Effects of Substrate Compliance on Buckling Delamination of Thin Films under Compression

Abstract. For films or coatings deposited on substrate at high temperature, residual compressive stresses are often induced in the surface layers because of the mismatch in the thermal expansion coefficients. Under such compressive residual stresses, the surface thin film is susceptible to buckling-driven delamination. Various shapes of buckled region are observed, including long straight-sided blisters, circular and the 'telephone cord' blister. Many studies have been done on systems with rigid substrates. Recent studies have shown that substrate compliance has an importance influence on both the film buckling stress and the energy release rate of the interface delamination crack, and when the substrate is very soft, another buckling mode may occur. This report will focus on the effects of substrate compliance on a straight–sided delamination buckle.

Keywords: Thin film, buckling, elastic mismatch, compliant substrate.

1. Introduction

Film/substrate structures are increasingly used in a variety of industrial applications. Residual compressive stresses are often induced in thin films because of the mismatch in the thermal expansion coefficients and high deposition temperature. Different stress relief mechanisms have been observed in thin films. For thin film bonded on relatively stiff substrate, one of the mechanisms involves buckling-driven delamination of thin films from substrate, as in the case of a ceramic thermal barrier coating or a diamond-like carbon wear resistant coating on a metallic substrate. (L.B.Freund and S.Suresh,2003) Various shapes of buckled region are observed,

including long straight-sided blisters, circular and the 'telephone cord' blister.

Many studies have been done on systems with rigid substrates. Recent studies have shown that when the substrate is very compliant compared with the film, substrate compliance has an importance influence on both the film buckling stress and the energy release rate of the interface delamination crack, and even leads to the transition of buckling mode. In this report, we will focus on the effects of substrate compliance on a straight–sided delamination buckle. The last part of the report will present a qualitative picture of mode transition between wrinkling and buckling delamination.

2. Straight-sided delamination buckle

Consider a z-independent portion of the straight-sided blister shown in figure 1. The film is assumed to be elastic and isotropic, with Young's modulus E_f and Poisson's ratio v_f . The substrate is also taken to be uniform and isotropic, with the corresponding elastic characters E_s and v_s . The substrate is assumed to be very thick compared with the film. The film is subject to an equi-biaxial compressive mismatch stress of magnitude σ . There exists an unattached region $-b \le x \le b$ in the interface of film and substrate. The problem that governs the behavior for the section A-A' far behind the curved front of the straight-sided blister is analyzed as a plane strain problem. Dundurs' elastic parameters are defined to denote the elastic mismatch between the film and the substrate:

$$\alpha = \frac{\overline{E}_f - \overline{E}_s}{\overline{E}_f + \overline{E}_s}$$

$$\beta = \frac{1}{2} \frac{\mu_f (1 - 2\nu_s) - \mu_s (1 - 2\nu_f)}{\mu_t (1 - \nu_s) + \mu_s (1 - \nu_f)}$$
(1)

with $\overline{E} = \frac{1 - v^2}{E}$, the plane strain elastic modulus. Typically α is the more important of the two parameters for most bilayer crack problems.

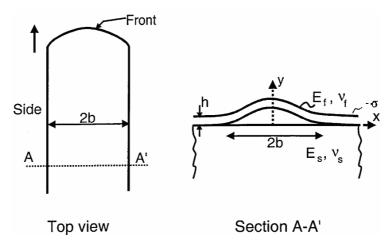


Figure 1. Schematic illustration of a straight-sided blister.

2.1 Buckling of films on rigid substrates

When the substrate is stiff compared with the film, under the assumption of h << b, the film is modeled as a wide, clamped Euler column of width 2b. M and ΔN are the moment and change in resultant force per unit length at the right-hand end of the column, shown in figure 2. By Von Karman nonlinear plate theory with fully clamped conditions at the boundary, the solutions are given (J.W. Hutchinson and Z. Suo, 1992):

$$M = \frac{\pi^2}{2} \frac{Dh}{b^2} \delta$$
, $\Delta N = \frac{3\pi^2}{4} \frac{D}{b^2} \delta^2$, where $D = \frac{\overline{E}_f h^3}{12}$ is the bending stiffness.

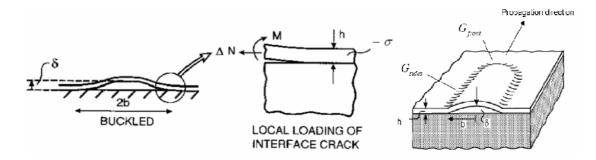


Figure 2. Illustration of film after buckling

the energy release rate: $G = \frac{6}{\overline{E}_f h^3} \left(M^2 + \frac{h^2 \Delta N}{12} \right) = \frac{h}{2\overline{E}_f} \left(\sigma - \sigma_0 \right) \left(\sigma + 3\sigma_0 \right), \text{ where}$

 $\sigma_0 = \frac{\pi \overline{E}_f}{12} \left(\frac{h}{b}\right)^2$ is the classical buckling stress of a wide plate with clamped edges.

The mode mixity parameter ψ (defined relative to the reference length l=h):

$$\tan \psi = \frac{4\cos\omega + \sqrt{3}\delta\sin\omega}{-4\sin\omega + \sqrt{3}\delta\cos\omega}$$
, where δ is the amplitude of the buckling deflection

and $\omega = \omega(\alpha, \beta)$ is the phase factor. The normalized energy release rate is

$$\frac{G}{G_0} = \left(1 - \frac{\sigma_0}{\sigma}\right) \left(1 + 3\frac{\sigma_0}{\sigma}\right) \tag{2}$$

It is plotted in figure 4, together with the phase angle, with $G_0 = \frac{\sigma^2 h}{2E_f}$ (the elastic energy density in the film with plane strain constraint). The energy release rate along the curved propagation front is:

$$G_{front} = \frac{1}{2b} \int_{-b}^{b} G_{sides} dy = \frac{h}{\overline{E}_{f}} (\sigma - \sigma_{c})^{2}$$
(3)

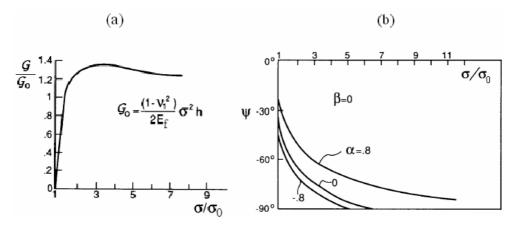


Figure 3. Normalized energy release rate and mode-mixity for film bonded on rigid substrate

2.2 Buckling of films on compliant substrates

The foregoing discussion does not mention the energy changes in the portion of the film that remains bonded to the substrate and that in the substrate itself, because the delaminated portion of the film is usually regarded as being compliant compared to the substrate. Consequently, the edge of the buckled portion of the film can be viewed as being rigidly clamped along this boundary. However, recent studies (Cotterell and Chen, 2000; H.H.Yu and J.W. Hutchinson, 2002) have shown that if the lateral amplitude of the buckling deflection is not very large compared to the thickness of the film or if the substrate is very compliant compared with the film, substrate compliance has an important effect on the condition of the onset of film buckling, as well as the energy release rate of the interface delamination crack. The following part focuses on the influence of the substrate compliance on the straight-sided delamination buckle.

As the delaminated film buckles, the normal axial compressive force at the edge of the delamination relaxes from the applied value N to the critical buckling value N_c , with resultant force change $\Delta N = N - N_c$, shown in figure 4 (Cotterell, B. and Chen, Z.,2000). If the substrate is not so stiff compared with the film, the relaxation in the force in the film will cause an axial displacement, u_0 , at the edge of the buckled film. At the same time a bending moment, M, arises to constrain the buckling and causes a rotation, ϕ , at the edge of the buckled film. In addition the change in the axial force causes a rotation and the end moment causes an axial deformation. The problem of the film-substrate system after buckling of the delaminated film can be decomposed into two problems: the buckled film and the remaining film/substrate system.

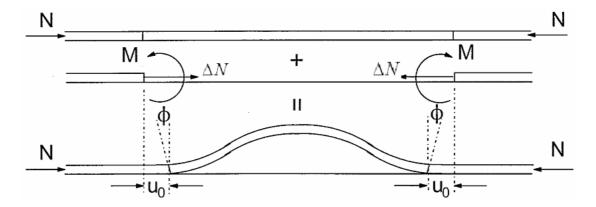


Figure 4. Superposition for a film/substrate system after buckling of the delaminated film

2.2.1 The solution of the buckled film

For the delaminated part of film, the important pre-stress component is $\sigma_{xx} = -\sigma$.

After buckling, shown as figure 5, T and M are the resultant force and moment per unit length at the edge of the buckled film, which is modeled by Von Karman nonlinear plate theory. The solutions are obtained (Yu and Hutchinson, 2002) as follows:

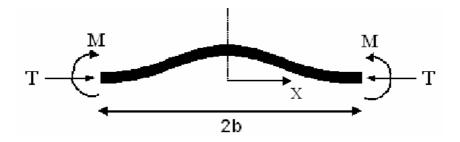


Figure 5. The delaminated part of film

$$u\Big|_{x=b} = \frac{\sigma h - T}{\overline{E}_f} - \frac{\lambda h}{8} \left(\frac{M}{bF\cos\lambda}\right)^2 (2\lambda - \sin 2\lambda)$$

$$\phi\Big|_{x=b} = -\frac{M\lambda}{Fb} \tan\lambda$$
(4)

with $\lambda = \pi \sqrt{\frac{T}{\sigma_0 h}}$, $\sigma_0 = \frac{\pi \overline{E}_f}{12} \left(\frac{h}{b}\right)^2$ is the classical buckling stress of a wide plate

with clamped edges, σ is the pre-compressive stress, so $T - \sigma h$ is the change of resultant force per unit length at the delaminated edge.

2.2.2 The solution of the remaining film/substrate system

The plane strain problem for the film/substrate system after buckling of the delaminated film can be reduced to the plane strain problem shown in figure 6, with the delaminated film removed.

By linearity, the relations that define the effective displacement and rotation at the attached edges are:

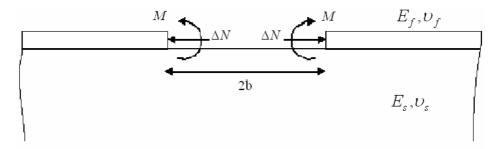


Figure 6. The remaining film/substrate system.

$$u_{0} = u \Big|_{x=b} = \frac{N - N_{c}}{\overline{E}_{f}} a_{11} + \frac{M_{0}}{\overline{E}_{f} h} a_{12} = \frac{\Delta N}{\overline{E}_{f}} a_{11} + \frac{M}{\overline{E}_{f} h} a_{12}$$

$$\phi = \phi \Big|_{x=b} = \frac{N - N_{c}}{\overline{E}_{f} h} a_{21} + \frac{M_{0}}{\overline{E}_{f} h^{2}} a_{22} = \frac{\Delta N}{\overline{E}_{f} h} a_{21} + \frac{M}{\overline{E}_{f} h^{2}} a_{22}$$
(5)

where a_{ij} are the compliance coefficients, and are functions of both b/h and the Dundurs' elastic mismatch parameters. To simplify the analysis, set $\beta = 0$ in the calculation. The constants can be determined numerically either by direct finite element calculations or by solving integral equation formulation as described in the previous studies (Yu et al.,2001).

In the reduced film/substrate system, h is the only significant physical length, and the stress intensity factors have the form:

$$K_{II} = c_{11} \frac{\Delta N}{\sqrt{h}} + c_{12} \frac{2\sqrt{3}M}{h\sqrt{h}}, \qquad K_{I} = c_{21} \frac{\Delta N}{\sqrt{h}} + c_{22} \frac{2\sqrt{3}M}{h\sqrt{h}}$$
 (6)

The coefficients c_{ij} also depend on b/h and α .

The energy release rate of the interface crack between the two isotropic materials in figure 6 is

$$G = \frac{\left(1 - \beta^2\right)\left(K_I^2 + K_{II}^2\right)}{2} \left(\frac{1}{\overline{E}_f} + \frac{1}{\overline{E}_s}\right) \tag{7}$$

2.2.3 The solution for the original problem

The solutions of the two separate problems are coupled by continuity at the edges of the delaminated film. By equating the displacement at the detached edges for the film/substrate system and the delaminated part of film, the eigenvalue equation is obtained (H.H.Yu and J.W. Hutchinson, 2002):

$$\frac{12b}{\pi h} \sqrt{\frac{\sigma_0}{\sigma_c}} \tan(\pi \sqrt{\frac{\sigma_c}{\sigma_0}}) + a_{22} - \frac{a_{12}^2}{1 + a_{11}} = 0$$
 (8)

3. The effect of substrate compliance

First, consider the effect of substrate compliance on the condition of onset of film buckling. For three different b/h, the normalized critical stress by the plane stress elastic modulus is shown in figure 7.

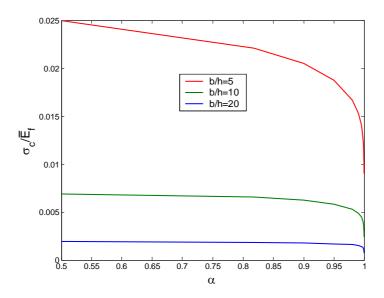


Figure 7. The normalized critical stress as a function of parameter α

Then the energy release rate and mode mix along the sides of the blister is examined. After the stress intensity factors are calculated from (4), the mode mixity is defined as:

$$\psi = \tan^{-1}(K_{II}/K_{I}) \tag{9}$$

Define b_0 to be the corresponding critical half width for case of film with clamped edges:

$$b_0 = \frac{\pi h}{2\sqrt{3}} \sqrt{\frac{\overline{E}_f}{\sigma}}$$

so we have $\frac{\sigma_c}{\sigma_0} = \left(\frac{b_c}{b_0}\right)^2$. The computed results for G/G_0 as a function of

 b/b_0 (H.H.Yu and J.W. Hutchinson, 2002) are shown in figure 8.

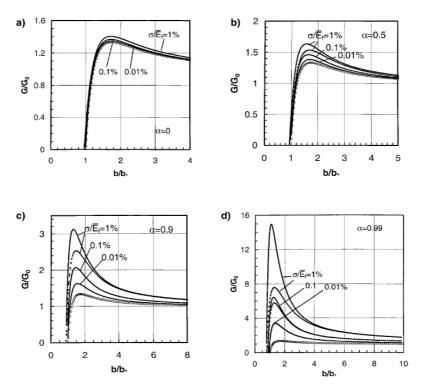


Figure 8. Normalized energy release rate along the sides of the delamination as function of normalized blister width for several levels of pre-stress and for the elastic mismatch: (a) $\alpha=0$; (b) $\alpha=0.5$;(c) $\alpha=0.9$,(d) $\alpha=0.99$. The solid line curves are computed using (6) and (7). The curve plotted as open circles is computed using (2).

The higher energy release rates for film bonded on compliant substrate is from the

release of elastic energy in the regions of the film attached to the substrate, as well as that from the delaminated portion of film with less constraint by the substrate. For sufficient large b, G can approach to G_0 .

The mode mixty associated with the interface crack is plotted in figure 9 as a function of b/b_0 (H.H.Yu and J.W. Hutchinson, 2002). From the figure we can see that the tendency for a higher proportion of mode I to mode II for blisters on more compliant substrates.

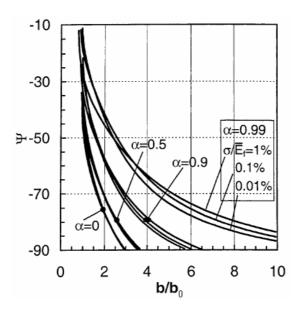


Figure 9. Mode mixty along the delamination edges as a function of the normalized blister width, elastic mismatch, and pre-stress.

Now consider the energy release rate averaged along the curved front of a tunneling delamination. The average energy release rate of the curved front is $G_{ss} = \frac{\Delta U}{2b}$, where ΔU is the total strain energy released per unit length of delamination. Curves of G_{ss}/G_0 versus b/b_0 are plotted as solid lines in figure 10. The figure shows that the result for $\alpha = 0$ is very close to that calculated from (3). From the results we can see that when the substrate is very compliant, with a big enough blister width, the energy release rate can exceed the energy release rate along the sides, which means that such a blister would propagate at its front once formed.

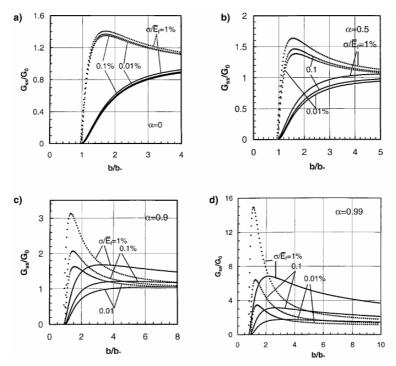


Figure 10. The normalized average energy release rate along the curved front of a steadily propagating straight-sided blister (solid lines) for the elastic mismatches: (a) $\alpha=0$; (b) $\alpha=0.5$; (c) $\alpha=0.9$, (d) $\alpha=0.99$. The dashed lines are the energy release rate along the sides of the delamination.

4. Transition between buckling-delamination and wrinkling

The above discussion only considers the delamination buckling mode. When the substrate is very soft, the compressive stress can lead to the wrinkling over the film surface without delamination. Recent experiments have observed co-existing of both as well as transition of the buckling modes. A qualitative understanding is represented as figure 11(R. Huang, 2005), so $\alpha \to 1$ is the interesting region.

For a thin elastic film on a thick substrate, the critical stress for wrinkling depends on the elastic moduli of the film and the substrate (R. Huang, 2005),

$$\sigma_{w} = \frac{3^{2/3}}{4} \left(\frac{1 - \alpha}{1 + \alpha} \right)^{2/3} \overline{E}_{f} \tag{10}$$

A comparison between the critical stresses for wrinkling and buckling-delamination for three different delaminated width b/h is presented in figure 12, both stresses are

normalized by the plane-strain modulus of the film and plotted versus the elastic mismatch parameter α in the region of very complaint substrates. From the figure we can see that the buckle mode of wrinkle start to compete with the delamination buckle when the substrate becomes very soft. For a given interfacial delamination width, there exists a critical value α_c : when $\alpha < \alpha_c$, the buckling stress is lower; when $\alpha > \alpha_c$, the wrinkling stress is lower. Therefore the buckling mode transition is predicted as the elastic mismatch between the film and the substrate varies.

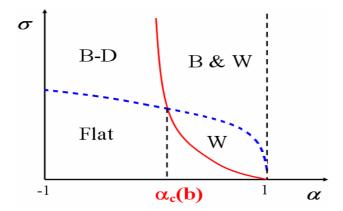


Figure 11. A qualitative understanding of the transition of the two buckling modes.

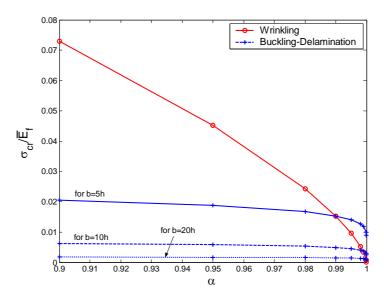


Figure 12. Comparison of the critical stress for wrinkling and for buckling-delamination

5. Conclusions

Substrate compliance has a significant effect on both the critical stress of thin film buckling and the energy release rate of the interface delamination crack for straight-sided blister. A qualitative change in buckle mode may appear when the elastic mismatch parameter α reaches a certain value for a given delamination size, and the two types of buckling modes co-exist and interact.

Reference:

- Freund, L.B., Suresh S. (2003). Thin Film Materials: Stress, Defect Formation and Surface Evolution. Cambridge University Press, UK.
- Hutchinson, J.W., Suo, Z., (1992). Mixed Mode Cracking in Layered Materials. Advances in Applied Mechanics **29**, 63-191
- Hutchinson, J.W., "Lecture Overheads on Delamination Mechanics." *Unpublished notes*, (2006).
- Yu, H.H., He, M.Y. and Hutchinson, J.W.(2001). Edge effects in thin film delamination. *Acta Mater.* **49**, 93-107
- Cotterell, B. and Chen, Z. (2000). Buckling and crackling of thin films on compliant substrates under compression. International Journal of Fracture **104**, 169-179.
- Huang, R., Stress-induced wrinkling in thin films, Polymers Division, NIST, Gaithersburg, MD, July 8, 2005. (Invited Talks)
- Huang, R., Dynamics of surface pattern evolution in thin films, Max-Planck Institute for Metals Research, Stuttgart, Germany, August 18, 2005. (Invited Talks)