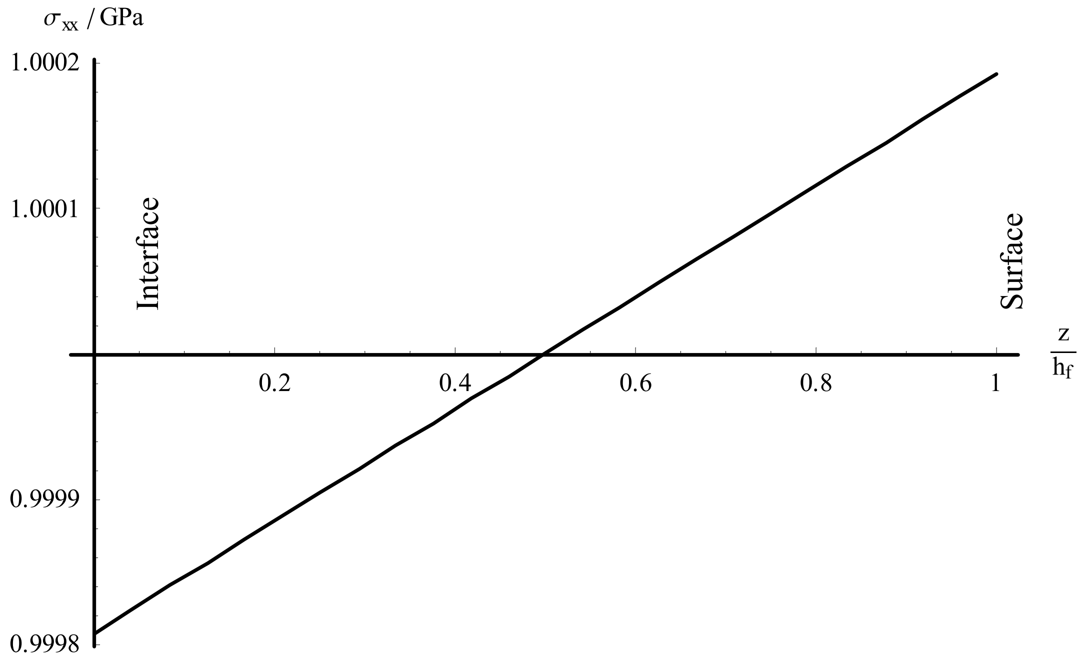


**Fig. 3:** **z-dependence of film stress as evaluated applying the three dimensional approach given in appendix B with 99 terms.**

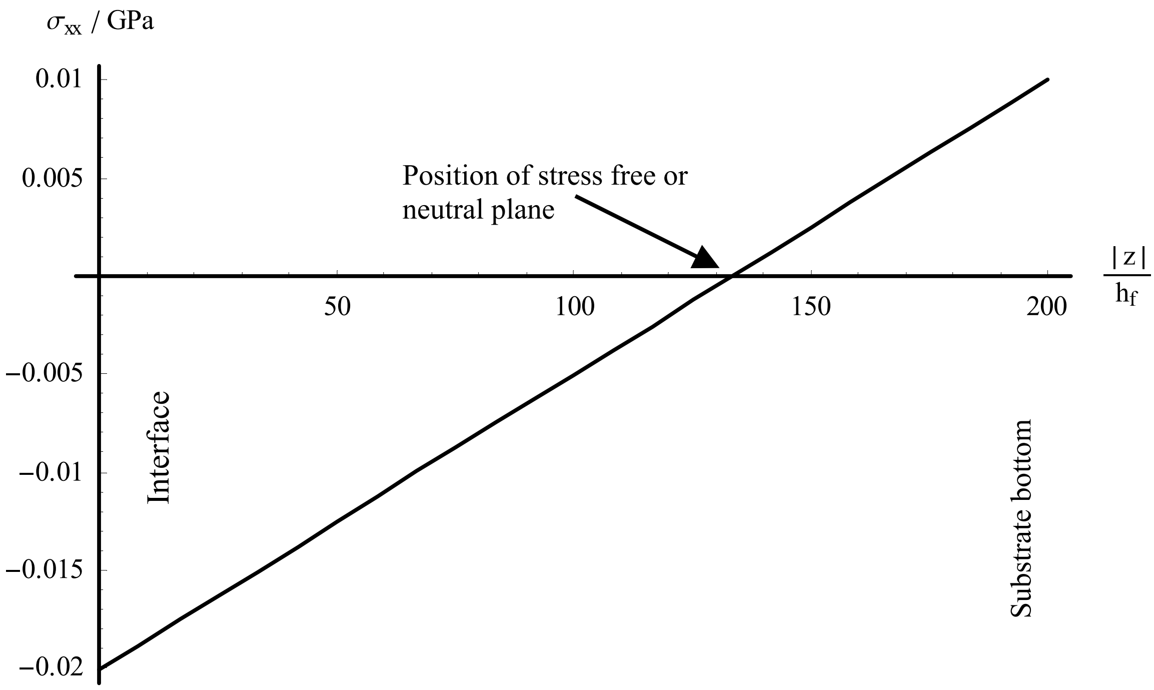


**Fig. 4:** **z-dependence of substrate stress as evaluated from the three dimensional approach given in appendix B with 99 terms.**

Now we compare the radius of curvature of the 3-D–approach (cf. Appendix B) with the results corresponding to equations (20) and (21) for a variety of different geometrical conditions.

In Figures 5 and 6 the ratio between the 3-D-approach and the Stoney value are plotted for five different aspect ratios a/b as a function of the substrate thickness.

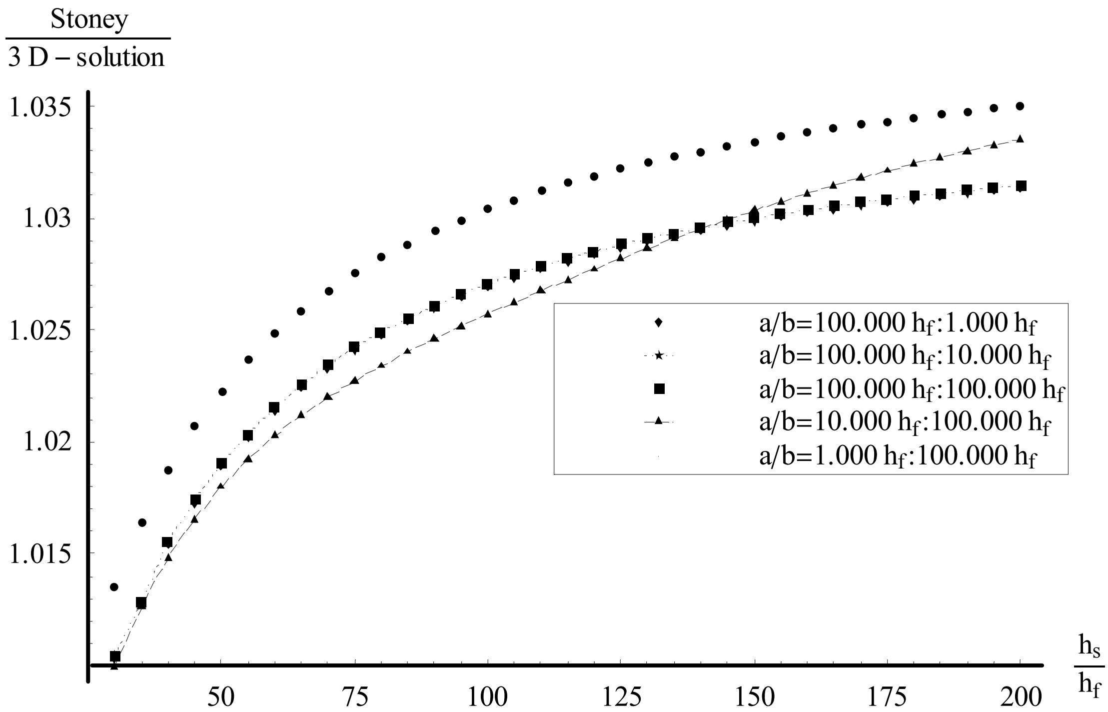


**Fig. 5:** **Ratio between the substrate bending of the "Stoney equation" (21) and the 3-D-approach of appendix B as a function of the substrate thickness for 5 different aspect ratios a/b of the rectangular substrate**

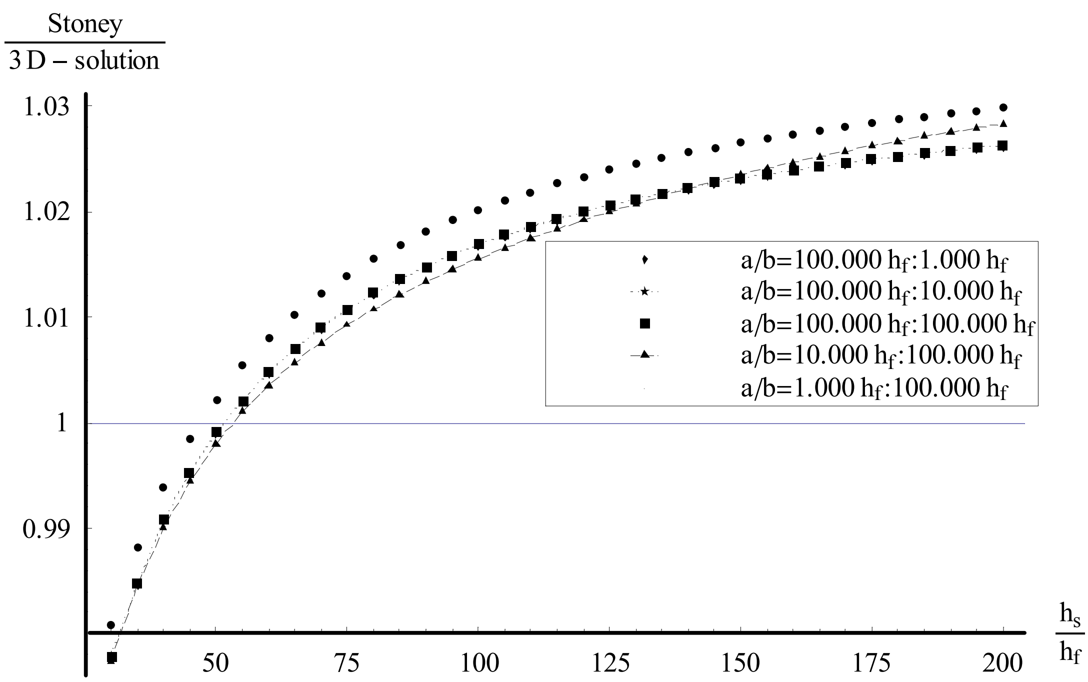


**Figure 6:** **Ratio between the substrate bending of equation (20) and the 3-D-approach of appendix B as a function of the substrate thickness for 5 different aspect ratios a/b of the rectangular substrate**

It is not surprising, that the apparently less approximated formula (20) provides a better agreement (see Fig. 6) especially in the case of bigger ratios $h_f/h_s$ while the so-called Stoney-formula (21) yields significantly higher deviations from the 3-D-approach within the investigated parameter field (Fig. 5).

We also find (figures 5, 6 and especially 7), that for thin to middle thick plates ($b/(h_f+h_s) > 10$) the influence of the aspect ratio b/a on the curvature $w_{yy}$ in direction of the varied side length is relatively small while the influence on the curvature $w_{xx}$ in direction of the side length held constant is almost none existent. The dependence of the ratio of curvatures from the Stoney result using equation (21) at one hand and the 3 D calculation on the other hand on the aspect ratio b/a is shown in figure 7 ($h_f = 1$ µm, $h_s = 200$ µm). Here we see, that in fact the difference between the Stoney result and the 3-D approach never exceeds 3.5 %.

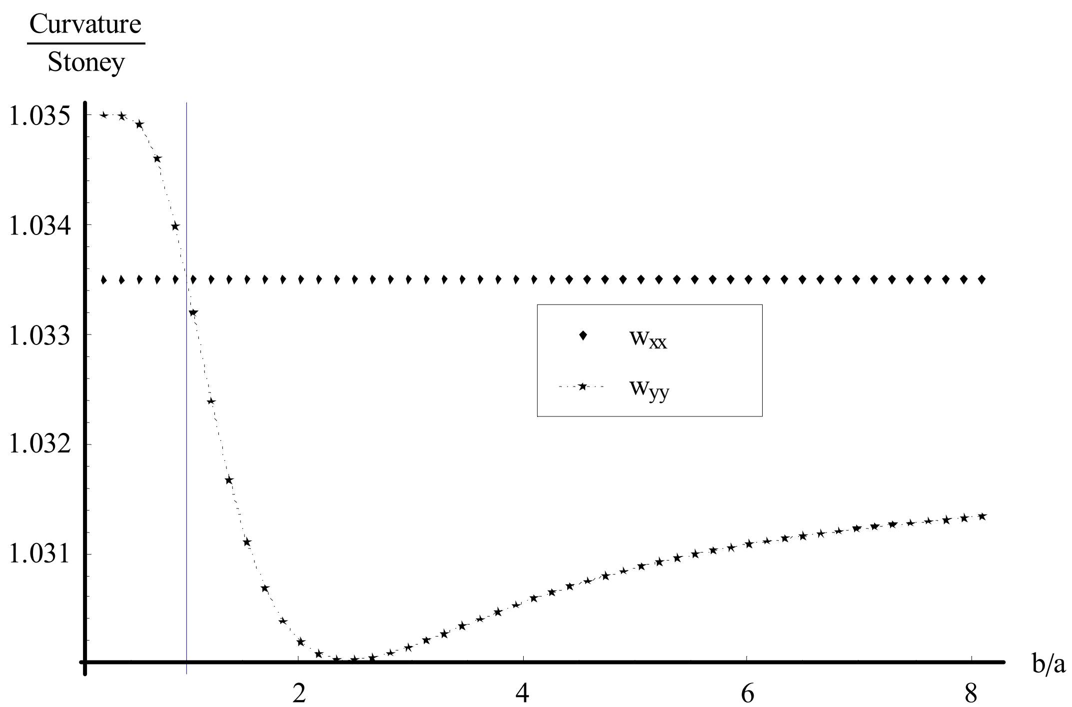


**Figure 7:** **Influence of the aspect ratios b/a of the rectangular substrate on the curvature in x- and y-direction, $w_{xx} = \frac{\partial^2 w}{\partial x^2}$ and $w_{yy} = \frac{\partial^2 w}{\partial y^2}$, as calculated using the 3D approach, in units of the Stoney-value (eq. 21)**

For thin plates this also holds in the case of relatively big or small b/a ratios (b/a>100/1 or b/a<1/100), which are not shown in figure 7. One would also expect symmetry between the two sides. So one can evaluate for b/a=100/1 with a=50*$h_s$:

$$w_{Stoney}/w_{xx}=1.034 \text{ and } w_{Stoney}/w_{yy}=1.031$$

and for b/a=1/100 b=50*$h_s$:

$$w_{Stoney}/w_{xx}=1.031 \text{ and } w_{Stoney}/w_{yy}=1.034.$$

Concerning the effect of the thickness of the plate we find (Fig. 8), that the plate approximation (both equation (20) and the Stoney equation (21)) provides a good agreement of below 5% with our 3-D solution as long as the total thickness $h_{tot}$ is at least 11 times smaller than the shortest side of the rectangular substrate (concerning experiments, this of course holds only apart from other uncertainties, like for example substrate roughness and coating inhomogeneities of course).

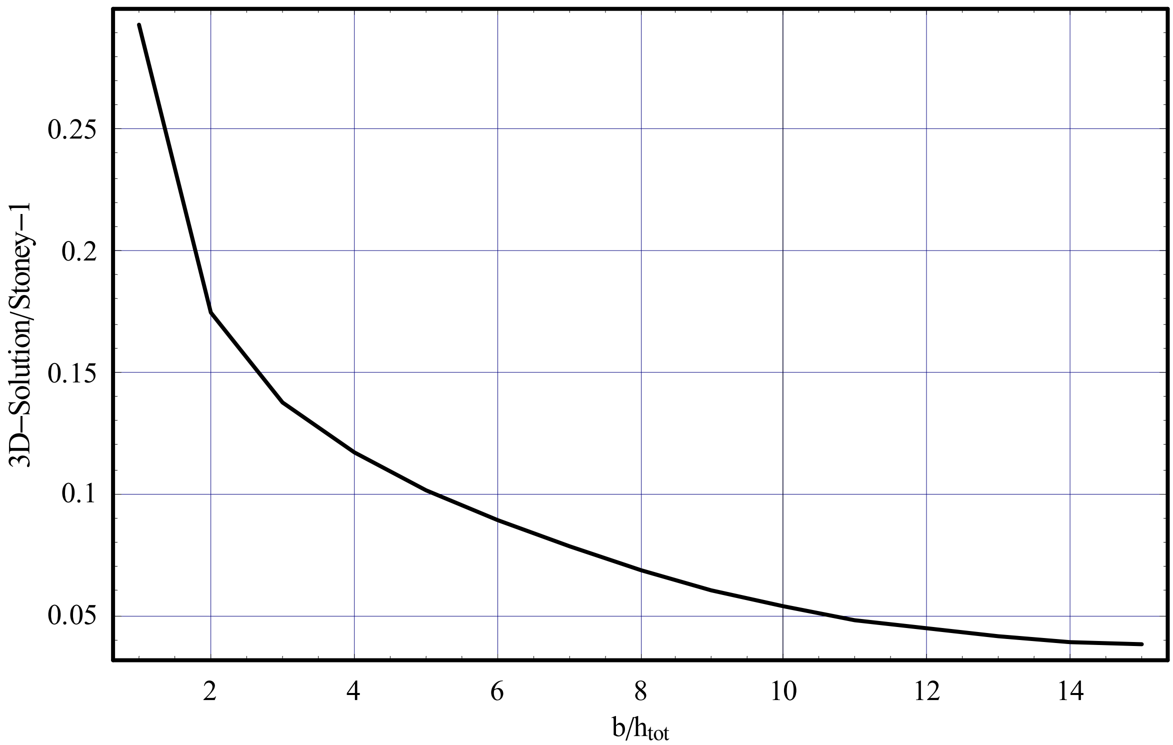


**Figure 8: Error function for the Stoney-value – calculated from the ratio of the centre curvature of the 3D-approach (appendix B) and the approximated solution (eq. 21).**

As we see in the case of a bent circular thick plate one obtains about the same limits for external loading, too. The formulae for this example are already at hand. They have been presented by Lurje 1964 (see also Schwarzer 2002). Comparing them with the thin plate case we extract the error behaviour given in figure 9.

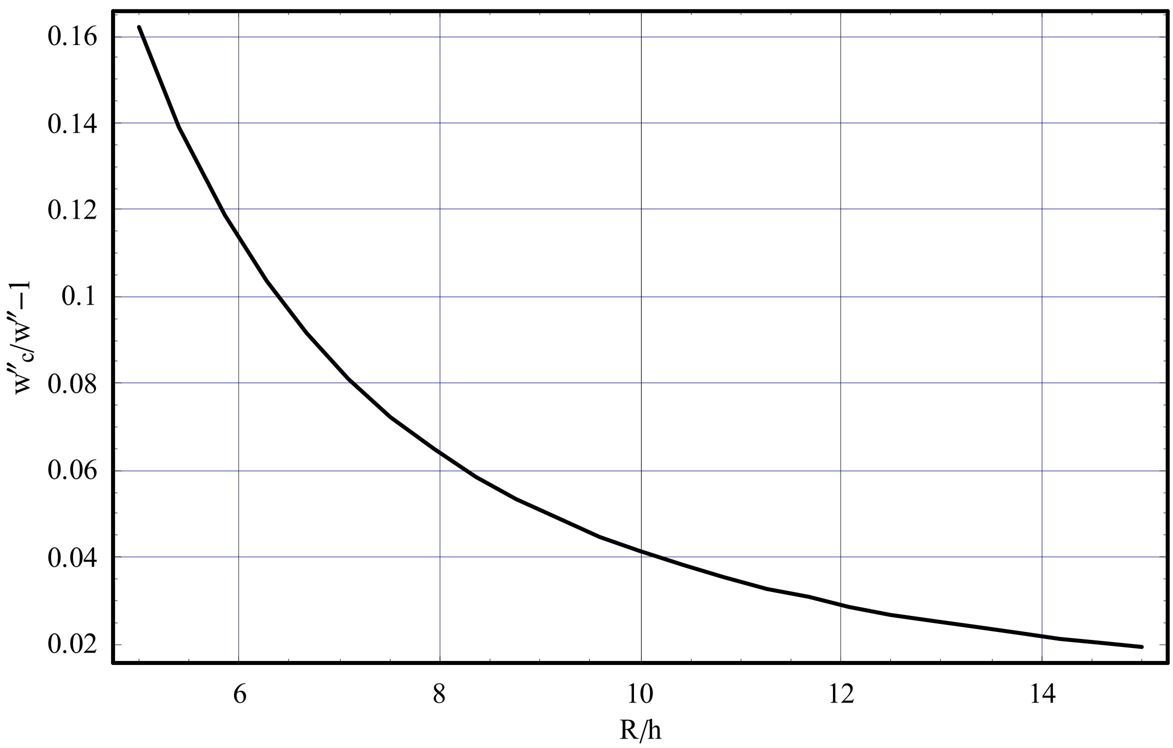


**Figure 9:** **Error function for the plate approximation – calculated from the ratio of the curvature at the edge of the correct and approximated solution for a bent circular plate fixed at the edge and loaded at the centre (both solutions from Lurie 1964).**

There the quotient $w''_c/w''$ between the correct solution $w''_c$ and the plate approximation $w''$ is given as a function of the ratio $b/h_{tot}$ (b now denoting the radius of the plate). We see, that the radius of the substrate b should not fall short of at least 9 times the thickness of the compound in order to fulfil the conditions (6) such that the plate-formulae of the external loading case will provide an accuracy of about 5%. So we see, that at least concerning the curvature, a 1:10-ratio between the plate thickness and the shortest side of the plate seems to make the much simpler plate-formulae applicable with an error of about 5% in both cases internal and external loading.

## Conclusion

The investigation has shown that the nature of deformation is determined by the ratio of substrate thickness to the lateral dimension of the substrate. Provided that

- $h_s << b$ ($b<a$ with a and b denoting the two sides of the rectangular substrate) , i.e. provided the plate approximation is valid and
- the film thickness $h_f$ is small compared to the substrate thickness $h_s$, thereby assuring a constant film stress over the whole substrate surface,

the coated substrate gets a constant curvature everywhere on its surface. In particular, even for an elongated, strip-like substrate a cap or bowl-shaped deformation is formed, as far as the smaller side of the strip is large in comparison to the substrate thickness. Hence, replacing the YOUNG´s modulus in eq. (1) by the biaxial modulus is appropriate, yielding equations (20) and (21), resp.. Using the plate modulus instead would deliver stress values which are too big by a factor of $(1 - \nu_s^2) / (1 - \nu_s) = 1 + \nu_s$, i.e. by 20...30 % for typical $\nu_s$ values of 0.2...0.3. It has been shown, that a ratio of about $b/h_{tot} \geq 11$ assures the validity of Stoney's equation (eq. (21)) with maximum deviation to the results of the 3D calculation of less than 5% no matter what aspect ratio a to b of the side lengths of the rectangular substrate is used.

So, as $b/h_{tot} \geq 11$ is the case for many substrates, both macroscopic strips and micromechanical cantilevers used in laboratories for stress measurement, Stoney's equation (eq. (21)) provides the suitable tool for the analysis of these experiments.

## References


Berry BS (1988) Anelastic relaxation and diffusion in thin-layer Materials in: Gupta D, Ho PS (eds.) Diffusion Phenomena in Thin Films and Microelectronic Materials, Noyes, Park Ridge, pp. 73.

Berry BS, Pritchet WC (1990) Internal stress and internal friction in thin-layer microelectronic materials, J. Appl. Phys. 67 (8), 15 April 1990, pp. 3661.

Elwenspoek M, Jansen HV (1998) Silicon Micro Machining, Cambridge University Press

Landau LD, Lifschitz EM (1989) Elastizitätstheorie, Akademie-Verlag Berlin, in German

Ljungcrantz H, Hultman L, Sundgren JE, Johansson S, Kristensen N, Schweitz JA, Shute CJ (1993) Residual stresses and fracture properties of magnetron sputtered Ti films on Si microelements, J. Vac. Sci. Technol. A 11(3) May/Jun. 1993, pp. 543

Lurje AI (1964) Three Dimensional Problems of the Theory of Elasticity, Interscience Publishers

Ohring M (1992) The Materials Science of Thin Films, Academic Press, San Diego, pp. 413.

Schwarzer N (2002) About the theory of thin coated plates, published in the internet at: http://archiv.tu-chemnitz.de/pub/2002/0005/index.html

Schwarzer N (2000) Arbitrary load distribution on a layered half space, ASME Journal of Tribology, Vol. 122, No. 4, October 2000, 672 - 681

Stoney G (1909) The tension of metallic films deposited by electrolysis, Proc. Royal Soc. London, A82 (1909) 172.

## *Appendix A*

We start with the approach

$$w = \sum_{j,k=1}^{\infty} c_{ik} \cdot \left[ \sin\left[ \frac{j\pi x}{a} \right] + \sin\left[ \frac{k\pi y}{b} \right] \right] \quad \text{(A.1)}$$

and apply the conditions (15). For the reason of simplification we set $\frac{\sigma_{xx}^f - \nu_s \sigma_{yy}^f}{\left(\nu_s^2 - 1\right)} = p_x$; $\frac{\sigma_{yy}^f - \nu_s \sigma_{xx}^f}{\left(\nu_s^2 - 1\right)} = p_y$, which allows us to split the coefficient matrix $c_{jk}$ into two separate series of coefficients $c_j$ and $c_k$

$$c_{jk} \longrightarrow c_j + c_k .$$

Thus we obtain

$$p_x(x) = \sum_{j=1}^{\infty} c_j \cdot N \cdot \frac{j^2 \pi^2}{a^2} \cdot \sin\left[ \frac{j\pi x}{a} \right] \quad \text{(A.2)}$$

$$p_y(y) = \sum_{k=1}^{\infty} c_k \cdot N \cdot \frac{k^2 \pi^2}{b^2} \cdot \sin\left[ \frac{k\pi y}{b} \right] \quad \text{(A.3)}$$

and can now determine the coefficients $c_j$ and $c_k$

$$c_j = \frac{2}{a} \cdot \int_0^a \frac{1}{N} \cdot \left( \frac{a}{j\pi} \right)^2 \cdot p_x \cdot \sin\left[ \frac{j\pi x}{a} \right] \cdot dx , \quad \text{(A.4)}$$

$$c_k = \frac{2}{b} \cdot \int_0^b \frac{1}{N} \cdot \left( \frac{b}{k\pi} \right)^2 \cdot p_y \cdot \sin\left[ \frac{k\pi y}{b} \right] \cdot dy . \quad \text{(A.5)}$$

Assuming a constant stress distribution in x- and y-direction one obtains the simple result

$$c_j = \frac{2}{a} \cdot \int_0^a \ldots = \frac{2}{a} \frac{1}{N} \left( \frac{a}{j\pi} \right)^2 \cdot p_x \left( \frac{a}{j\pi} - \frac{a}{j\pi} \cos\left( j\pi \right) \right) = \begin{cases} \frac{4 p_x}{a N} \cdot \left( \frac{a}{j\pi} \right)^3 & j = 1,3,5,\ldots \\ 0 & j = 2,4,6,\ldots \end{cases} \quad \text{(A.6)}$$

$$c_k = \frac{2}{b} \cdot \int_0^b \ldots = \frac{2}{b} \frac{1}{N} \left( \frac{b}{k\pi} \right)^2 \cdot p_y \left( \frac{b}{k\pi} - \frac{b}{k\pi} \cos\left( k\pi \right) \right) = \begin{cases} \frac{4 p_y}{b N} \cdot \left( \frac{b}{k\pi} \right)^3 & k = 1,3,5,\ldots \\ 0 & k = 2,4,6,\ldots \end{cases} \quad \text{(A.7)}$$

## *Appendix B*

In order to come to a suitable three dimensional approach for thick substrates we assume the coating as to be separated from the substrate and pressed at its rim such, that exactly the bi-axial intrinsic stress state with a defined $\sigma_{xx}$ and $\sigma_{yy}$ appears. This pre-stressed coating is now "stuck" on the substrate. The external forces $F_x$ and $F_y$ producing the pre-stress-state are removed allowing the coating-substrate-system to find its equilibrium. The former forces acting on the rim of the coating must be now taken on by the elastic stiffness of the substrate. They, the forces, couple into the substrate as shearing forces $S_x$ and $S_y$ via its surface. In order to simplify the calculation we consider a substrate of rectangular geometry with the side lengths a and b. We do not know yet the distribution of this shearing stress on the substrate surface so we start with a general solution of the problem, which can be given due to the displacements. Thus, for both substrate and film we apply the following approach for the displacements $\vec{u} = (u, v, w)$ in x, y and z-direction:

$$\vec{u} = \sum_{i,k=1}^{\infty} c_{ik} \begin{pmatrix} c^2\left(\left(A+Bcz\right)e^{cz}+\left(D+Fcz\right)e^{-cz}\right)\sin\left[cx\right]+u^2\left(Ce^{uz}+Ge^{-uz}\right)\cos\left[uy\right] \\ u^2\left(\left(\tilde{A}+\tilde{B}uz\right)e^{uz}+\left(\tilde{D}+\tilde{F}uz\right)e^{-uz}\right)\sin\left[uy\right]+c^2\left(\tilde{C}e^{cz}+\tilde{G}e^{-cz}\right)\cos\left[cx\right] \\ c^2\left(\left(-A-\left(-3+4\nu+uz\right)B\right)e^{cz}+\left(D+\left(3-4\nu+uz\right)F\right)e^{-uz}\right)\cos\left[cx\right] \\ +u^2\left(\left(-\tilde{A}-\left(-3+4\nu+uz\right)\tilde{B}\right)e^{uz}+\left(\tilde{D}+\left(3-4\nu+uz\right)\tilde{F}\right)e^{-uz}\right)\cos\left[uy\right] \end{pmatrix} \quad \textbf{(B.1)}$$

with properly chosen c and u (a and b denoting the side lengths of the rectangular substrate) it can be assured that the shearing stresses $\sigma_{xy}$, $\sigma_{xz}$ and $\sigma_{yz}$ being zero at the substrate rim (with $\sigma_{xz}$ only at |x|=a/2 and $\sigma_{yz}$ only at |y|=b/2). The constants $A,B,C,D,F,G$ and $\tilde{A},\tilde{B},\tilde{C},\tilde{D},\tilde{F},\tilde{G}$ are different for film and substrate so altogether we have 24 constants to determine. In this case a suitable Fourier series would be necessary to construct the desired stress distribution for either the normal or shearing stresses within any chosen z=constant-plane of the compound. It can be shown that (B.1) satisfies the equation for equilibrium for an isotropic elastic medium (see e.g. Landau and Lifschitz 1989). The stress components can be found using the following identities:

$$\sigma_{jk} = \frac{E}{1+\nu}\left(u_{jk} + \frac{\nu}{1-2\nu}u_{ll}\delta_{jk}\right) \quad with \quad j,k = x,y,z;\ u_{xk} = \frac{\partial u}{\partial k};\ u_{yk} = \frac{\partial v}{\partial k};\ u_{zk} = \frac{\partial w}{\partial k}. \quad \textbf{(B.2)}$$

Setting the co-ordinate origin at the interface (z=0) the further boundary conditions:

$$\sigma_{zz}\big|_{z=h_f} = \sigma_{zz}\big|_{z=-h_s} = \sigma_{xz}\big|_{z=-h_s} = \sigma_{yz}\big|_{z=-h_s} = \sigma_{xz}\big|_{z=h_f} = \sigma_{yz}\big|_{z=h_f} = 0,$$

$$\sigma_{xz}\big|_{z=0+0} = \sigma_{xz}\big|_{z=0-0} = f_x\left(x,y\right), \sigma_{yz}\big|_{z=0+0} = \sigma_{yz}\big|_{z=0-0} = f_y\left(x,y\right),$$

$$\sigma_{zz}\big|_{z=0+0} = \sigma_{zz}\big|_{z=0-0}, \quad u_3\big|_{z=0+0} = u_3\big|_{z=0-0},$$

$$Fx = \sigma_{rr}^f h_f b = Sx = \int_{-b/2}^{b/2}\int_{0}^{a/2} \sigma_{xz} dxdy,$$

$$Fy = \sigma_{rr}^f h_f a = Sy = \int_{-a/2}^{a/2}\int_{0}^{b/2} \sigma_{yz} dydx.$$

give the equations necessary to determine all constants. One can extract from (B.1), that the structure of the normal stresses in lateral direction of the film-substrate-compound $\sigma_{xx}$ and $\sigma_{yy}$ can in principle be given in the following form:

$$\begin{aligned}\sigma_{xx} &= \sum_{i=1}^{\infty} fx_x(z)\, c_i \cos(\frac{i\pi x}{a}) + \sum_{k=1}^{\infty} fx_y(z)\, c_k \cos(\frac{k\pi y}{b}),\\ \sigma_{xx} &= \sum_{i=1}^{\infty} fy_x(z)\, c_i \cos(\frac{i\pi x}{a}) + \sum_{k=1}^{\infty} fy_y(z)\, c_k \cos(\frac{k\pi y}{b}).\end{aligned} \qquad \textbf{(B.3)}$$

Now we need to find equations for the determination of the Fourier coefficients $c_i$ and $c_k$. From the bi-axial stress conditions $\sigma^f_{xx} = \sigma^f_{yy} = \sigma$ at a distinct depth $z=z_0$ together with (B.3) we obtain:

$$\begin{aligned}c_i &= \frac{2}{a}\int_{-a/2}^{a/2} \frac{\sigma\left(fx_y(z_0) - fy_y(z_0)\right)}{fx_y(z_0)\, fy_x(z_0) - fx_x(z_0)\, fy_y(z_0)} \cos\left(\frac{i\pi x}{a}\right),\\ c_k &= \frac{2}{b}\int_{-b/2}^{b/2} \frac{\sigma\left(fx_y(z_0) - fy_y(z_0)\right)}{fx_y(z_0)\, fy_x(z_0) - fx_x(z_0)\, fy_y(z_0)} \cos\left(\frac{k\pi y}{b}\right).\end{aligned} \qquad \textbf{(B.4)}$$

In addition, in order to satisfy the condition that also the stress components $\sigma^{f,s}_{xx}$ and $\sigma^{f,s}_{yy}$ should be zero at the edges of the plate, namely

$$\sigma^{f,s}_{xx}\Big|_{x=\pm\frac{a}{2}} = 0 \quad and \quad \sigma^{f,s}_{yy}\Big|_{y=\pm\frac{b}{2}} = 0,$$

additional terms are necessary. However, the influence of these terms is insignificant as long as the length of the shortest side is big against the total thickness of the coating substrate compound.

## *Tables*

**Table 1: Mechanical parameters for a system of a 1µm TiN-coating on silicon**

| | Young's modulus | Poisson's ratio | Thickness |
|---|---|---|---|
| Coating | 450 GPa | 0.25 | $h_f$= 1µm |
| Substrate | 164.4 GPa | 0.224 | $h_s$ = 200µm |