Evaluation of Mechanical Parameters of an Elastic Thin Film System by Modeling and Numerical Simulation of Telephone-cord Buckles

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Abstract

The morphology of telephone-cord buckles of elastic thin films can be used to evaluate the initial residual stress and interface toughness of the filmsubstrate system. The maximum out-of-plane displacement δ , the wavelength λ and amplitude A of the wave buckles can be measured in physical experiments. Through δ , λ , and A, the buckle morphology is obtained by an annular sector model established using the von Karman plate equations in polar coordinates for the elastic thin film. The mode-mix fracture criterion is applied to determine the shape and scale parameters. A numerical algorithm combining the Newmark- β scheme and the Chebyshev collocation method is adopted to numerically solve the problem in a quasi-dynamic process. Numerical experiments show that the numerical results agree well with physical experiments.

Keywords:

telephone-cord buckles, elastic thin film, initial residual stress, interface toughness, von Karman plate equations, mode-mix fracture criterion, Chebyshev collocation method.

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1. Introduction

Thin film materials are wildly used in many fields, such as thermal barrier coatings [1], micro-electro -mechanical systems [2], magnetic recording media [3], etc. However, compressed residual stresses are generally inevitably introduced on the elastic thin films in manufacturing processes, which can lead to undesirable delamination in the interface of the thin film and the substrate. For this reason, various patterns of buckles, such as the most commonly observed circular buckles [4], straight-sided buckles [5] and telephone cord buckles [6], are formed.

In experiments, the telephone cord buckles are the most frequently observed. Unfortunately, due to its complexity compared with the other two kinds, the results on the telephone cord buckles are much less reported. In 1997, applying the Griffith criterion and assuming that the energy release rate is identical everywhere on the fracture front, Gioia and Ortiz established a model in which the zigzagged edges of a telephone cord buckle are approximated by a sequence of congruent connected circular arcs, and the propagation fronts are also approximated by circular arcs but in a different size. The model describes the shape of the edges successfully and fits experimental results well [7], however, it cannot determine the widths of the telephone cord buckles. In 2002, Moon et al. established a pinned circle model, in which the delamination area is characterized by a sequence of connected sectors and on each sector the deformation of the buckle is assumed to be rotationally symmetric with respect to the pinned center [8]. The model well describes both the shape of the edges and the width of the telephone cord buckle, and the corresponding numerical problem is reduced to one dimension. However, because of the rotationally symmetric assumption, the center of sector is a singular point of the energy release rate, and in addition the global deformation is discontinuous across the connection lines between the sectors. Another model uses the analytical solution of straight-sided buckles [9], which avoids numerical computation. The model is based on the similarity of the out-of-plane displacements on the connection lines and the straight-sided buckles, and approximates the buckle near a connection line as a straight-sided buckle. A similar model is adapted in [10], which approximates the telephone cord buckle by a straight-sided buckle measured on the middle line (l in Fig. 1) instead. Since they are all 1D models in nature, none of the models mentioned above makes sufficient use of the shape of the delamination area, for example, the wavelength and amplitude, and the width of the telephone cord buckles are neglected.



Figure 1: A typical section: O is the center of the sector, $\overline{OA_1}$ and $\overline{OA_2}$ are the outer and inner radii with $|\overline{OA_1}| = R$ and $|\overline{OA_2}|/|\overline{OA_1}| = r_0$, $\angle A_1OB_1 = 2\theta_0$ is the central angle. Q_1 and Q_2 with $|\overline{Q_1A_1}| = |\overline{Q_2B_2}|$ are the reciprocally corresponding connection points across which the deformation is smooth.

Because the morphology of the buckles can be measured conveniently, there is much effort and great interests of using the knowledge to evaluate the mechanic parameters, such as the residual stresses and adhesion energy. In 2004, Cordill et al. gave some results on the adhesion measurement by morphology of thin film buckles [9]. In 2007, through measuring the morphology of the telephone cord buckles (AFM), Cordill et al. evaluated the residual stresses and the interface toughness by using the pinned circle model and the straight-sided buckle approximation [10], they also reported a special telephone-cord to straight-sided buckle phenomenon, and they found that the mechanical parameters evaluated by the telephone cord buckles are comparable to those evaluated by the straight-sided ones, the latter are considered to be accurate for a given system (see the line labeled with Straight in Table 1 for the case of $h^* = 300 nm$). In 2009, Yu et al. prepared a wedge shaped iron film system with the thickness changing from zero to several hundred nanometers, and reported the telephone cord buckles phenomenon on it in detail [11].

In the present paper, the annular sector model established in [12], where a telephone cord buckle is characterized by a sequence of connected annular sectors as shown in Fig. 2, is adopted, the difference is that here the shape and size of the annular sector is determined by the mode-mix criterion, of which the Griffith criterion used in [12] is a special case. To obtain numerical



Figure 2: The annular sector model : delamination area is divided into congruent annular sectors. O is the center of the sector AOB. The dashed lines are the connection lines between adjacent sectors.

solutions for the governing static von Karman plate equations, a system of quasi-dynamic equations is introduced, and the Chebyshev collocation method and the Newmark- β scheme are adopted for the discretization of the dynamic system as in [12]. To efficiently solve the discrete system for various parameters, the continuation method is applied in the computing process. To verify the model, the evaluated interface toughness and initial residual stress are compared with those reported in [10], and the results from the telephone cord buckle match remarkably well with those given by the analytical solution of the straight sided buckle observed in the physical experiments on a same film system (see the line labeled with Straight in Table 1 for the case of $h^* = 300nm$).

The rest of the paper is organized as follows. The annular sector model and corresponding numerical method is briefly introduced in section 2 (for details see [12]). The numerical experiments and results are presented and discussed in section 3, where comparisons of our results with physical experiments and the results produced by the other models mentioned above are also made. The paper ends with a brief summary in section 4.

2. The annular sector model and the numerical method

Different from the straight-sided approach and the pinned circle approach of the telephone cord buckles, the annular sector model is a 2D model. The advantage of this is that the buckle's morphology can be better characterized by the shape and size of the buckling area. On the other hand, the computing complexity is increased when the computing area becomes to 2D. Numerical methods designed to deal with this difficulty is shown in section 2.2.

2.1. The annular sector model

To describe a typical telephone cord buckle as a sequence of reciprocally connected annular sectors, the shape and the width scale of the telephone cord buckle, which can be completely determined by three parameters, need to be determined. For simplicity, we choose the outer radius R of the annular sector as the scale parameter, the half central angle θ_0 and the normalized inner radius r_0 , i.e. the ratio of the inner radius against the outer radius, of the annular sector as the shape parameters (see Fig. 1).

The governing equations of the equilibrium state of the buckle can be reduced to the von Karman plate equations defined on an annular sector Ω^* . Naturally, it is convenient to express the equations in the polar coordinate system (r^*, θ^*) with the annular sector's center O as the polar origin and the sector's geometric symmetry line as the polar axis. For simplicity, we assume that the initial residual stress is equi-biaxial compressive, in Cartesian coordinates this is expressed as $-\sigma_{xx} = -\sigma_{yy} = \sigma_0^* > 0, \sigma_{xy} = 0.$

The von Karman equation is non-dimensioned by introducing the following normalized variables

$$u = \frac{Ru^{*}}{(h^{*})^{2}}, v = \frac{Rv^{*}}{(h^{*})^{2}}, w = \frac{w^{*}}{h^{*}}, r = \frac{r^{*}}{R}, \theta = \theta^{*}, h = \frac{h^{*}}{R},$$

$$\sigma_{c}^{*} = \frac{E}{1 - \nu^{2}} \frac{(\pi h)^{2}}{3(1 - r_{0})^{2}}, \sigma_{0} = \frac{\sigma_{0}^{*}}{\sigma_{c}^{*}}.$$
(1)

and is rewritten as (see [12] for details)

$$\begin{cases} \triangle^2 w - \frac{4\pi^2}{(1-r_0)^2} \sigma_0 \triangle w = N_W(w, u, v), \\ L_U(u, v) + N_U(w) = 0, \\ L_V(u, v) + N_V(w) = 0, \end{cases} (r, \theta) \in \Omega, \qquad (2)$$

where L_U , L_V are the linear parts of the last two equations in (2), and N_W , N_U , N_V are the non-linear parts of the von Karman equations under polar coordinate system, \triangle denotes the Laplacian operator, and the normalized annular sector region is defined as $\Omega = \{(r, \theta) | r_0 < r < 1, -\theta_0 < \theta < \theta_0\}$.

To reflect the experimental symmetry (l in Fig. 1 is the symmetric axis), the connection of the annular sectors through reciprocal points (Q_1, Q_2 in Fig.

1), and the film being clamped to the substrate on the arched edges of the annular sectors, the equations (2) are coupled with the following boundary conditions

$$\begin{cases} w(r_0, \theta) = 0, \ w_{,r}(r_0, \theta) = 0, \ u(r_0, \theta) = 0, \ v(r_0, \theta) = 0, \\ w(1, \theta) = 0, \ w_{,r}(1, \theta) = 0, \ u(1, \theta) = 0, \ v(1, \theta) = 0, \end{cases}$$
(3)

and the reciprocally periodic connection boundary conditions

$$\begin{cases} \frac{1}{r^{k}} \frac{\partial^{k} w}{\partial \theta^{k}} \Big|_{(r,-\theta_{0})} = \frac{1}{(1+r_{0}-r)^{k}} \frac{\partial^{k} w}{\partial \theta^{k}} \Big|_{(1+r_{0}-r,\theta_{0})}, \quad k = 0, 1, 2, 3, \\ u(r,-\theta_{0}) = -u(1+r_{0}-r,\theta_{0}), \quad \frac{u_{,\theta}\left(r,-\theta_{0}\right)}{r} = -\frac{u_{,\theta}\left(1+r_{0}-r,\theta_{0}\right)}{1+r_{0}-r}, \quad (4) \\ v(r,-\theta_{0}) = v(1+r_{0}-r,\theta_{0}), \quad \frac{v_{,\theta}\left(r,-\theta_{0}\right)}{r} = \frac{v_{,\theta}\left(1+r_{0}-r,\theta_{0}\right)}{1+r_{0}-r}. \end{cases}$$

Let E and ν be the Young's modulus and Poisson's ratio of the elastic thin film. In the polar coordinate system, the energy release rate G and the phase angle ψ are given as [13]

$$G(r_{0},\theta_{0}) = \frac{3(1-\nu^{2})h^{*}(\sigma_{c}^{*})^{2}}{8\pi^{4}E} \left((w_{,rr} + \frac{\nu}{r^{2}}w_{,r\theta})^{2} + 12u_{,r}^{2} \right),$$

$$\psi(r_{0},\theta_{0}) = \arctan\left(\frac{(w_{,rr} + \frac{\nu}{r^{2}}w_{,r\theta})\cos\omega + \sqrt{12}u_{,r}\sin\omega}{-(w_{,rr} + \frac{\nu}{r^{2}}w_{,r\theta})\sin\omega + \sqrt{12}u_{,r}\cos\omega} \right),$$
(5)

where ω is a function of Dundurs' parameter [13]. Let Γ_I be the mode I interface toughness. Then, the mode-mix fracture criterion [14] states that on the fracture front $G = \Gamma(\psi) \equiv \Gamma_I (1 + \tan^2((1 - \rho)\psi))$. It reduces to the Griffith criterion when $\rho = 1$. We choose the mode-mix criterion as our fracture criterion, and choose the shape parameters in such a way that the variance of Γ_I on the fracture front is minimized. The effect of the mode parameter ρ on the output of the model is studied numerically.

2.2. Numerical treatment

We adopt a partial dynamic approach to solve the static von Karman equations (2). Our aim is to find the equilibrium solution of the following

equations

$$\begin{cases} w_{,tt} + cw_{,t} + \Delta^2 w - \frac{4\pi^2}{(1 - r_0)^2} \sigma_0 \Delta w = N_W(w, u, v), \\ L_U(u, v) + N_U(w) = 0, \\ L_V(u, v) + N_V(w) = 0, \end{cases} (r, \theta) \in \Omega, \quad (r, \theta) \in \Omega, \quad (6)$$

The Newmark- β ($\gamma = 0.5, \beta = 0.25$) scheme [14] is adopted in temporal discretization of the first equation for w, which is in fact the only equation that is time dependent in equations (6). For simplicity, in N_W , u and v take the value of the previous time step, while w takes the unknown value in the current time step. This simplification will definitely reduce tremendous amount of computing cost, though it may also lose some temporal accuracy which is not of much concern for a static solution. The discrete scheme of the first equation of equations (6) is implicit and is solved by fixed point iterations.

The Chebyshev collocation method is adopted in spatial discretization. First, we map the normalized annular sector region to a standard computing region $\hat{\Omega} = \{(x, y) | -1 < x < 1, -1 < y < 1\}$ with $x = (2r - 1 - r_0)/(1 - r_0)$, $y = \theta/\theta_0$. The first equation in equations (6) is 4-order for the normalized out-of-plane displacement w, thus the boundary conditions of w need to be treated with special care. With a new variable q, set $w(x, y) = (1 - x^2)q(x, y)$ [14], then, the clamped boundary conditions (3) for w reduce to the homogenous boundary conditions for q, just the same as for u and v, which can be easily imposed with Gauss-Lobatto collocation points. Let $T_i(x)$ be the Chebyshev polynomials of degree i. The discrete form of the displacements u, v and w are given as

$$\begin{cases} w_n(x,y) = \sum_{i=0}^{M} \sum_{j=0}^{N+2} (1-x^2) \hat{q}_{ij}^n T_i(x) T_j(y), \\ u_n(x,y) = \sum_{i=0}^{M} \sum_{j=0}^{N} \hat{u}_{ij}^n T_i(x) T_j(y), \\ v_n(x,y) = \sum_{i=0}^{M} \sum_{j=0}^{N} \hat{v}_{ij}^n T_i(x) T_j(y). \end{cases}$$
(7)

For the reciprocally periodic connections (4), we have twice as much of boundary conditions for w as for u and v. Following the idea of constructing the Gauss-Lobatto type collocation points [15], we denote $P_i(x)$ polynomials of degree i which form the sequence of orthogonal polynomials on [-1, 1] with the weight function $\hat{W}(y) = (1 - y^2)^{\frac{3}{2}}$. Then, we construct the collocation points for the discrete form (7): the Gauss-Lobatto collocation points in the x direction are used for w_n, u_n, v_n (there are (M - 1) interior points and 2 boundary points), the Gauss-Lobatto collocation points in the y direction are used for u_n, v_n (there are (N - 1) interior points and 2 boundary points), and zeros of $P_{N-1}(y)$ are chosen to be the interior collocation points for w_n in the y direction, each of the boundary points are used twice in this case to match the number of the boundary conditions [12].

To conclude, we write the fully discrete system as

$$\left(\frac{4}{(\Delta t)^2} + \frac{2c}{\Delta t}\right) W_{M,N}^{n+1} = F(W_{M,N}^{n+1}, \mathbf{U}_{M,N}^n) + \left(\frac{3}{(\Delta t)^2} + \frac{c}{2\Delta t}\right) W_{M,N}^{n+1} + 2\left(\frac{1}{(\Delta t)^2} + \frac{c}{\Delta t}\right) W_{M,N}^n - \left(\frac{1}{(\Delta t)^2} + \frac{c}{2\Delta t}\right) W_{M,N}^{n-1}, \quad (8)$$

$$\mathcal{L}(\mathbf{U}_{M,N}^{n+1}) = \mathbf{f}(W_{M,N}^{n+1}),\tag{9}$$

where Δt is the time step length, $W_{M,N}^n, U_{M,N}^n$ stand for the vector value of $w, (u, v)^T$ at time $n\Delta t$ on the interior collocation points, F, \mathcal{L} and \mathbf{f} stand for $N_W - \Delta^2 w + 4\pi^2(1 - r_0)^{-2}\sigma_0\Delta w, (L_U, L_V)^T, -(N_U, N_V)^T$ respectively. As mentioned before, the first equation of (8) is solved by the fixed point iterations

$$\left(\frac{4}{(\Delta t)^2} + \frac{2c}{\Delta t}\right) W_{M,N}^{n+1,k+1} = F(W_{M,N}^{n+1,k}, \mathbf{U}_{M,N}^n) + \left(\frac{3}{(\Delta t)^2} + \frac{c}{2\Delta t}\right) W_{M,N}^{n+1,k} + 2\left(\frac{1}{(\Delta t)^2} + \frac{c}{\Delta t}\right) W_{M,N}^n - \left(\frac{1}{(\Delta t)^2} + \frac{c}{2\Delta t}\right) W_{M,N}^{n-1}, \quad (10)$$

where $W_{M,N}^{n+1,0}$ is set to be $W_{M,N}^{n}$.

In our numerical experiments, we set M = 20 and N = 10, which turned out to be sufficient to obtain reasonably accurate numerical results with acceptable efficiency [12].

3. Numerical results and discussions

In this section, our numerical results on the relationship between the geometrical and mechanical parameters are presented and compared with the experimental and numerical results reported in [10].



Figure 3: The relationship between $w_m = \delta/h^*$ and σ_0 established by the annular sector model with $\kappa = 2$.



Figure 4: The relationship between δ and Γ established by the annular sector model with $\kappa = 2$ and $h^* = 200 nm$.

3.1. The relationship between the geometrical and mechanical parameters

Since the shape parameter r_0 is not easily obtained in physical experiments, to apply our model, we would rather introduce another shape parameter that is more easily accessible and more stable in the computation. One of such a parameter is $\kappa = 4A\lambda^{-1}$, where A and λ are the wave amplitude and the wavelength of the telephone cord buckles [11], which can be conveniently measured in experiments and can be expressed, in the annular sector model, as functions of the shape parameters r_0 and θ_0 as follows

$$\lambda = (1 + r_0) \sin \theta_0, \quad A = 2 - (1 + r_0) \cos \theta_0.$$
(11)

By choosing κ and θ_0 as independent shape parameters of an annular sector, r_0 is then given as

$$r_0 = \frac{\kappa \sin \theta_0 + \cos \theta_0 - 2}{\kappa \sin \theta_0 - \cos \theta_0}.$$
 (12)

In this subsection, we present numerical results with $\kappa = 2$, which is the value measured in Fig.2 (a) in [10]. For a given set of mechanical parameters, the mode-mix criterion is used to obtain the shape parameters $(r_0(\kappa, \theta_0), \theta_0)$, and the shape and size of the corresponding buckle is then completely determined. The numerical results on such a relationship (see Fig. 3) can now be used conversely to obtain mechanical parameters, such as the initial stress σ_0 and the interface toughness Γ_I and $\Gamma(\psi)$ (see Fig. 4), of the elastic thin film system from the shape and size parameters measured in the telephone cord buckles observed in physical experiments. Other than κ and θ_0 , another parameter we use to evaluate σ_0 is the maximum out-of-plane displacement δ , which we will take the measurements either on the whole buckling area or restricted on the connection lines while the corresponding results will be labeled as (A-S/A) and (A-S/C) respectively (see Table 1). For the convenience of comparison, we also list in Table 1 the values obtained in [10] for the initial stress σ_0 and normalized one σ_0^* , which are denoted as σ_r/σ_b and σ_r in [10], as well as the interface toughness Γ_I and $\Gamma(\psi)$ (with $\rho = 0.3$) by the three 1D models mentioned in section 1 with the corresponding maximum out-of-plane displacement δ measured in physical experiments. We notice that, in computation, it is the relationship between the normalized parameters $w_m = \delta/h^*$ and σ_0 that is actually established by our model.

It is interesting to point out here that the data on the initial stress and the interface toughness given by our model in Table 1 for the case of $h^* = 300nm$ are in fact predicted by the linear functions reconstructed by applying the least square method on the data shown in Fig. 3 and Fig. 4. The results corresponding to A-S/C match the physical experiments remarkably well, and thus justify in a way the validity of our model with the A-S/C approach.

A typical phase angle distribution along the arcs of an annular sector is

Table 1: Recovered values of the initial residual stress and interface toughness with $\kappa = 2$ by the annular sector model, compared with the data obtained with three 1D models in [10], where $w_m = \delta/h^*$.

h^*	Meas/model	δ	w_m	σ_0^*	σ_0	Γ_I	$\Gamma(\psi)$
(nm)		(μm)	(ratio)	(GPa)	(ratio)	(J/m^2)	(J/m^2)
	A-S/C	0.633	3.17	4.8	9.5	4.8	16.3
200	A-S/A	0.67	3.33	5.3	10.5	4.8	16.5
(case 1)	Str-str	0.633	3.17	4.7	5.96		9.56
	Curv-str	0.67	3.33	4.75	9.43		6.01
	Pincrc-pincrc	0.67	3.33	3.74	6.87		2.93
	A-S/C	1.47	4.9	2.14	18.8	0.4	1.58
	A-S/A	1.73	5.77	1.87	22.8	0.14	0.61
300	Straight	1.31	4.7	2.07	15.4		1.6
(case 2)	Str-str	1.47	4.9	2.18	19.1		1.8
	Curv-str	1.73	5.77	2.14	26.1		1.67
	Pincrc-pincrc	1.73	5.77	1.64	18.5		0.86



Figure 5: The phase angle of a typical telephone-cord buckles' fracture front with $\kappa = 2$, $\theta_0 = 0.81$, and $\sigma_0 = 10$.

shown in Fig. 5, where

$$\eta = \begin{cases} -\frac{\theta + \theta_0}{2\theta_0}, & r = r_0, \\ \frac{\theta - \theta_0}{2\theta_0}, & r = 1. \end{cases}$$
(13)

From this figure, we see that the fracture front is clearly not mode-I dominant. This justified the use of the mode-mix instead of the Griffith criterion in our model. Furthermore, we see that numerically $\psi < -90^{\circ}$ almost everywhere on the inner radius boundary, that means the inner radius boundary is not the exact fracture front, where the crack should be pure mode-II with $\psi = -90^{\circ}$. In addition, we notice that the error of ψ reaches the maximum in the middle of the arc and the minimum on the connection points, which could partially explain why the results produced by A-S/C are much more accurate than those by A-S/A (see Table 1).

3.2. The effect of the fracture mode parameter

It is interesting to see the actual effect of the mix mode parameter ρ on the numerical results of the proper shape parameters. Fig. 6 shows a typical numerical result for such an effect with $\kappa = 2$ and $\sigma_0 = 10$. We notice that, in general, there is essentially no effect for $\rho < 0.5$, while the effect is clearly not negligible for $\rho > 0.5$. In fact, the effect of ρ on r_0 should be considered quite significant for $\rho > 0.5$. We would also like to point out here that the result shown in Fig. 6 is typical in the sense that for various normalized initial residual stress σ_0 , the graphs are qualitatively the same, in particular, the value of the proper shape parameter θ_0 changes only slightly (within 5% when σ_0 varies from 8 to 14).



Figure 6: The relationship between ρ and the shape parameters r_0, θ_0 with $\kappa = 2, \sigma_0 = 10$.

4. Conclusion

For a given set of mechanical parameters, the morphology of the telephone cord buckles developed on an elastic thin film system can be fully determined numerically by the 2D annular sector model coupled with the mode-mix fracture criterion. This in fact establishes a relationship between the mechanical parameters of the elastic thin film system and the geometrical parameters of the telephone cord buckles. It turns out that the relationship can be used to evaluate the system's mechanical parameters by the measurements of some easily accessible shape and size parameters of the telephone cord buckles observed in physical experiments. The numerical results well match the physical experiments and justified the use of the mode-mix fracture criterion. Furthermore, for the telephone cord buckles, the mechanical parameters recovered by our 2D model are in general much more accurate than those evaluated by the three well known 1D models.

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