About the theory of thin coated plates

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1. Introduction

For lots of applications and theoretical deliberations it would be a great help if one would be able to describe the elastic field of inhomogeneous bodies like thin film-substrate-compounds directly from the known conditions at the boundary and interfaces and the material parameters like Young's modulus and Poisson's ratio.

There exist two principal methods for the simplification of elastic problems of coated materials:

• the infinite space or halfspace, used for crack, defect and contact mechanical problems and

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• the plate or shell simplification, widely used for all problems where one dimension of the body can be considered as small compared to the others.

The problem considered in this paper is that of a coated plate under arbitrary deformation. If the thickness of the compound can be considered as small in comparison to the radial extensions of the plate and in addition the displacement is small compared to the thickness, the approximation of the weakly bent plate (see [1], pp. 48 - 57) can be used. In this case it is rather simple to extend the theory of homogeneous plates to that for layered ones using the calculus of the Free Energy of a deformed body. This method will be used in this work and the corresponding equations will be completely calculated for the cases of the supported and the fixed plate. In addition we will present illustrative examples of the equations obtained.

However, if concentrated local forces cause large stress gradients the plate or shell simplification is often not sufficient to explain the elastic and inelastic effects occurring in thin film-substrate-compounds. Possible reasons are interfacial forces caused by different deformation of film and substrate as well as asperity contact and defect problems. Taking i.e. the problem of a simply bent plate, one can use the plate approximation as long as

1. the geometrical parameters (film and substrate thickness, bending length etc.) justify the plate simplification and in addition
2. one is not interested in the complete stress distribution of the bent plate at all of its positions.

But especially in thin film problems one often needs exactly those stress components and deformations which the ordinary plate approximation neglects, setting (with z being parallel to the plate’s normal):

\[ \sigma_{xz} = \sigma_{zx} = \sigma_{zz} = 0, \]

i.e., contact stress normal to the plate surface, shearing stress at the interface, the exact shape of the neutral surface, etc. ([1], p. 49). Thus, because the theory presented here is based upon the theory of the weakly bent plate it is valid and practicable only in those cases, where one is not interested in specific information about the exact stress distribution and deformation within the inhomogeneous body.

2. Boundary conditions for the plate approximation

In order to obtain the range of validity of the thin plate approximation concerning the plate’s geometry we simply compare the correct solution of the thick plate with that one of the thin plate for a suitable problem and extract an error function giving the deviation of the thin plate approximation from the correct solution as a function of the ratio of the plate’s diameter to its thickness. We consider the problem of a circular plate of radius R fixed at the edge and loaded at the centre by a concentrated force. The solution for both the thick and the thin plate can be found in [8]. Figure 1 gives the quotient \( \frac{w_c}{w} \) between the correct solution \( w_c \) and the plate approximation \( w \). It is given as a function of the ratio R/h. From this figure one can deduce that one for example needs a ratio of at least R/h\(=22 \) if one wants to stay in the accuracy range of about 5%. For bigger ratios R/h the accuracy of the thin plate approximation increases relatively rapidly, so that for about R/h>60 the error of the theory lays well below 1% and thus can be neglected. In order to allow the reader to estimate himself the error for concrete examples, the author has written a short Mathematica®-package, which calculates the ratio \( \frac{w_c}{w} \) for arbitrary mechanical and geometrical parameters of the plates in question (see appendix).
Figure 1: Error function for the plate approximation – calculated from the ratio of the normal displacements of the correct and approximated solution for a bent circular plate fixed at the edge and loaded at the centre (see appendix).

3. Thin Plate Approximation for the Free Energy in the Case of Isotropy

From Hooke's law ([1], p. 11) and the simplification of the thin plate given by eq. (1) we get for the Free Energy of any infinitesimal small volume element of the bent plate ([1], pp. 50)

\[ F_{\alpha \alpha} = (z - \alpha)^2 \frac{E}{2(1 - \nu^2)} (\Phi_1 + 2(1 - \nu)\Phi_2), \]  

where \( E \) denotes the Young's modulus of the plate and \( \nu \) the Poisson's ratio. As \( \alpha \) stands for the position of the neutral surface we have laid the origin \( z=0 \) at the substrates bottom. In the general case of an arbitrary inhomogeneous body \( E \) and \( \nu \) are functions of all co-ordinates \( x, y, z \) but under the assumption of a coated plate we have to write \( E=E(z) \) and \( \nu=\nu(z) \). \( \Phi_{1,2} \) are functions of \( x \) and \( y \). If we denote the displacement in \( z \) direction with \( w \) we can write:

\[ \Phi_1 = \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right)^2; \quad \Phi_2 = \left( \frac{\partial^2 w}{\partial x \partial y} \right)^2 - \frac{\partial^2 w}{\partial x^2} \frac{\partial^2 w}{\partial y^2}. \]

4. The weakly bent Coated Plate

4.1. The Position of the Neutral Surface in a Multilayer-Substrate-Compound (pure external bending state)

To get the position of the neutral surface (that surface in the plate which is not compressed or stretched but purely bent) one has to find the minimum of the Free Energy (2) for the given geometry of the plate and the given boundary conditions. For homogenous plates one obtains in the case of pure bending that this position is exactly at the middle of the plate. If the plate is coated with \( n-1 \) coatings (the coating with number \( i \) extends from \( h_{i-1} \) to \( h_i \) and has the elastic parameters \( E_i \) and \( \nu_i \) as elastic modulus and Poisson's ratio, respectively, the substrate
extends from \( h_0 = 0 \) to \( h_1 \) and has the parameters \( E_1 \) and \( \nu_1 \) one gets for the total Free Energy of the plate

\[
F_{\text{ges}} = \int_0^{h_x} \int (z - \alpha)^2 \left( \frac{E(z)}{2(1 - \nu^2(z))} \right) (\Phi_1 + 2(1 - \nu(z))\Phi_2) \, dz \, dx \, dy,
\]

where only the inner integral interests for the determination of the position \( \alpha \) of the neutral surface:

\[
F = \int_{-\alpha}^{h_x - \alpha} (z - \alpha)^2 \left( \frac{E(z)}{2(1 - \nu^2(z))} \right) (\Phi_1 + 2(1 - \nu(z))\Phi_2) \, dz.
\]

To find the minimum one has to solve the following equation:

\[
\frac{\partial F}{\partial \alpha} = \sum_{i=1}^{n} \left[ \frac{E_i}{2(1 - \nu_i^2)} \left( \Phi_1 + 2(1 - \nu_i)\Phi_2 \right) \right] \left[ (h_i - \alpha)^2 - (h_i - h_{i-1})^2 \right] = 0
\]

The solution may be obtained as:

\[
\alpha = \frac{\sum_{i=1}^{n} \frac{E_i}{2(1 - \nu_i^2)} \left[ \Phi_1 + 2(1 - \nu_i)\Phi_2 \right] (h_i^2 - h_{i-1}^2)}{2 \sum_{i=1}^{n} \frac{E_i}{2(1 - \nu_i^2)} \left[ \Phi_1 + 2(1 - \nu_i)\Phi_2 \right] (h_i - h_{i-1})}.
\]

This equation simplifies significantly in those cases where \( w \) is independent of \( y \), i.e. \( w = w(x) \). Here we have

\[
\Phi_2 = \left( \frac{\partial^2 w}{\partial x \partial y} \right) - \frac{\partial^2 w}{\partial x^2} \frac{\partial^2 w}{\partial y^2} = 0 - \frac{\partial^2 w}{\partial x^2} \frac{\partial^2 w}{\partial y^2} = 0,
\]

which subsequently leads to the simple term:

\[
\alpha = \frac{\sum_{i=1}^{n} \frac{E_i}{2(1 - \nu_i^2)} (h_i^2 - h_{i-1}^2)}{2 \sum_{i=1}^{n} \frac{E_i}{2(1 - \nu_i^2)} (h_i - h_{i-1})}.
\]

For cases of symmetry of revolution one obtains from

\[
\Phi_1 = \left( \frac{\partial^2 w}{\partial r^2} + \frac{1}{r} \frac{\partial w}{\partial r} \right)^2, \quad \Phi_2 = -\frac{1}{r} \frac{\partial^2 w}{\partial r^2} \frac{\partial w}{\partial r};
\]

\[
\alpha = \frac{\sum_{i=1}^{n} \frac{E_i}{2(1 - \nu_i^2)} \left[ \left( \frac{\partial^2 w}{\partial r^2} \right)^2 + \left( \frac{1}{r} \frac{\partial w}{\partial r} \right)^2 + 2\nu_i \frac{\partial^2 w}{\partial r^2} \frac{\partial w}{\partial r} \right] (h_i^2 - h_{i-1}^2)}{2 \sum_{i=1}^{n} \frac{E_i}{2(1 - \nu_i^2)} \left[ \left( \frac{\partial^2 w}{\partial r^2} \right)^2 + \left( \frac{1}{r} \frac{\partial w}{\partial r} \right)^2 + 2\nu_i \frac{\partial^2 w}{\partial r^2} \frac{\partial w}{\partial r} \right] (h_i - h_{i-1})}.
\]

In most practical cases it is possible to assume the Poisson's ratio as to be approximately equal for all coatings and the substrate. Now we obtain a very simple form for the equation of \( \alpha \):
Because of its practical importance we now consider explicitly an arbitrary coating-substrate-compound with $E_f, E_s, \nu_f, \nu_s$ as Young's modulus and Poisson's ratio and $h_f, h_s$ as thickness of coating and substrate, respectively.

We present two forms of solutions, which could be obtained from each other by simple interchanging of the material parameters. Let's consider a coated plate which is bent in directions of the coating's normal in the first case and in direction of the substrate's normal in the second one. The deformation functions $\Phi_1 = \Phi_1(x,y)$ and $\Phi_2 = \Phi_2(x,y)$ may be given as $\Phi_1^u$ and $\Phi_2^u$ for the first (film in the range $h_s < z \leq h_{tot} = h_s + h_f$) and $\Phi_1^d$ and $\Phi_2^d$ for the second case (film in the range $0 < z \leq h_s$). The figure 1 makes the geometrical conditions clear. Thus we can write now the two different solutions:

- concavely bent in direction of the coating's normal,

$$\alpha = \frac{\sum_{i=1}^{n} E_i (h_i^2 - h_{i-1}^2)}{2 \sum_{i=1}^{n} E_i (h_i - h_{i-1})}.$$  

- convexly bent in direction of the coating's normal

$$\alpha = \frac{E_s}{2(1-\nu_s^2)}[\Phi_1^u + 2(1-\nu_s)\Phi_2^u]h_s^2 + \frac{E_f}{2(1-\nu_f^2)}[\Phi_1^u + 2(1-\nu_f)\Phi_2^u](h_{tot} - h_s)$$
\[ \alpha_t = \frac{E_f}{2(1-\nu_f)} \left[ \Phi_1^d + 2(1-\nu_f)\Phi_2^d \right] h_f^2 + \frac{E_s}{2(1-\nu_s)} \left[ \Phi_1^u + 2(1-\nu_s)\Phi_2^u \right] h_{tot}^2 - h_f^2 \]  
\[ 2h_f \frac{E_f}{2(1-\nu_f)} \left[ \Phi_1^d + 2(1-\nu_f)\Phi_2^d \right] + \frac{E_s}{2(1-\nu_s)} \left[ \Phi_1^u + 2(1-\nu_s)\Phi_2^u \right] h_{tot} - h_f \]. \quad (10)

The index \( t \) may be considered as an abbreviation for "turned" because one obtains \( \alpha_t \) in the case \( \Phi_i^d = \Phi_i^u \) (\( i = 1, 2 \)) from a coating-substrate system which is upside down compared to the \( \alpha \) case (see figure 1). The reader may prove, that the equations (9) and (10) are equal in the case of a homogeneous plate. Assuming a displacement \( w = w(x) \) we are able to simplify the two equations above according to (6) and can now evaluate the influence of the compound parameters on the position of the neutral surface within the coated plate.

\[ \alpha, \alpha_t/(h_s+h_f) \]

Figure 3: Position of the neutral Surface within a coating-substrate-compound (in units of its total thickness) in dependence on the coating's Poisson's ratio \( \nu_f \)

The following three figures show the influence of the coating parameters \( \nu_f, E_f \) and \( h_f \). All known variable parameters in the figures were fixed by the following conditions:

Figure 3: \( E_f = E_s, \nu_s = 0.3, h_s = 9h_f \).
Figure 4: \( \nu_s = \nu_f, h_s = 9h_f \),

Figure 5: \( E_f = xE_s (x = 3, 5, 10), \nu_s = \nu_f, h_s + h_f = 1 \).

We obtain a rather small influence of the coating's Poisson's ratio \( \nu_f \) on the position of the neutral surface (figure 3). In contrary to this result one gets significant dependence on the ratios \( E_f \) to \( E_s \) (figures 4 and 5) and the coating thickness to the substrate thickness (figure 5).

For coating thickness of about 1:100 of the substrate thickness the deviation of the neutral surface from the middle position is always smaller than 0.01 of the total compound thickness \( h_{tot} \).

\[ \alpha, \alpha_t/(h_s+h_f) \]

Figure 4: Position of the neutral Surface within a coating-substrate-compound (in units of its total thickness) in dependence on the ratio of the coating's Young's modulus \( E_f \) to the substrate Young's modulus \( E_s \).
4.2. Equilibrium Condition for the weakly bent, coated Plate

If we denote the force which acts on a surface unit of the coated Plate with P we can write for the condition of the minimum of the total Free Energy of the plate:

$$\partial F_{pl} - \int P \delta w dx dy = 0.$$  \hspace{1cm} (11)

The variation of the Free Energy $\partial F_{pl}$ for a coated plate yields (c.f. [1], p. 52):

$$\partial F_{pl} = \int (z - \alpha)^2 \frac{E(z)}{1 - \nu^2(z)} \left[ \int \frac{\partial \Delta w}{\partial n} + (1 - \nu(z)) \frac{\partial}{\partial l} \left( \sin \theta \cos \phi \left( \frac{\partial^2 W}{\partial y^2} - \frac{\partial^2 W}{\partial x^2} \right) \right) \right] dw dl$$

$$+ \int \Delta^2 w \delta w dx dy - \frac{\partial}{\partial n} \left[ \int \Delta w (1 - \nu(z)) \left( 2 \sin \theta \cos \phi \frac{\partial^2 W}{\partial x \partial y} - \cos^2 \phi \frac{\partial^2 W}{\partial y^2} \right) \right] dw dl.$$  \hspace{1cm} (12)

Here the surface integral must be evaluated over the whole plate surface, while the line integrals have to be calculated along the boundary of the plate. The symbols l, n and $\theta$ are defined at the plate edge (boundary), where n means the direction normal and l tangential to $\alpha, \alpha_t/(h_s+h_f)$
the edge curve. The symbol \( \theta \) describes the angle between the x-axis and \( n \). The following relations may be useful:

\[
\frac{\partial}{\partial x} = \cos \theta \frac{\partial}{\partial n} - \sin \theta \frac{\partial}{\partial l} ; \quad \frac{\partial}{\partial y} = \cos \theta \frac{\partial}{\partial n} + \sin \theta \frac{\partial}{\partial l} .
\]

From the two equations above one obtains the following three boundary conditions for the coated plate:

\[
\int (z-\alpha)^2 \frac{E(z)}{1-\nu^2(z)} \left[ \int \Delta^2 w dx dy \right] dz - \int P dx dy = 0
\]

\[
\Rightarrow \int \left[ \int (z-\alpha)^2 \frac{E(z)}{1-\nu^2(z)} \Delta^2 w \right] dz - P = 0,
\]

\[
\int (z-\alpha)^2 \frac{E(z)}{1-\nu^2(z)} \left[ -\frac{\partial \Delta w}{\partial n} + (1-\nu(z)) \frac{\partial}{\partial l} \left( \sin \theta \cos \theta \left( \frac{\partial^2 w}{\partial y^2} - \frac{\partial^2 w}{\partial x^2} \right) \right) \right] dz = 0,
\]

\[
\int (z-\alpha)^2 \frac{E(z)}{1-\nu^2(z)} \left[ \Delta w + (1-\nu(z)) \left( 2 \sin \theta \cos \theta \left( \frac{\partial^2 w}{\partial x^2} \right) \right) \right] dz = 0.
\]

Because here is not the place to discuss these conditions in detail, we refer to the literature (e.g. [1] pp. 50 – 57). The reader should realise that the only difference to the homogeneous case is caused by the integration with respect to \( z \).

### 4.3. Illustrative Example: Circular coated plate

The task we consider now is that of a circular coated plate loaded at the centre by a concentrated force and supported at the edge. Therefore we have to evaluate the following differential equation ([1], p. 55)

\[
\Delta^2 w = 0; \quad \Delta = \frac{1}{r} \frac{d}{dr} \left( r \frac{d}{dr} \right)
\]

The general non singular solution is

\[
w = ar^2 + b + cr^2 \ln \frac{r}{R},
\]

where \( R \) denotes the radius of the plate. The constants \( a, b \) and \( c \) as well as the position of the neutral plane can be determined from the following boundary conditions:

1. **At the centre of the coated plate at \( r=0 \) acts the force \( f \).**

Varying the Free Energy of the plate (c.f. equation (11)) yields:
where $D$ has to be calculated from:

$$D = \int_0^h (z - \alpha)^2 \frac{E(z)}{2[1 - \nu^2(z)]} dz,$$

in order to consider the coated constitution of the plate. This follows directly from equation (13).

2. The plate is supported at the edge

$$w(r=R) = 0,$$

while the first condition directly leads to $\partial w(r=R) = 0$ and thus equation (14) is already fulfilled one obtains the second one by a consequent transition to differentiations with respect to $n$ and $l$. In addition one has to realise that because of $w(r=R) = 0$ all differentiations of $w$ with respect to $l$ yield $0$.

3. The position of the neutral plane must lead to a minimum for the Free Energy

$$0 = \frac{\partial}{\partial \alpha} F = \frac{\partial}{\partial \alpha} \left[ \int_0^h (z - \alpha)^2 \frac{E(z)}{2[1 - \nu^2(z)]} \left( \Phi_1 + 2(1 - \nu(z))\Phi_2 \right) dz \right],$$

with equation (6) as solution for $\alpha$.

Substitution of the solution (17) of the biharmonic equation (16) in the boundary condition (18) yields:

$$2\pi \int_0^R r\Delta^2 wdr = 2\pi \int_0^R \left( \frac{1}{r} \frac{d}{dr} 4c \right) wdr = \frac{f}{D} \Rightarrow c = \frac{f}{8\pi D}.$$

The conditions (20) and (21) provide:

$$b = -aR^2,$$

$$a = -c \int_0^h (z - \alpha)^2 \frac{E(z)}{2[1 - \nu^2(z)]} [3+\nu(z)] dz.$$

Thus we can give now the complete solution of the task above for a coated plate consisting of substrate and $n-1$ coatings (arbitrary number of coatings and arbitrary thickness of each coating):

$$w = w(r) = \frac{f}{16\pi D} \left[ \xi (R^2 - r^2) + 2r^2 \ln \frac{r}{R} \right],$$

\[(22)\]
where:

\[
\xi = \sum_{i=1}^{n} \left( h_i^3 - h_{i-1}^3 - 3\alpha(h_i^2 - h_{i-1}^2) + 3\alpha^2(h_i - h_{i-1}) \right) \frac{E_i}{(1 - \nu_i^2)} \left[ 3 + \nu_i \right]
\]

\[
D = \sum_{i=1}^{n} \left( h_i^3 - h_{i-1}^3 - 3\alpha(h_i^2 - h_{i-1}^2) + 3\alpha^2(h_i - h_{i-1}) \right) \frac{E_i}{3(1 - \nu_i^2)}
\]

and \( \alpha \) must be determined using equation (6).

The results presented in this chapter were experimentally proved on metal coating – glass substrate systems ([2], [3]).

4.4 Arbitrary rectangular coated plate, supported at its corners and loaded homogeneously over its surface

We consider now a coated rectangular plate of arbitrary ratio of the length of both sides. Again we call \( w = w(x, y) \) the displacement in direction if \( z \) and lay the \( z \)-axis parallel to the normal of the non-deformed plate. The following boundary conditions must be satisfied:

\[
w(0,0) = w(0, b) = w(a, 0) = w(a, b) = 0,
\]

\[
\Delta w(0,0) = \Delta w(0, b) = \Delta w(a, 0) = \Delta w(a, b) = 0.
\]

As figure 6 shows are \( a \) and \( b \) the length of the two edges of the rectangle in direction of \( x \) and \( y \), respectively. We are able to find a solution choosing an approach consisting of Fourier series as follows:

\[
w = w(x, y) = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} c_{j,k} \left( \sin \frac{j\pi x}{a} + \sin \frac{k\pi y}{b} \right)
\]

(23)

In addition to the above mentioned boundary conditions the approach must satisfy the corresponding differential equation for a bent plate ([1], 53).

\[
N \Delta \Delta w(x, y) = p(x, y),
\]

(24)

with:

\( p(x, y) \) – pressure distribution on the plate surface

\( N \) – flexural rigidity of the plate

To calculate \( N \) we distinguish here two cases. The simple one is the homogeneous case, where we have to set:

\[
N_{\text{hom}} = \frac{E \cdot h^3}{12 \cdot (1 - \nu^2)},
\]

(25)

with:

\( h \).... thickness of the plate,
Young’s modulus, 

Poisson’s ratio.

In the non-homogeneous case one has to evaluate the following integral in order to obtain the flexural rigidity:

\[ N = \int_a^b \frac{\alpha^2}{2(1 - \nu^2(z))} \, dz, \tag{26} \]

with:

- \( h_{tot} \): total thickness of the compound,
- \( E(z) \): Young’s modulus as function of \( z \),
- \( \nu(z) \): Poisson’s ratio as function of \( z \),
- \( \alpha \): position of the neutral surface with \( z=0 \) \( \equiv \) substrate bottom.

Equation (24) yields

\[ N\Delta w = \sum_{j,k=1}^{\infty} c_{jk} \left[ \frac{j^4 \pi^4}{a^4} \cdot \sin \left( \frac{j \pi x}{a} \right) + \frac{k^4 \pi^4}{b^4} \cdot \sin \left( \frac{k \pi y}{b} \right) \right] \cdot N = p(x, y). \tag{27} \]

For the reason of simplification we set

\[ p_{x}(x, y) = p_{x}(x) + p_{y}(y) \]

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

\[ p_{x}(x) = \sum_{j=1}^{\infty} c_{j} \cdot N \cdot \frac{j^4 \pi^4}{a^4} \cdot \sin \left( \frac{j \pi x}{a} \right) \]

\[ p_{y}(y) = \sum_{k=1}^{\infty} c_{k} \cdot N \cdot \frac{k^4 \pi^4}{b^4} \cdot \sin \left( \frac{k \pi y}{b} \right) \]

and can now determine the coefficients \( c_{j} \) and \( c_{k} \):

\[ c_{j} = \frac{2}{a} \cdot \int_{0}^{a} \frac{1}{N} \cdot \left( \frac{a}{j \pi} \right)^{4} \cdot p_{x} \cdot \sin \left( \frac{j \pi x}{a} \right) \cdot dx, \tag{30} \]

\[ c_{k} = \frac{2}{b} \cdot \int_{0}^{b} \frac{1}{N} \cdot \left( \frac{b}{k \pi} \right)^{4} \cdot p_{y} \cdot \sin \left( \frac{k \pi y}{b} \right) \cdot dy. \tag{31} \]

Assuming a constant load in x- \( p_{x} \) and y-direction \( p_{y} \) one obtains the simple result

\[ c_{j} = \frac{2}{a} \cdot \int_{0}^{a} \frac{1}{N} \cdot \left( \frac{a}{j \pi} \right)^{4} \cdot p_{x} \left( \frac{a}{j \pi} - \frac{a}{j \pi} \cos(j \pi) \right) \begin{cases} \frac{4p_{x}}{aN} \left( \frac{a}{j \pi} \right)^{5} & \text{for } j=1,3,5,\ldots \\ 0 & \text{for } j=2,4,6,\ldots \end{cases} \tag{32} \]

\[ c_{k} = \frac{2}{b} \cdot \int_{0}^{b} \frac{1}{N} \cdot \left( \frac{b}{k \pi} \right)^{4} \cdot p_{y} \left( \frac{b}{k \pi} - \frac{b}{k \pi} \cos(k \pi) \right) \begin{cases} \frac{4p_{y}}{bN} \left( \frac{b}{k \pi} \right)^{5} & \text{for } k=1,3,5,\ldots \\ 0 & \text{for } k=2,4,6,\ldots \end{cases} \tag{33} \]

From the original approach (23) and the last two equations we obtain subsequently for the displacement \( w \):

\[ w = \frac{4}{N \pi^{5}} \sum_{j=1}^{\infty} a^{4} \sin \left( \frac{j \pi x}{a} \right) + \sum_{k=1}^{\infty} b^{4} \sin \left( \frac{j \pi y}{b} \right), \quad (j,k=1,3,5,\ldots). \tag{34} \]

with \( \alpha \) already given throughout the equation (5).

Now we are interested in the curvature at the centre of the plate. Therefore we define the new co-ordinate system \( x' \) and \( y' \) with the origin in the centre of the plate and find with the fundamental relations \( \sin \left( \frac{\pi}{2} + \alpha \right) = \cos \alpha \) and \( \sin \left( \frac{3\pi}{2} + \alpha \right) = -\cos \alpha \):
\[
\begin{align*}
\frac{w}{N\pi^2} &= \frac{4}{N\pi^2} \left[ p_x \sum_{j=1}^{\infty} \frac{a^4}{j^5} \sin \left( j\pi \left( x' + \frac{a}{2} \right) \right) + p_y \sum_{k=1}^{\infty} \frac{b^4}{k^5} \sin \left( j\pi \left( y' + \frac{b}{2} \right) \right) \right] \\
&= \frac{4}{N\pi^2} \left[ p_x \sum_{j=1}^{\infty} \frac{a^4}{j^5} (-1)^{j-1} \left( \frac{j\pi}{a} \right) + p_y \sum_{k=1}^{\infty} \frac{b^4}{k^5} (-1)^{k-1} \left( \frac{j\pi}{b} \right) \right] \quad (j, k=1, 3, 5, \ldots)
\end{align*}
\]

For small \(x'\) and \(y'\) one can develop the cos-functions into a Taylor series and obtains after neglecting of quantities which are small of higher order

\[
\begin{align*}
\left. \frac{w''(\vec{n})}{R(\vec{n})} \right|_{\text{centre}} &= -\frac{4}{N\pi^2} \left[ \sum_{j=1}^{\infty} (-1)^{j-1} \frac{a^4}{j^5} p_x \vec{n} \cdot \vec{e}_x + \sum_{k=1}^{\infty} (-1)^{k-1} \frac{b^4}{k^5} p_y \vec{n} \cdot \vec{e}_y \right] \quad (j, k=1, 3, 5, \ldots) \quad (36)
\end{align*}
\]

Here the vector \(\vec{n}\) \((|\vec{n}| = 1)\) gives the direction of the line where the curvature is calculated for.

The vectors \(\vec{e}_x\) and \(\vec{e}_y\) are unit vectors of the co-ordinate system \(x', y'\). Using equation (38) we may obtain the radius of curvature for the centre of the rectangular plate with

\[
\left. \frac{1}{R(\vec{n})} \right|_{\text{centre}} = \frac{4}{N\pi^2} \left[ \sum_{j=1}^{\infty} (-1)^{j-1} \frac{a^4}{j^5} p_x \vec{n} \cdot \vec{e}_x + \sum_{k=1}^{\infty} (-1)^{k-1} \frac{b^4}{k^5} p_y \vec{n} \cdot \vec{e}_y \right] \quad (j, k=1, 3, 5, \ldots) \quad (37)
\]

Thus, we may assume with an accuracy of about 10% a constant radius of curvature (does not depend significantly on \(x\) and \(y\)) in any direction \(\vec{n}\) within an area of \(|x'| \frac{\pi}{a} \leq 0.45\) and \(|y'| b \leq 0.45\) around the centre of the plate. We will see in the next section that a similar result occurs in the case of a bending resulting from intrinsic or thermal stresses within the film coated on a substrate. Thus, the curvature of bending of a compound caused by an external homogeneously distributed load shows a similar behaviour at the plate centre than the bending caused by film stresses.

### 5. Intrinsic and Thermal Stresses in Multilayer-Substrate-Compounds

The evaluation of the deformation and stresses of multilayer-substrate-compounds is very complicated because one has to note that all layers added to the compound (as long as they are under stress) do not only deform the substrate but all the other layers, too. In addition there are differences between intrinsic and thermal stresses because the first one occurs directly when the layer is deposited while for the second one a temperature difference between the moments of deposition and stress measurement is necessary. Thus, we will start here with the simple case of a single homogeneous coating on a homogeneous substrate.

#### 5.1. The Equation of Stoney

Let us consider a coated plate of arbitrary symmetry. The curvature \(R\) of this plate in the direction of \(x\) may be described by (see figure 7):

\[
\frac{1}{R} = \frac{d\varphi}{ds} = \frac{(\arctan(w'))'dx}{\sqrt{dx^2 + dw'^2}} = \frac{w''dx}{\left(1 + w'^2\right)^{3/2}} \equiv w''
\]

\(w\) means again the displacement in \(z\)-direction, in addition we have with \(s\) and \(\varphi\) the length and the angle of the arc, which follows the deformation curve of the plate.

Further we get from the plate approximation (chapter 1, see also [1], p. 48):

---

2 This equation was first published from G. G. Stoney [4] for narrow coated strips. The evaluation we follow here is based on assumptions which are valid for thin coated plates.
\[
\begin{align*}
\frac{\partial^2 w}{\partial x^2}; \quad u_{yy} = -z \frac{\partial^2 w}{\partial y^2}; \quad u_{zz} = \frac{z v}{1-v} \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right),
\end{align*}
\]

which yields with ([1], p. 17):
\[
\sigma_{jk} = \frac{E}{1+\nu} \left( u_{jk} + \frac{\nu}{1-2\nu} u_{0} \delta_{jk} \right),
\]

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

after few simplifications:
\[
\begin{align*}
\sigma_{xx} &= -\frac{Ez}{1-\nu^2} \left[ \frac{\partial^2 w}{\partial x^2} + \nu \frac{\partial^2 w}{\partial y^2} \right], \\
\sigma_{yy} &= -\frac{Ez}{1-\nu^2} \left[ \nu \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right].
\end{align*}
\]
5.1.1. Symmetry of Revolution

In those cases, where $\frac{\partial^2 w}{\partial x^2} = \frac{\partial^2 w}{\partial y^2}$ (e.g. constant radius of curvature over a sufficiently big area of the plate\(^3\)) one obtains finally:

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

where const stands for being constant along x and y, but not z of course. This directly yields $\sigma_{xy} = 0$ and $\sigma_{rr} = \text{const}$, because we have the general transformation rule:

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

---

\(^3\) As one obtains from the results of Suhir [6] this condition is approximately satisfied for a lot of coating substrate compounds bent by thermal and / or intrinsic stresses.
Now we assume a homogeneous stress distribution within the coating and demand, that the sum of forces and torques within the body yields zero in the case of equilibrium. With these two conditions both the curvature \( \frac{\partial^2 w}{\partial r^2} = \text{const} \) of the plate and the position of the neutral surface \( \alpha \) will be determined.

Force free:

\[
F = 0 = \int_0^{h_f} \sigma_{rr} \, dz = \int_0^{h} \frac{E(z)}{1-n(z)} \frac{\partial^2 w}{\partial r^2} (z-\alpha) \, dz + \int_{h_f}^{h} \sigma_{rr}^f \, dz ,
\]

(42)

torque free:

\[
M = 0 = \int_0^{h_f} \sigma_{rr} \, z \, dz = \int_0^{h} \frac{E(z)}{1-n(z)} \frac{\partial^2 w}{\partial r^2} (z-\alpha)^2 \, dz + \int_{h_f}^{h} \sigma_{rr}^f (z-\alpha) \, dz ,
\]

(43)

where we set here for the reason of simplicity \( \sigma_{rr}^f (z) \)=constant in the coating (Index \( f \) stands for the coating) and a \( z \)-proportional stress distribution in the substrate \( \sigma_{rr}^s (z) \)=constant*\( z \) which follows directly from the derivation above. Note, that we have to lay the origin such that we obtain \( \sigma_{rr}^s = 0 \) at the neutral surface (here in our notation we have to set \( z=0 \) at the substrate bottom).

With the following separation of the total force \( F \) into two parts namely one coming from the substrate and one from the coating

\[
F = F_f + F_s = 0
\]

(44)

one obtains from equation (42):

\[
F_f = \int_0^{h_f} \sigma_{rr}^f \, dz = \sigma_{rr}^f \cdot h_f = -F_s = -\int_0^{h} \frac{E_s \cdot \partial^2 w}{1-\nu_s} (z-\alpha) \, dz
\]

(45)

Thus, we can give now the exact solution for the equations (43) and (45):

\[
\alpha = \frac{h_s \left(3h_f + 2h_i\right)}{6(h_f + h_i)} ,
\]

(46)

\[
\frac{\partial^2 w}{\partial r^2} = \frac{1-\nu_s}{E_s} \sigma_{rr}^f \frac{6(h_f^2 + h_s^2)}{h_i^3} ,
\]

(47)

through which we straight forward derive a relation between the coating stress \( \sigma_{rr}^f \) and the curvature of the compound:

\[
\sigma_{rr}^f = -\frac{E_s}{1-\nu_s} \frac{1}{2h_f} \left[ (z-\alpha)^2 \right]_0^h \frac{\partial^2 w}{\partial r^2} = -\frac{E_s}{1-\nu_s} \frac{h_s^3}{h_f} \frac{1}{6(h_f + h_i)} \frac{\partial^2 w}{\partial r^2}
\]

\[
\cong -\frac{E_s}{1-\nu_s} \frac{h_s^3}{h_f} \frac{1}{6(h_f + h_i)} \frac{1}{R} ,
\]

(48)

In the case of very thin films one can neglect \( h_i \) against to \( h_s \) and obtains \( \alpha \cong 1/3 * h_s \) and further:

\[
\sigma_{rr}^f = -\frac{E_s}{1-\nu_s} \frac{\partial^2 w}{\partial x^2} \frac{1}{6h_f} \frac{h_s^2}{1-\nu_s} \frac{1}{6h_f} R.
\]

(49)

This last equation is well known as the so called Stoney equation [4], [5] and widely used in thin film techniques.
5.1.2. The rectangular substrate

The case of the rectangular substrate has been discussed elsewhere [9]. Thus, here we only give the main results.

Assuming a homogeneous deposition process, the biaxial film stress should be isotropic and homogeneous, i.e. \( \sigma_{xx} = \sigma_{yy} = \sigma_{rr} \) at any single point and \( \sigma_{rr} \) being constant everywhere on the surface. We then obtain again an approximately circular symmetric deformation and equation (48) gives the connection between film stress and curvature. The maximum effect of the non circular geometry of the substrate can be estimated by the following formula:

\[
\frac{\sigma_{b}^f}{\sigma_{rr}} = \frac{1 - \nu}{E} \left( 6h_j^2 + 9h_jh_s + 4h_s^2 \right) h_j^3,
\]  

with \( \sigma_{b}^f \) giving the film stress reduction due to the bending process. This yields low values for \( \sigma_{b}^f/\sigma_{rr} \) in all cases where the \( h_j/h_s \) ratios are small.

5.1.3. The coated bar

Reduction of one edge of the rectangular substrate until it reaches the size of its thickness leads us to the problem of the coated bar.

Let’s consider now a co-ordinate system with the z-axis parallel to the long side of the coated bar. The bar shall be bent perpendicular to this axis. Under the assumption, that all stress components within the bar are small compared to the component normal to z, \( \sigma_{zz} \), we find from (40) the following three simple equations

\[
\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0, \quad \frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x} = 0, \quad \frac{\partial u_z}{\partial x} + \frac{\partial u_z}{\partial y} = 0,
\]

where \( R \) denotes the radius of curvature of the bar. Integration yields:

\[
u = \frac{1}{2R} (z^2 + \nu((x - \alpha)^2 - y^2)), \quad u_y = -\nu \frac{(x - \alpha)y}{R}, \quad u_z = \frac{(x - \alpha)z}{R}.
\]

To find the position of the neutral surface \( \alpha \) one has to satisfy that the bar must be free of forces and torque. The corresponding equations may be found directly from the terms above. Under the assumption that the coatings normal is approximately parallel to the x-axis and the stress in the coating is homogenous over the whole thickness one can write:

\[
\int_0^h \sigma_{zz}(x - \alpha)dx = \int_0^{h} E_s u_z^f dx + \int_0^{h} \sigma_{zz}(x - \alpha)dx = \int_0^{h} E_s \frac{(x - \alpha)^2}{R} dx + \int_0^{h} \sigma_{zz}(x - \alpha)dx = 0,
\]

The origin of the x-axis was laid at the substrate bottom. The final result is an \( \alpha \) already given through equation (46) and the original Stoney equation [10] for the coated bar:

\[
\sigma_{zz}^f = -E_s \frac{h_j^3}{h_s} \left[ \frac{1}{6(h_j + h_s)} \right] \frac{1}{R} \approx -E_s \frac{h_j^3}{6h_j} \frac{1}{R}.
\]
where the last approximation is valid in the case of very thin films compared to the substrate thickness.

5.1.4. Non-isotropic substrates

To give the reader the possibility to follow our calculation we will present it in detail despite the fact, that this could be considered a long and boring development for those who are more familiar with tensor evaluations. We start with Hook's relation between stress \( \sigma_{ij} \) and strain tensor \( u_{ij} \)

\[
\sigma_{ij} = C_{ijkl} e_{kl},
\]

\[
u_{ij} = S_{ijkl} \sigma_{kl},
\]

where \( C_{ijkl} \) denotes the tensor of Young's moduli and \( S_{ijkl} \) the tensor of compliance. The stress and strain tensors may be transformed into a rotated co-ordinate system using the rotation matrix \( l_{ij} \) as

\[
\sigma'_{ij} = l_{ik} l_{jl} \sigma_{kl},
\]

\[
u'_{ij} = l_{ik} l_{jl} \epsilon_{kl}. \tag{52}
\]

Here we present the rotation matrices \( l_{x_{ij}}, l_{y_{ij}}, l_{z_{ij}} \) as functions of the angle of rotation \( \phi \) for all three axes \( x, y \) and \( z \), respectively:

\[
l_{x_{ij}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \phi & \sin \phi \\ 0 & -\sin \phi & \cos \phi \end{pmatrix}, \quad l_{y_{ij}} = \begin{pmatrix} \cos \phi & 0 & \sin \phi \\ 0 & 1 & 0 \\ -\sin \phi & 0 & \cos \phi \end{pmatrix}, \quad l_{z_{ij}} = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\]

We put the \( z \)-axis parallel to the normal of the plate and use the thin plate approximation ([1], 49) with

\[
\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{yx} & \sigma_{yy} & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\]

Usually the tensor of compliance or modulus is given as a 6x6 matrix and one has to recapitulate that the indexes 1,2,3,4,5,6 stand for \( xx, yy, zz, yz, zx, xy \), respectively. Thus, one could find the tensor of strain as follows:

\[
\begin{pmatrix} u_{xx} \\ u_{yy} \\ u_{zz} \\ u_{yz} \\ u_{zx} \\ u_{xy} \end{pmatrix} = S_{ij} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{pmatrix}, \quad (i, j = 1...6)
\]

But to get additional information about the single strain components one needs the contrary relation. Because of their importance as substrates (for instance silicon) we will concentrate here on cubic systems which leads to the following relation

\[
\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{pmatrix} = C_{ijkl} \begin{pmatrix} u_{xx} \\ u_{yy} \\ u_{zz} \\ u_{yz} \\ u_{zx} \\ u_{xy} \end{pmatrix},
\]

where the last approximation is valid in the case of very thin films compared to the substrate thickness.
The resulting equations are:

\[ u_{zz} = - \frac{C_{12}}{C_{11}} (u_{xx} + u_{yy}), \quad \frac{\partial u_x}{\partial z} = - \frac{\partial u_z}{\partial x}, \quad \frac{\partial u_y}{\partial z} = - \frac{\partial u_z}{\partial y}, \]

where we have used the relation between strain and displacement \( u_{ik} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right) \). Now we set according to the isotropic case \( u_z = w(x,y) \). Integration yields

\[ u_x = -z \frac{\partial w}{\partial x}, \quad u_y = -z \frac{\partial w}{\partial y}, \]

and we obtain for the strain components:

\[ u_{xx} = -z \frac{\partial^2 w}{\partial x^2}, \quad u_{yy} = -z \frac{\partial^2 w}{\partial y^2}, \quad u_{xy} = -z \frac{\partial^2 w}{\partial x \partial y}, \quad u_{zz} = u_{yz} = 0. \]

Similar to the evaluation for the plate of symmetry of revolution we are now able to find a relation between the stress in a homogeneous thin film which is fixed on the substrate and the curvature of this compound. We assume, that the substrate shall have symmetry of revolution. We measure the curvature along the x axis as this is one of the main axes of the cubic substrate. The evaluation starts with the equation \( \sigma_{xx} = C_{11} u_{xx} + C_{12} (u_{yy} + u_{zz}) \) and the assumption of force and torque freedom of the whole compound. The final result is an \( \alpha \) already given through equation (46) and the Stoney equation for the cubic substrate with symmetry of revolution:

\[ \sigma_{xx}^f = \left( \frac{2C_{12}}{C_{11}} - C_{11} - C_{12} \right) \left( \frac{1}{6h_f + h_s} \right) \left( \frac{1}{R_x} \right) \approx \left( \frac{2C_{12}^2}{C_{11} - C_{12}} \right) \left( \frac{h_s^3}{6h_f^2 R_s} \right). \quad (53) \]

Unfortunately this result is valid only in those cases, where the main crystal axes of the cubic substrate are falling together with the x, y and z axes of our co-ordinate system. In many other cases where the substrates normal for instance is not (100) oriented one has to rotate the tensors of modulus and compliance according to

\[ C'_{ijkl} = l_{im} l_{jn} l_{ko} l_{lp} C_{mnop}, \]

\[ S'_{ijkl} = l_{im} l_{jn} l_{ko} l_{lp} S_{mnop}, \]

and thus obtains much more complex formulae.

This calculation may be performed easily by a program package which contains in addition all main formulae of this paper and which is published in the internet [7].

An other way to avoid the above mentioned cumbersome calculation could be to apply bar-shaped substrates for film stress measurement and to evaluate them using equation (51). To evaluate the effective Young's modulus \( E_s \) for any crystal orientation of the bar one has to use the following equations:

Cubic substrates:

\[ E_s = \frac{C_{11} + C_{12}}{(C_{11} + 2C_{12})(C_{11} - C_{12})} + \left( 1 + \frac{2}{C_{44}} \right) \left( n_2^2 n_2^2 + n_2^2 n_2^2 + n_2^2 n_2^2 \right)^{-1}, \]

Hexagonal substrates:
\[
E_s = \frac{2C_{44}C_{66}\left((C_{11} + C_{12})C_{33} - 2C_{13}^2\right)}{
C_{44}C_{33}C_{11}(n_x^2 + n_y^2)^2 - 4C_{66}C_{13}C_{44}(n_x^2 + n_y^2)n_z^2 + C_{13}\left(C_{44}(n_x^2 + n_y^2)^2 + 4C_{66}(n_x^2 + n_y^2)n_z^2\right) + (C_{11} - C_{12})n_z^2\left(C_{33}(n_x^2 + n_y^2) + C_{44}n_z^2\right)}.
\]

Substrates of general anisotropy:
\[
E_s = (S_{ijkl}n_i n_j n_k n_l)^{-1},
\]
where \(n_i (i=x,y,z)\) are the components of the unified vector of the crystal orientation and \(C_{66}\) is defined as \(C_{66} = 1/2(C_{11} - C_{12})\). We will explain these formulae with the help of an example. Let us consider a bar of silicon which is (111)-oriented along the z-axis according to the coordinate system we have used in section above. With the corresponding elastic parameters \(C_{11} = 166\) GPa, \(C_{12} = 64\) GPa, \(C_{44} = 79.6\) GPa for silicon [10] and \(n_x = n_y = n_z = \frac{1}{\sqrt{3}}\) one obtains \(E_s = 187.9\) GPa as the effective substrate modulus to be used in eq. (1.51).

### 5.2. Multilayer Systems 1: Each Additional Layer Deforms the Multilayer-Compound

At first we will consider a system, where each layer deforms the whole compound as soon as it has been deposited. As an example one could assume a system which contains no thermal stress but intrinsic stress. The film substrate system is fixed on the substrate holder in such a manner that it can follow the stress (i.e. it can be deformed) during the growth process.

The system shall consist of a substrate and \(n\) layers, where the first layer \(n = 1\) lays directly on the substrate. Now we imagine to add an additional layer \(n+1\) and try to evaluate its influence on the total compound deformation. The stress in that layer no. \(n+1\) be . Its effect can be described independently of any predeformations in those cases, where

1. all deformations are totally linear elastic and
2. the predeformation is small enough to allow to consider the whole system as a flat plate instead of a shell.

Thus, regarding the substrate together with the primary layers \(i = 1\) to \(i = n\) as a whole which interacts with the additional one, we can formulate the equations of equilibrium as follows:

**Force free:**
\[
F_{n+1} = 0 = \int_{0}^{h_{n+1}} \sigma_{xx}(z)dz = -\int_{0}^{h_{n+1}} E_s \frac{\partial^2 w}{\partial x^2} (z - \alpha_{n+1})dz - \sum_{i=1}^{n} \int_{h_{i-1}}^{h_{i}} E_i \frac{\partial^2 w}{\partial x^2} (z - \alpha_{n+1})dz + \int_{h_{n}}^{h_{n+1}} \sigma_{xx}^{n+1}(z)dz,
\]

**Torque free:**
\[
M_{n+1} = 0 = \int_{0}^{h_{n+1}} \sigma_{xx}(z)dz = -\int_{0}^{h_{n+1}} E_s \frac{\partial^2 w}{\partial x^2} (z - \alpha_{n+1})^2 dz - \sum_{i=1}^{n} \int_{h_{i-1}}^{h_{i}} E_i \frac{\partial^2 w}{\partial x^2} (z - \alpha_{n+1})^2 dz + \int_{h_{n}}^{h_{n+1}} \sigma_{xx}^{n+1}(z)(z - \alpha_{n+1})dz,
\]

where the \(i\)'th layer ranges from \(h_{i-1}\) to \(h_i\) (\(h_0\) denotes the substrate top surface, \(h_n = h_0; z = 0\) stands for the substrate bottom) and has the elastic parameters \(E_i\) and \(\nu_i\) for Young's modulus and Poisson's ratio, respectively.
Now it would be interesting to know how the stress in the layer i will have changed from its primary value \( \sigma_{xx}^i \) it has had immediately after deposition to the final stress distribution \( \sigma_{xx}^i(z) \) one obtains after deposition of the other layers \( i+1 \) to \( n+1 \):

\[
\sigma_{xx}^j(z)_{i+1} = \sigma_{xx}^j - \frac{E_i}{1-\nu_i} \sum_{j=i+1}^{n+1} \left( \frac{\partial^2 W}{\partial z^2} \right)_j (z - \alpha_j).
\]  

(56)

Thereby the term \( \left( \frac{\partial^2 W}{\partial z^2} \right)_j (z - \alpha_j) \) in principle describes a product of the curvature \( \frac{\partial^2 W}{\partial z^2} \), which belongs to the displacement \( w_j \) caused by the stress \( \sigma_{xx}^j \) in the layer \( j \) and the corresponding "lever" \( z - \alpha_j \).

Instead of a specific layer-stress \( \sigma_{xx}^j \) one is often more interested in the resulting average stress \( \overline{\sigma} \) one would get for the whole layer system after finishing the deposition process:

\[
\overline{\sigma} = \frac{\sum_{j=1}^{n+1} h_j \int_{z_{i+1}}^{z_{n+1}} \sigma_{xx}^j(z) \, dz}{\sum_{j=1}^{n+1} (h_j - h_{i-1})} - \frac{1}{2(1-\nu_i)} \sum_{j=1}^{n+1} \left( \frac{\partial^2 W}{\partial z^2} \right)_j (h_i^2 - h_{i-1}^2 - 2\alpha_j (h_j - h_{i-1}))}.
\]  

(57)

For very thin films \( (h_i << h_s) \), the equation above may be simplified significantly by taking into account that:

\[
\sigma_{xx}^j >> \frac{E_i}{1-\nu_i} \sum_{j=i+1}^{n+1} \left( \frac{\partial^2 W}{\partial z^2} \right)_j (z - \alpha_j).
\]  

(58)

Then, one obtains from equation (0) a quite simple term for the average coating stress:

\[
\overline{\sigma} = \frac{\sum_{j=1}^{n} \sigma_{xx}^j (h_j - h_{i-1})}{\sum_{j=1}^{n} (h_j - h_{i-1})}.
\]  

(59)

Now we are able to represent the equations (0) and (0) for the more realistic case, that each of the \( n+1 \) layers deforms the compound according to their intrinsic stresses. This means that each layer \( i \) influences the deformation of the substrate and all layers 1 to \( i-1 \) below itself by the stress \( \sigma_{xx}^i \) and is in addition deformed by the layers \( i+1 \) to \( n+1 \) deposited above itself.

Force free:

\[
0 = F_f + F_s = \int_{0}^{h_i} - \frac{E_s}{1-\nu_s} \sum_{j=1}^{n+1} \left( \frac{\partial^2 W}{\partial z^2} \right)_j (z - \alpha_j) \, dz + \sum_{i=1}^{n+1} \frac{h_i}{h_{i-1}} \int_{z_{i+1}}^{z_{n+1}} \sigma_{xx}^i(z) \, dz
\]
\[
\frac{\sigma_{xx}}{E_s} \sum_{i=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz + \frac{h_i - E_s}{1 - \nu_s} \sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz \\
= \frac{h_i - E_s}{1 - \nu_s} \sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz \\
= \frac{h_i - E_s}{1 - \nu_s} \sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz
\]

\[
\sigma_{xx}^\beta (h_i - h_{i-1}) = \frac{h_i - E_s}{1 - \nu_s} \sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz - \sum_{j=1}^{n_{xx}} \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz
\]

where the term (3rd line)

\[
\sigma_{xx}^\beta (h_i - h_{i-1}) = \frac{h_i - E_s}{1 - \nu_s} \sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz - \sum_{j=1}^{n_{xx}} \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz
\]

emphasise the above mentioned fact that the stress \( \sigma_{xx}^\beta \) of the \( i \)th layer does not only bend the substrate but all the layers below \( \left( - \sum_{j=1}^{n_{xx}} \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right) \) and it is changed itself by all the layers above \( \left( - \sum_{j=1}^{n_{xx}} \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right) \). In the same manner the condition for the freedom of torque yields:

\[
0 = M_f + M_s = \frac{h_i - E_s}{1 - \nu_s} \sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz + \sum_{i=1}^{n_{xx}} \int_{h_{i-1}}^{h_i} (z - \alpha_i) \sigma_{xx}^\beta (z) \right)_i dz
\]

\[
= \frac{h_i - E_s}{1 - \nu_s} \sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz + \sum_{i=1}^{n_{xx}} \int_{h_{i-1}}^{h_i} (z - \alpha_i) \sigma_{xx}^\beta (z) \right)_i dz
\]

\[
= \frac{h_i - E_s}{1 - \nu_s} \sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz + \sum_{i=1}^{n_{xx}} \int_{h_{i-1}}^{h_i} (z - \alpha_i) \sigma_{xx}^\beta (z) \right)_i dz
\]

\[
\sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz
\]

\[
= \frac{h_i - E_s}{1 - \nu_s} \sum_{j=1}^{n_{xx}} \left[ \int_{h_{i-1}}^{h_i} \left( \frac{\partial^2 w}{\partial \alpha^2} \right)_j (z - \alpha_j) \right] dz + \sum_{i=1}^{n_{xx}} \int_{h_{i-1}}^{h_i} (z - \alpha_i) \sigma_{xx}^\beta (z) \right)_i dz
\]
\[ \sum_{j=1}^{n+1} \left[ \frac{1}{31-v_j} \sum_{i=1}^{n+1} \left\{ \frac{\partial^2 w}{\partial x^2} \right\}_j (h^3_i - 3\alpha_i h^2_i + 3\alpha_i^2 h_i) \right] + \sigma_{xx} \frac{h_i^2 - h_{i-1}^2 - 2\alpha_i(h_i - h_{i-1})}{2} \]

\[ \sum_{i=1}^{n+1} \left[ -\frac{1}{31-v_i} \sum_{j=i+1}^{n+1} \left\{ \frac{\partial^2 w}{\partial x^2} \right\}_j (h^3_i - h^3_{i-1} - 3\alpha_i (h^2_i - h^2_{i-1}) + 3\alpha_i^2 (h_i - h_{i-1})) \right] - \frac{1}{3} \sum_{j=1}^{n+1} \left\{ \frac{E_j}{1-v_j} \frac{\partial^2 w}{\partial x^2} \right\}_j (h^3_j - h^3_{j-1} - 3\alpha_j (h^2_j - h^2_{j-1}) + 3\alpha_j^2 (h_j - h_{j-1})) \]

From these conditions one may evaluate successively all necessary parameters of the whole compound.

5.3. Multilayer Systems 2: The Deformation of the Multilayer-Compound starts after deposition and cooling down (fixed substrate case)

The case we will now consider is that one of a substrate-multilayer system where absolutely no deformation occurs during the deposition process. The compound deforms completely after depositing all single layers. As an illustrative example one could assume a system with only thermal but without any intrinsic stresses. Now all the layers influence each other and we obtain the new conditions of equilibrium by rewriting the last two equations in the following form:

**Force free:**

\[ 0 = F_j + F_s = \int_0^{h_j} - \frac{E_s}{1-v_s} \sum_{i=1}^{n+1} \left\{ \frac{\partial^2 w}{\partial x^2} \right\}_j (z - \alpha) \, dz + \sum_{i=1}^{n+1} \left[ \sigma_{xx} \frac{h_i}{h_{i-1}} \right] \, dz \]

\[ = \int_0^{h_j} - \frac{E_s}{1-v_s} \sum_{i=1}^{n+1} \left\{ \frac{\partial^2 w}{\partial x^2} \right\}_j (z - \alpha) \, dz + \sum_{i=1}^{n+1} \left[ \sigma_{xx} \frac{h_i}{h_{i-1}} \right] \, dz \]

\[ = -\frac{1}{2} \frac{E_s}{1-v_s} \sum_{i=1}^{n+1} \left\{ \frac{\partial^2 w}{\partial x^2} \right\}_j (h_i^2 - 2\alpha h_i) \]

\[ - \sum_{i=1}^{n+1} \left[ \sigma_{xx} \frac{h_i}{h_{i-1}} - \frac{1}{2} \frac{E_i}{1-v_i} \sum_{j=1}^{n+1} \left\{ \frac{\partial^2 w}{\partial x^2} \right\}_j (h_j^2 - h_{j-1}^2 - 2\alpha(h_j - h_{j-1})) \right] \]

Now we have a case, where the stress \( \sigma_{xx} \) of the \( i \)th layer does not only bend the substrate but all other layers (below and above) and itself \( -\sum_{j=1}^{n+1} \int_{h_{j-1}}^{h_j} \frac{E_j}{1-v_j} \left\{ \frac{\partial^2 w}{\partial x^2} \right\}_j (z - \alpha) \, dz \) and it is in addition changed by the stress in all the other layers \( -\int_{h_{j-1}}^{h_j} \frac{E_j}{1-v_j} \sum_{j=1, j \neq i}^{n+1} \left\{ \frac{\partial^2 w}{\partial x^2} \right\}_j (z - \alpha) \, dz \),

which results in the double summation given above.

**Torque free:**
5.4. Multilayer Systems 3: Arbitrary Combination of Intrinsic and Thermal Stresses – Illustrative Example

In the most practical cases both intrinsic and thermal stresses will occur in each layer of a multilayer-substrate compound. Thus we must combine the results of 5.2. and 5.3. to obtain the correct and complete conditions of equilibrium for the compound.

As an simple example we will consider here a two-layer-substrate system with the following parameters:

<table>
<thead>
<tr>
<th>Layer</th>
<th>Young’s modulus</th>
<th>Poisson’s ratio</th>
<th>thermal stress</th>
<th>Intrinsic stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substrate</td>
<td>$E_s$</td>
<td>$\nu_s$</td>
<td>$\tau_s = 0$</td>
<td>$\sigma_s = 0$</td>
</tr>
<tr>
<td>1st Coating</td>
<td>$E_1$</td>
<td>$\nu_1$</td>
<td>$\tau_1 = 0$</td>
<td>$\sigma_1$</td>
</tr>
<tr>
<td>2nd Coating</td>
<td>$E_2$</td>
<td>$\nu_2$</td>
<td>$\tau_2$</td>
<td>$\sigma_2 = 0$</td>
</tr>
</tbody>
</table>

The concrete conditions of equilibrium may be obtained now from the equations of the two sections above. One gets:

**Force free:**

$$0 = \frac{1}{2} \frac{E_s}{1-\nu_s} \left[ \frac{\partial^2 w_{th}}{\partial x^2} \right]_1 \left( h_2^2 - 2\alpha_{th} h_s \right) + \tau_2 \left( h_2 - h_1 \right)$$

$$- \frac{1}{2} \frac{E_1}{1-\nu_1} \left[ \frac{h_1^2 - h_2^2 - 2\alpha_{th} (h_1 - h_s)}{1-\nu_2} \right] \frac{\partial^2 w_{th}}{\partial x^2} + \frac{E_2}{1-\nu_2} \left( h_2^2 - h_1^2 - 2\alpha_{th} (h_2 - h_1) \right) \left[ \frac{\partial^2 w_{th}}{\partial x^2} \right]_2,$$

$$0 = - \frac{1}{2} \frac{E_s}{1-\nu_s} \left[ \frac{\partial^2 w_{th}}{\partial x^2} \right]_1 \left( h_s^2 - 2\alpha_{th} h_s \right) + \sigma_1 \left( h_1 - h_s \right),$$

where the index "th" stands for thermal and "int" for intrinsic.

**Torque free:**
\[
0 = -\frac{E_s}{3(1-\nu)} \left( \frac{\partial^2 w_{th}}{\partial x^2} \right)_2 \left( h_i^3 - 3\alpha_{th} h_i^2 + 3\alpha_{th}^2 h_i \right) + \tau_2 \left( h_i^2 - h_i^2 - 2\alpha_{th}(h_i^2 - h_i) \right)
\]
\[
-\frac{1}{3} \left( \frac{E_i}{1-\nu_i} \right) \left( h_i^3 - h_i^3 - 3\alpha_{int} (h_i^2 - h_i^2) + 3\alpha_{int}^2 (h_i - h_i) \right)
\]
\[
0 = -\frac{E_s}{3(1-\nu)} \left( \frac{\partial^2 w_{int}}{\partial x^2} \right)_2 \left( h_i^3 - 3\alpha_{int} h_i^2 + 3\alpha_{int}^2 h_i \right) + \sigma_1 \left( h_i^2 - h_i^2 - 2\alpha_{int}(h_i^2 - h_i) \right).
\]

In this special example one would be able to evaluate e.g. the positions of the neutral surfaces \(\alpha_{th}\) and \(\alpha_{int}\) and the curvatures \(\frac{\partial^2 w_{th}}{\partial x^2}\) and \(\frac{\partial^2 w_{int}}{\partial x^2}\) for thermal and intrinsic stress cases, respectively if the material constants and the values of the stresses \(\sigma_1\) and \(\tau_2\) are known.

6. Experimental example

In an experimental application [2] some of the results given above (eq. (22)) were used to determine the elastic modulus \(E\) of two different thin films on glass substrates. The experimental part of the work was performed by A. K. Jänting and J. M. Bell of Queensland University of Technology, Brisbane, Australia and M. V. Swain of CSIRO, Lindfield, Australia. The precise measurement of the force and deflection during the biaxial loading of the discs were achieved using a UMIS 2000, a commercially available micromechanical probe [11]. The force was applied and recorded stepwise and the deflection of the disc was measured for each step of the applied force. The loading cycle was divided into 20 steps which enabled a close monitoring of the bending response of the tested discs. The test set-up is schematically described in Figure 8. The force was applied using a blunt indenter (a ruby ball, diameter=500µm) on a brass shaft. The support of the disc from below was realised using 4.04 mm diameter steel ball bearings. The loads used were 5, 10 and 15 mN, giving deflections up to approximately 2300 nm for the thinnest discs. To ensure statistical reliability, each disc was tested three times, with a rotation of 120° between measurements. The differences in deflection between the positions were small (<0.1% for the uncoated discs and about 0.6% for the coated ones). Each load cycle was repeated five times and the values were then averaged for the analysis. The substrates used were glass cover slips, 15 mm in diameter with a thickness of 151-155 µm. Two different metal films, copper and aluminium, were deposited on the glass discs using magnetron sputtering. These metals were chosen to provide values of significantly different elastic modulus (bulk values: 71GPa and 130GPa [12] for aluminium and copper, respectively).
The film thicknesses were up to 1 µm for the copper and up to 2 µm for the aluminium films. For the theoretical analysis, the following Poisson's ratios were assumed:

- substrate [13]: $\nu_s = 0.21$
- copper film [12]: $\nu_{Cu} = 0.343$
- aluminium film [12]: $\nu_{Al} = 0.345$

The average values of the elastic modulus for the magnetron sputtered copper and aluminium films determined in this way were $116\pm8$GPa and $84\pm5$GPa, resp.. These values are relatively close to the bulk values. A more detailed presentation and discussion of the experimental results is to be found in [2].

**Conclusions**

On the basis of the calculus of the Free Energy the author has evaluated formulae for the equilibrium conditions of thin coated plates. Here the three cases thermal stress, intrinsic stress and external forces were considered. Some of the results published in this paper are of common knowledge, in particular Stoney’s equation is widely used [5, 17]. Others have been proved experimentally [2]. It was demonstrated in the paper that the deformation of a coating substrate compound must be separated in two different parts, namely:

1. the deformation which occurs during the deposition where every sub-layer is bent only by those layers being coated above him and
2. the deformation occurring completely after the deposition where every sub-layer bends the whole compound.

The main simplification in this evaluation is the assumption of a homogeneous stress distribution within a certain layer or coating. But as one considers a single layer or coating as a sum of sub-layers of equal mechanical parameters like Young's modulus and Poisson's ratio one can reduce the uncertainty of this approximation by increasing the amount of sub-layers involved in the calculation. For instance in-situ measurement of the curvature of the compound during the deposition process will thus provide as more accurate information about the stress distribution as more sub-layers will be taken into consideration in the evaluation. In the same manner one would be able to get information about the distribution of the mechanical parameters within the film along its normal direction by either making an assumption about the stress distribution or having such additional information from other measurements (e.g. infrared spectroscopy [15, 16]).

The problem which appears then is the cumbersome treatment of the rather voluminous formulae. To overcome these difficulties a software package was written and published in the internet [7] which takes over the formal and cumbersome evaluation for cases with bigger amounts of sub-layers.

In addition the case of a coated plate bent due to an external force was investigated and evaluated completely for a special example namely the problem of a circular coated plate loaded at the centre by a concentrated force and supported at the edge. It has been shown experimentally that such investigations may be used for the determination of mechanical parameters of coatings [2], [14], [17].
Acknowledgement

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References

[10] Landolt-Börnstein, Neue Serie, Vol. III/1, pp. 1 – 16

Appendix

Mathematica package for the evaluation of the displacement of a circular plate fixed at the edge and loaded at the centre by a concentrated load

The first instruction loads a package for the solution of the equation $J_n(\lambda_n)=0$, with $J_n$ denoting the Bessel function of order $n$.

```mathematica
<< NumericalMath`BesselZeros`
```

Now we define a depth parameter $n$ of the calculation and evaluate the roots of the Bessel function of order zero.
\[ n = 20; \]
\[ \lambda_s = \text{BesselJZeros} [0, n]; \]

We give values for the Poisson's ratio \( v \), the Young's modulus \( E_{\text{mod}} \) and the total load \( Q \)
\[ v = 0.3; \]
\[ E_{\text{mod}} = 0.169; \]
\[ Q = 1; \]

and define all constants and functions used in the calculation.
\[ m = \frac{1}{v}; G = E_{\text{mod}} \frac{m}{2} / (m + 1); Nn[h_] := \frac{4}{3} G h^3 \frac{m}{(m - 1)}; \]
\[ \text{sh}[x_] := \text{Sinh}[x]; \text{ch}[x_] := \text{Cosh}[x]; \]
\[ \text{J1}[x_] := \text{BesselJ}[1, x]; \text{J0}[x_] := \text{BesselJ}[0, x]; \]
\[ \Delta_1[x_] := 2 x - \text{sh}(2 x); \]

Finally the two solutions of the displacement of the middle surface of the plate for the thick and the thin plate are given as functions of the radius \( r \) (measured from the plate's centre), the plate's diameter \( r_0 \) and its thickness \( h \).

\[ w_{0\text{thickplate}}[r_, r0_, h_] := \]
\[ \frac{Q}{2 \pi G r_0} \sum_{s=1}^{n} \left( \left( \frac{2 (m - 1)}{m} \text{ch} \left[ \frac{\lambda_s [[s]] h}{r_0} \right] + \frac{\lambda_s [[s]] h}{r_0} \text{sh} \left[ \frac{\lambda_s [[s]] h}{r_0} \right] \right) \right) \]
\[ \left( \frac{1}{2} \frac{1}{2} \frac{r^2}{r_0^2} - \frac{\text{J0} \left[ \lambda_s [[s]] \frac{r}{r_0} \right]}{\text{J1} \left[ \lambda_s [[s]] \right]} \right) \frac{1}{\text{J1} \left[ \lambda_s [[s]] \right]} \frac{1}{\Delta_1 \left[ \lambda_s [[s]] \frac{h}{r_0} \right]}; \]

\[ w_{0\text{thinplate}}[r_, r0_, h_] := -\frac{Q r_0^2}{8 \pi Nn[h]} \left( \frac{r^2}{r_0^2} \text{Log} \left[ \frac{r}{r_0} \right] + \frac{1}{2} \left( 1 - \frac{r^2}{r_0^2} \right) \right) \]