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ANALYSIS OF THE LEFM CONCEPT FOR INTERFACIAL CRACKS APPLICATION TO COATING BUCKLING DELAMINATION IN TERMS OF SUBSTRATE ELASTIC CHARACTERISTICS

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In this paper the buckling delamination of a coating on a flat substrate in form of a straight-sided blister with special attention paid to the influence of elastic characteristics of the substrate is considered. Conditions for the buckling initiation are analyzed as well as the energy release rate and mode mixity of the interface crack as functions of the difference in elastic characteristics of the coating and the substrate. The problem is discussed from the aspect of application of the linear elastic fracture mechanics (LEFM) concept for the interfacial crack. The real angle function ω of the Dundurs parameters α and β and the ratio of thicknesses of the two layers are used for determination of the energy release rate and the load phase angle. Both the energy release rate along the sides of the blister and the average energy release rate at the front of the blister were calculated. The results thus obtained justify the application of the LEFM concept for interfacial cracks to the considered problem.

Key words: coating, buckling delamination, LEFM concept, interfacial cracks

1. Introduction

When thin films and coatings are exposed to significant residual compressive stresses, they delaminate by buckling. This is particularly valid for ceramic coatings on a metal substrate like wear resistant coatings on cutting tools and thermo-insulating coatings. The residual stresses appear due to the fact that the coatings are deposited at temperatures which are significantly higher than the operating ones. Those stresses appear during temperature changes as a consequence of the difference in the thermal expansion coefficients of the coating and substrate materials. The same phenomenon is noted in metal films on polymer substrates which are visco-elastic materials, and the present analysis does not extend to those cases. Examples where this type of buckling appears are the oxide layer in a thermal barrier coating such as Al_2O_3 on Ni-Cr-Al and Fe-Cr-Al alloys, hard transparent coatings on optical polymers and metal fibers on polymer substrates in electronics packages. These surface layers are prone to buckling delamination if the interface has lower toughness. High residual compressive stresses can cause various forms of buckling of coatings like: straight-sided blister, circular or elliptical blister and the so-called "telephone cord" blister. In the present paper, the coating delamination in form of a straight-sided blister, shown in Fig. 1, depending on the elastic characteristics of the substrate is analyzed.

For determination of the stress intensity factor, energy release rate and load phase angle, the real angle function ω is used, which is the function of the two Dundurs parameters α and β and

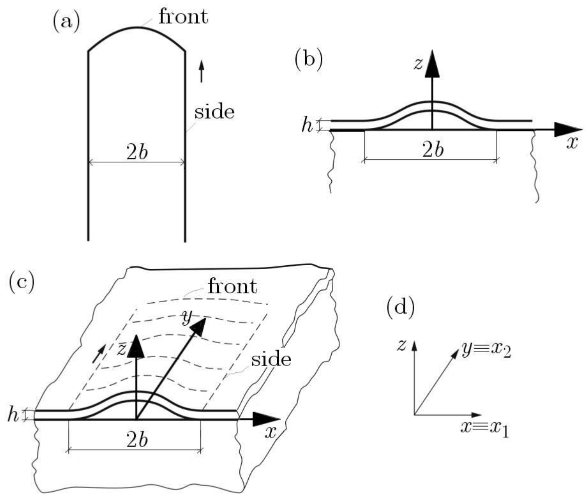

Fig. 1. The straight-sided blister appearance and parameters; (a) top view, (b) front view, (c) 3D appearance, (d) reference frame notation for derivations in Appendix

the layers thickness ratio h/H, as defined by Suo and Hutchinson (1990), which is different from the analysis presented by Yu and Hutchinson (2002), where the integral equations method was used for definition of coefficients a_{ij} and c_{ij} and other variables mentioned above. Also, instead of the method of integral equations, used by Suo and Hutchinson (1990), for determination of the ω function, an approximation of the tabular results, presented there, is done by application of symbolic programming, and an analytical expression is obtained for ω in terms of α, β and h/H.

2. Formulation of the problem

The considered problem of the straight-sided blister delamination is shown in Fig. 2. The coating is separated from the substrate in the area $-b \leqslant x \leqslant b$. Between the coating and the substrate, there exists an interfacial crack at a distance b from the coordinate system origin, in the plane strain conditions. Here $2b$ and δ are width and height of the blister, respectively, while h is the coating thickness.

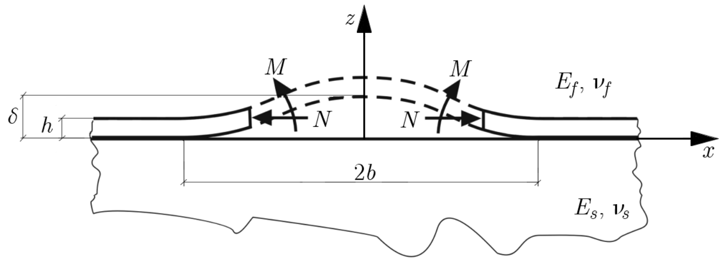

Fig. 2. Geometry and tractions for a straight-sided blister

Considering the behavior of an indium-tin oxide coating on the substrate of polymers, where there is a large difference in the elastic characteristics of the coating and the substrate, Cotterell and Chan (2000) showed that the elastic characteristics of the substrate have influence on the stress value, which leads to appearance of a blister and affects the energy release rate at the interface when the modulus of the substrate is significantly lower than that of the coating. Yu and Hutchinson (2002) extended those results to arbitrary combinations of materials and sizes of the blister. In this paper, the results shown by Cotterell and Chan (2000) and Yu and Hutchinson (2002) using the concept of Linear Elastic Fracture Mechanics (LEFM) for the crack on the interface are analyzed. All the numerical simulations were done by application of symbolic programming package Mathematica®.

The assumption is made that the coating material is elastic and isotropic with Young's modulus E_f and Poisson's ratio ν_f. It is also assumed that the substrate is elastic with Young's modulus E_s and Poisson's ratio ν_s, and has an infinite thickness.

The coating is exposed to uniform, equi-biaxial compressive stress. The resulting force and moment per unit length, N and M, respectively, which act at the edge of the coating, are in directions as shown in Fig. 2. Using the LEFM concept for the interface between the two layers presented in Veljkovic and Nikolic (2003) and Nikolic and Djokovic (2011), for the case of infinite substrate thickness, one defines the stress intensity factor, the energy release rate and the mode mixity as

$$\begin{aligned} K &= K_1 + \mathrm{i}K_2 = h^{-\mathrm{i}\varepsilon}\Big(\frac{F}{\sqrt{12h}} - \mathrm{i}\frac{M}{\sqrt{h^3}}\Big)\mathrm{e}^{\mathrm{i}\omega}\sqrt{\frac{6(1-\alpha)}{1-\beta^2}} \\ G &= \frac{1-\beta^2}{2}\Big(\frac{1}{\overline{E}_f} + \frac{1}{\overline{E}_s}\Big)(K_1^2 + K_2^2) = \frac{6}{\overline{E}_f h^3}\Big(M^2 + \frac{F^2h^2}{12}\Big) \\ \tan\psi &= \frac{K_2}{K_1} = \frac{\mathrm{Im}(Kh^{\mathrm{i}\varepsilon})}{\mathrm{Re}(Kh^{\mathrm{i}\varepsilon})} = \frac{\sqrt{12}M\cos\omega + hF\sin\omega}{-\sqrt{12}M\sin\omega + hF\cos\omega} \end{aligned} \tag{2.1}$$

respectively, where α and β are the Dundurs parameters defined as

$$\alpha = \frac{\overline{E}_f - \overline{E}_s}{\overline{E}_f + \overline{E}_s} \qquad \beta = \frac{\overline{E}_f(1-\nu_f)(1-2\nu_s) - \overline{E}_s(1-\nu_s)(1-2\nu_f)}{2[\overline{E}_f(1-\nu_f)(1-2\nu_s) + \overline{E}_s(1-\nu_s)(1-2\nu_f)]} \tag{2.2}$$

and $\overline{E}_f = E_f/(1-\nu_f^2)$ and $\overline{E}_s = E_s/(1-\nu_s^2)$, $\omega \equiv \omega(\alpha,\beta,h/H = 0)$. The function ω is a real angular function of the two Dundurs parameters and the ratio of the two layers thicknesses $\eta = h/H$ introduced by Suo and Hutchinson (1990) by which the stress intensity factor is completely determined

$$\omega = \frac{1+\eta}{1.1+\eta}\sqrt{\frac{1+\alpha-\beta}{1-\alpha^2+\beta^2}}\,\frac{180}{\pi}\,[^\circ] \tag{2.3}$$

Determination of ω requires that the crack problem should be solved for a single case of load, for given values of α, β and η. Suo and Hutchinson (1990) did that using the integral equations method. They presented their results in a tabular form. Those results were approximated with an analytical expression for ω, given by (2.3), in Veljkovic and Nikolic (2003). When there is no difference in elastic characteristics of the materials, $\omega = 52.1^\circ$. Considering that the influence of the coefficient β on solving the problem presented in Fig. 1 is much smaller than the influence of the coefficient α, in further considerations it was adopted that $\beta = 0$.

The parameter ε is called the bielastic constant; it is a characteristics of the interfacial crack and was defined by Rice (1988) as

$$\varepsilon = \frac{1}{2\pi}\ln\frac{1-\beta}{1+\beta} \tag{2.4}$$

The parameter ε is equal to zero for a homogeneous material, i.e. when the two materials are the same.

The problem shown in Fig. 2 can be observed in terms of buckling theory of Euler's bars and described by von Karman's nonlinear plate theory, for which the governing equations for the displacement along the z-axis and the membrane stress along the x-axis are (cf. Appendix (A.3))

$$\frac{\overline{E}_f h^3}{12}\frac{d^4w}{dx^4} + (\sigma h + F)\frac{d^2w}{dx^2} = 0 \qquad \frac{dN}{dx} = 0 \tag{2.5}$$

where w is the displacement along the y-axis (vertical in Fig. 2). Solutions to equation (2.5) for boundary conditions $w = 0$ and $dw/dx = 0$ for $x = \pm b$ are

$$w = \frac{h}{2}\Big(1 + \cos\frac{\pi x}{b}\Big)\sqrt{\frac{4}{3}\Big(\frac{\sigma}{\sigma_c} - 1\Big)} \qquad M = \sigma_c\frac{h^2}{2}\sqrt{\frac{4}{3}\Big(\frac{\sigma}{\sigma_c} - 1\Big)}\cos\frac{\pi x}{b} \qquad N = -h\sigma_c \tag{2.6}$$

where: $\sigma_c = (\pi^2/12)\overline{E}_f(h/b)^2$ is the critical stress at the onset of buckling for a plate which is clamped on its edges.

The residual compressive stress σ must be bigger than the critical value σ_c in order for a blister to appear and buckling delamination of the coating to start as an interfacial crack of length $2b$. The ratio σ/σ_c is a dimensionless stress parameter. Considering that the increasing size of b reduces σ_c, it means that the dimensionless stress parameter σ/σ_c increases with an increase of b.

Substituting equations $(2.6)_{2,3}$ into equation $(2.1)_2$, one obtains the energy release rate along sides of the blister as

$$G = \frac{\sigma^2 h}{2\overline{E}_f}\Big(1 - \frac{\sigma_c}{\sigma}\Big)\Big(1 + 3\frac{\sigma_c}{\sigma}\Big) \tag{2.7}$$

Substitution of equations $(2.6)_{2,3}$ into equation $(2.1)_3$ gives the mode mixity as

$$\tan\psi = \frac{2\cos\omega + \sqrt{\Big(\frac{\sigma}{\sigma_c} - 1\Big)}\sin\omega}{-2\sin\omega + \sqrt{\Big(\frac{\sigma}{\sigma_c} - 1\Big)}\cos\omega} \tag{2.8}$$

If the elastic energy, which exists in the unbuckled coating exposed to compressive stress, is defined as

$$G_0 = \frac{1}{2}\frac{\sigma^2 h}{\overline{E}_f} \tag{2.9}$$

equation (2.7) can be then written as

$$G = G_0\Big(1 - \frac{\sigma_c}{\sigma}\Big)\Big(1 + 3\frac{\sigma_c}{\sigma}\Big) \tag{2.10}$$

The crack propagation along the interface strongly depends on modes of the crack loading (Nikolic and Veljkovic, 2006). The criterion for crack propagation along the interface, in conditions of mode mixity, was defined by Hutchinson and Suo (1992) as

$$G = G_I^c f(\psi) = G_I^c(1 + (1-\lambda)\tan^2\psi) \tag{2.11}$$

where G_I^c is pure Mode 1 toughness and λ is a parameter that takes into account the influence of Mode 2 on the crack propagation criterion. The parameter λ has a value in the range from 0 to 1. When $\lambda = 1$, the condition for crack propagation is reduced to the condition for crack propagation along an ideally brittle interface, i.e., $G = G_I^c$ for all the modes combinations. When $\lambda = 0$, the crack advance only depends on Mode 1 component.

Since in the coating delamination in form of a straight-sided blister, the width of the blister, $2b$, remains constant, the delamination is carried out through the interfacial crack that is expanding along more or less circular front of the blister. The average energy release rate at the blister front is defined by an expression for the energy release rate of a circular blister whose radius is b (Hutchinson and Suo, 1992)

$$G_{ss} = G_0\Big(1 - \frac{\sigma_c}{\sigma}\Big)^2 \tag{2.12}$$

3. Results and discussion

In Fig. 3, the change in the mode mixity, ψ, at the crack tip in terms of the σ/σ_c ratio for different values of parameter α and for $\beta = 0$ is shown. The diagrams were obtained based on equation (2.8) using symbolic programming package Mathematica®.

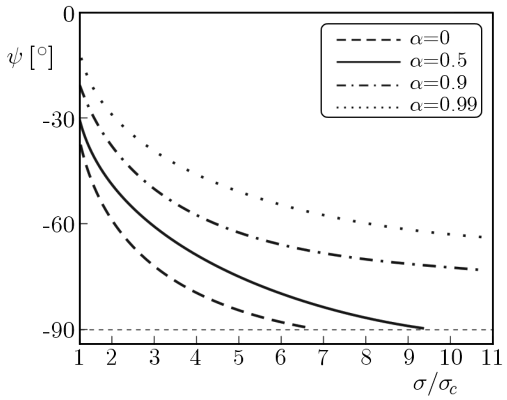

Fig. 3. The mode mixity ψ as a function of σ/σ_c for different values of the parameter α

The influence of different elastic characteristics of the coating and substrate material are contained within the parameter ω. When there is no difference between the elastic characteristics of the coating and the substrate, i.e. for $\alpha = 0$, the curve of dependence of ψ on σ/σ_c starts at $\psi = -37.9°$. From Fig. 3 can be seen that when σ/σ_c increases, the proportion of Mode 2 relative to Mode 1 for a given value of α also increases. Figure 3 also shows that the point where there is only Mode 2 ($\psi = -90°$ depends on the difference between the elastic characteristics of the coating and the substrate. For systems with a more compliant substrate, for example, for $\alpha = 0.9$ $(\overline{E}_f/\overline{E}_s = 10)$ or $\alpha = 0.99$ $(\overline{E}_f/\overline{E}_s = 100)$, the portion of Mode 1 with respect to Mode 2 is higher for the same values of σ/σ_c. The influence of elastic characteristics of the substrate is thus such that more elastic substrates favours the process of coating delamination due to predominance of Mode 1.

In Fig. 4, the normalized energy release rate needed for the expansion of the interfacial crack along the sides of the blister in terms of σ/σ_c for different values of parameter α for $\beta = 0$ and $\lambda = 0.25$ is shown. The diagrams were obtained on the basis of equations (2.10) and (2.11).

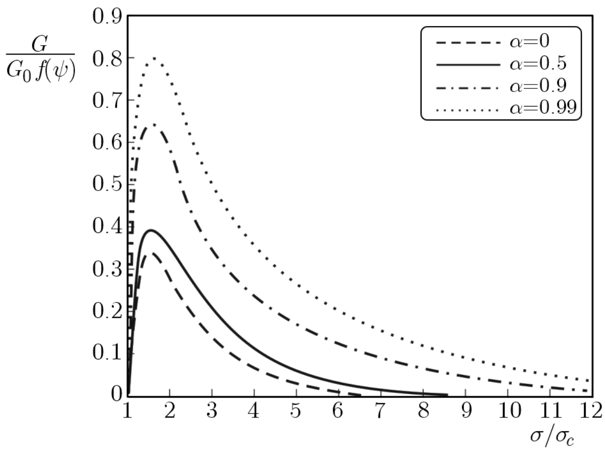

Fig. 4. The influence of differences between elastic characteristics of the coating and the substrate on the energy release rate along sides of the blister for different values of the parameter α

Figure 4 shows that the influence of differences between the elastic characteristics of the coating and the substrate is not big, even for $\alpha = 0.5$ $(\overline{E}_f/\overline{E}_s = 3)$. This influence becomes more significant only for $\alpha > 0.5$. It can also be seen that the peak of the curve of energy release rate has significantly higher values for $\alpha = 0.9$ and $\alpha = 0.99$. This increase in the energy release rate in systems with more compliant substrates comes from the release of the elastic energy in the areas where the coating is bonded to the substrate and the energy of the delaminated part of the coating. When the substrate is more compliant, the width of the area in which the influence of delamination is felt is be bigger and, therefore, the energy release rate is higher. For very compliant substrates, the width at which additional elastic energy is released can be even bigger than the width of the blister. However, if the width of the blister increases, this influence is reduced and for b big enough, the energy release rate G is closing to G_0.

In Fig. 5, the normalized average energy release rate needed for the expansion at the front of the blister as a function of σ/σ_c for different values of the parameter α and for $\beta = 0$ and $\lambda = 0.25$ is shown. The diagrams were obtained on the basis of equations (2.11) and (2.12).

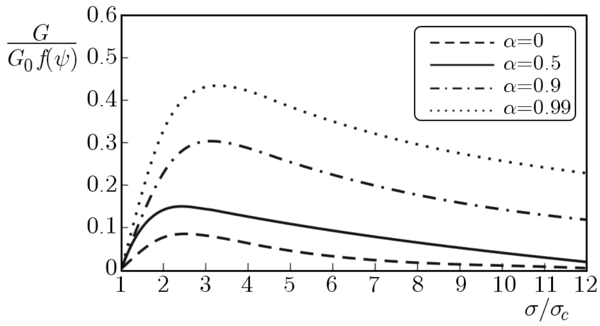

Fig. 5. The influence of differences between elastic characteristics of the coating and the substrate on the average energy release rate at the front of the blister for different values of the parameter α

From Fig. 5, it can be seen that the influence of differences between elastic characteristics of the coating and the substrate are not big until the coating is not stiff enough in comparison to the substrate, i.e. while $\alpha < 0.5$. The average energy release rate at the front of the blister is smaller than the energy release rate along sides of the blister. This conclusion can be drawn when Figs. 4 and 5 are compared to each other. The influence of differences between the elastic characteristics of the coating and the substrate becomes obvious for very compliant substrates, i.e. $\alpha \geqslant 0.9$. The average energy release rate at the front of the blister increases as the substrate becomes more compliant, i.e. as the difference between elastic characteristics of the coating and the substrate increases.

Comparison of Figs. 4 and 5, for values $\alpha = 0.9$ and $\alpha = 0.99$, shows that the average energy release rate at the front of the blister is bigger than the energy release rate along the sides of the blister. This explains why the coating delamination in form of a straight-sided blister occurs at the front of the blister and not along its sides.

4. Conclusions

For determination of the stress intensity factor, energy release rate and the load phase angle, Yu and Hutchinson (2002) used the integral equations method for definition of coefficients a_{ij} and c_{ij}, while in the present paper the real angular function ω in terms of the Dundurs parameters α and β and the ratio of the layers thicknesses, as defined by Suo and Hutchinson (1992), is used. Instead of the integral equations method for determination of the ω function, an approximation of their tabular values is used, which was obtained by the symbolic programming routine what enabled obtaining an analytical expression for ω in terms of α, β and h/H. This was further used in obtaining all the diagrams presented in the paper.

Based on diagrams presented in Figs. 3, 4 and 5, one can conclude that elastic characteristics of the substrate have significant influence on buckling delamination of the coating in form of a straight-sided blister when the ratio of Young's moduli of the coating and substrate is bigger than 3. This influence is particularly pronounced in metal and ceramic coatings on polymer substrates in which the ratio of moduli is bigger than 100 or for ceramic coating on a metal substrate (e.g. Al_2O_3 on Al) where the moduli ratio is 10. The influence of elastic characteristics of the substrate is such that more elastic substrates favour the process of coating delamination due to predominance of Mode 1. The influence of differences between the elastic characteristics of the coating and the substrate is not big, even for $\alpha = 0.5$, and it becomes more significant only for $\alpha > 0.5$. The average energy release rate at the front of the blister is smaller than the energy release rate along the sides of the blister. This explains why the coating delamination in form of a straight-sided blister occurs at the front of the blister and not along its sides.

The analysis presented in this paper, which is based on the concept of linear elastic fracture mechanics for the interfacial crack and nonlinear plate theory, with the use of symbolic programming, confirms the results shown by Cotterell and Chen (2000) and Yu and Hutchinson (2002). This justifies the application of this concept for explaining the influence of elastic characteristics of the substrate on buckling delamination of the coating with improvement of the model given by Cotterell and Chen (2000) and Yu and Hutchinson (2002) by application of equations from Suo and Hutchinson (1992) combined with symbolic programming. An analysis, considered in Nikolic and Djokovic (2012) of the coating delamination on a cylindrical substrate, has also proven the validity of this concept for those types of problems. Thus, the further investigation of coating delamination on both types of surfaces should concentrate on trying to improve the mathematical model to describe the real, physical problem of coating delamination better. The analysis should also be extended to considering problems of coating delamination in other forms like elliptical and "telephone cord" blisters.

Appendix A. A short survey of Föppl-von Karman plate equations

In order to clarify equations (2.6), a Cartesian frame, $\{x_k\} \stackrel{def}{=} \{x_\alpha, z\} = \{x, y, z\}$, shown in Fig. 1d is introduced, with the x_2 axis along the fixed sides of the blister. The displacement vector is then defined as $\{u_k\} \stackrel{def}{=} \{u_\alpha, w\} = \{u, v, w\}$. In the following text, thework by Wierzbicki (2007) is mainly consulted. Assumptions of the Föppl-von Karman theory are listed below:

1. The plate is thin such that its thickness h is much smaller than the typical plate dimension.
2. The magnitude of the transverse deflection is of the same order as the thickness of the plate (but according to Wierzbicki (2007), even for $w \sim 10h$ the theory is valid).
3. Products of the in-plane displacements u_α are negligibly small.
4. Love-Kirchhoff's hypothesis is satisfied (i.e. the in-plane displacements are linear functions of z).

The in-plane strain tensor and the curvature tensor have the form (comma means differentiation with respect to the coordinates $\{x_\alpha\} = \{x_1, x_2\}$)

$$2E_{\alpha\beta} = u_{\alpha,\beta} + u_{\beta,\alpha} + w_{,\alpha}w_{,\beta} \qquad \kappa_{\alpha\beta} = -w_{,\alpha\beta} \tag{A.1}$$

Introducing the bend-twist moment and the in-plane (membrane) force by means of

$$M_{\alpha\beta} = \int\limits_{-h/2}^{h/2} \sigma_{\alpha\beta} z \, dz \qquad N_{\alpha\beta} = \int\limits_{-h/2}^{h/2} \sigma_{\alpha\beta} \, dz$$

under the assumption of material linearity in the elastic range as well as geometric nonlinearity, one obtains the constitutive equations

$$\begin{aligned} M_{\alpha\beta} &= D[(1-\nu)\kappa_{\alpha\beta} + \nu\kappa_{\gamma\gamma}\delta_{\alpha\beta}] \\ N_{\alpha\beta} &= \overline{E}h[(1-\nu)E_{\alpha\beta} + \nu E_{\gamma\gamma}\delta_{\alpha\beta}] - F\delta_{\alpha\beta} \equiv \Delta N_{\alpha\beta} - F\delta_{\alpha\beta} \end{aligned} \tag{A.2}$$

where $D = \overline{E}h^3/12$ is the bend-twist rigidity with $\overline{E} \equiv E/(1-\nu^2)$. In the second moment--curvature constitutive equation, it is assumed that the in-plane equi-biaxial compressive pre-stress $F = h\sigma$ is applied (see also Hutchinson, 2001). With these preliminaries, the equilibrium equations read

$$M_{\alpha\beta,\alpha\beta} + (N_{\alpha\beta}w_{\beta})_{,\alpha} = 0 \qquad (N_{\alpha\beta})_{,\alpha} = 0 \tag{A.3}$$

Due to the geometrical and boundary conditions – clamped edges of the blister along the x_2-axis, it is reasonable to assume that $w_{,2} = 0$. Then $(A.3)_1$ is simplified into

$$-w_{,1111} + \frac{N_{11}}{D}w_{,11} = 0 \tag{A.4}$$

while $(A.3)_2$ becomes $N_{11,1} = 0$. Thus, the above non-zero component of the membrane force $(A.2)_2$

$$N_{11} = \overline{E}hE_{11} - F = \overline{E}h\Big(u_{1,1} + \frac{1}{2}w_{,1}^2\Big) - F \tag{A.5}$$

must be constant. The clamped edges of the blister imply the boundary conditions $u_1(x_1 = \pm b) = w(x_1 = \pm b) = 0$ as well as $w_{,1}(x_1 = \pm b) = 0$ (see Hutchinson and Suo, 1992). These are satisfied by the following solution to (A.4)

$$w = C\Big(1 + \cos\frac{\pi x_1}{b}\Big) \tag{A.6}$$

which provides the buckling stress

$$N_{11c} = -h\sigma_c = -D\Big(\frac{\pi}{b}\Big)^2 \tag{A.7}$$

The displacement u_1 is found from (A.5). After integration, one arrives at

$$u_1(x_1) = \frac{\pi}{8b}C^2\sin\frac{2\pi x_1}{b} \tag{A.8}$$

with

$$C^2 = \frac{h^2}{3}\Big(\frac{\sigma}{\sigma_c} - 1\Big) \tag{A.9}$$

which leads to $(2.6)_1$. Finally, moment $(2.6)_2$ is found by applying (A.6) and $(A.1)_2$ into $(A.2)_1$.

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