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Spallation of thin films driven by pockets of energy concentration

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ABSTRACT

A hypothesis is made that delamination can be driven by pockets of energy concentration (PECs) in the form of pockets of tensile stress and shear stress on and around the interface between a thin film and a thick substrate, where PECs can be caused by thermal, chemical or other processes. Based on this hypothesis, three analytical mechanical models are developed to predict several aspects of the spallation failure of elastic brittle thin films including nucleation, stable and unstable growth, size of spallation and final kinking off. Both straight-edged and circular-edged spallations are considered. The three mechanical models are established using partition theories for mixed-mode fracture based on classical plate theory, first-order shear-deformable plate theory and full 2D elasticity. Experimental results show that all three of the models predict the initiation of unstable growth and the size of spallation very well; however, only the 2D elasticity-based model predicts final kinking off well. The energy for the nucleation and stable growth of a separation bubble comes solely from the PEC energy on and around the interface, which is 'consumed' by the bubble as it nucleates and grows. Unstable growth, however, is driven both by PEC energy and by buckling of the separation bubble. Final kinking off is controlled by the fracture toughness of the interface and the film and the maximum energy stored in the separation bubble. This work will be particularly useful for the study of spallation failure in thermal barrier coating material systems.

1. Introduction

Thin solid films are found in many different applications fulfilling various roles [1] such as confinement of electric charge in integrated electronic circuits, thermal insulation in thermal barrier coatings (TBCs), and protection against corrosion, friction and wear in surface coatings. Although thin films are not usually expected to have a primary load-carrying capability, they often experience residual stresses due to the fabrication process and/or working conditions. One typical example is the in-plane compressive stress in TBCs caused by the mismatch of thermal expansion coefficient between the coating and alloy substrate. Residual stresses are a major cause of film cracks and debonding. Buckling-driven delamination is a typical example of film failure under in-plane compressive residual stress, which has been extensively studied in the last few decades. Among many others, Refs. [2–6] report studies on buckling-driven delamination with straight edges [2,4,6], circular edges [2,3], elliptical edges [2], and 'telephone cord'-shaped edges [5].

In studies on buckling-driven delamination, it is conventional to assume either a pre-existing interface crack which is larger than the critical buckling characteristic dimension or a pre-existing imperfection [3,7,8]; however, some examples of thin-film delamination show no evidence of any pre-existing interface crack or imperfection, but still display buckling behavior [9,10]. A new hypothesis was proposed by Wang et al. [11] to explain this behavior. According to this hypothesis, delamination can be driven by pockets of energy concentration (PECs) in the form of pockets of tensile stress and shear stress, with the former being dominant [9,10] on and around the interface between a thin film and a thick substrate, where PECs can be caused by a number of different processes, including thermal cooling. Based on this hypothesis, Wang et al. [11] developed an analytical mechanical model to predict several aspects of thin-film spallation failure including nucleation, stable and unstable growth, size of spallation and final kinking off. The predictions agree very well with experimental results in Refs. [9,10].

The present work aims to extend Wang et al.'s work [11] on delamination driven by PECs in two ways: First, to consider straight-edged delamination in addition to circular-edged

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Nomenclature

A	amplitude of upward deflection of film bubble
b	width of through-width straight-edged delamination
h	thickness of film
E	Young's modulus of film
$\bar{E}$	effective Young's modulus of film
G, G_I, G_{II}	total, mode I and mode II ERRs
G_{Ic}, G_{IIc}	film-substrate pure mode I and II interface fracture toughness
G_c	film-substrate mode-dependent interface fracture toughness
$\bar{G}_c$	film-substrate interface fracture toughness averaged over delamination
G_{cf}	fracture toughness of film material
M_{xB}, N_{xBe}	crack tip longitudinal bending moment and effective force
M_{rB}, N_{rBe}	crack tip radial bending moment and effective force
r, θ	radial and circumferential coordinates of circular film bubble
R_B	half-crack length of straight-edged delamination; radius of circular-edged delamination
u_0	residual strain energy density in the film
U_a	'bubble energy'; increase in combined strain energy and surface energy due to bubble separation
U_b	bending strain energy of film bubble
U_i	in-plane strain energy of film bubble
U_s	surface energy of delaminated surfaces of film bubble
U_0	strain energy of film bubble before separation
w	upward deflection of film bubble
x, y	lengthwise and widthwise coordinates of straight-edge film bubble
z	out-of-plane coordinate
α	buckling correction factor (e.g. due to initial imperfection)
β	kink-off angle
ε_x^R, σ_x^R	averaged axial relaxation strain and stress due to bending deflection
ε_r^R, σ_r^R	averaged radial relaxation strain and stress due to bending deflection
ε_0, σ_0	uniform residual compressive strain and stress in film
ν	Poisson's ratio of film
ψ	ratio of film-substrate pure mode II and I interface fracture toughness

delamination in Ref. [11]. Second, to develop analytical mechanical models for PEC-driven delamination based on the classical and the first-order shear-deformable plate mixed-mode-fracture partition theories [12–14] in addition to the analytical mechanical model [11] which was based only on the 2D elasticity mixed-mode-fracture partition theory [15–20]. The mechanical model for delamination with straight edges is developed in Section 2 while the model for delamination with circular edges is developed in Section 3. Theoretical predictions are compared with experimental results [9,10] in Section 4. Conclusions are drawn in Section 5.

2. Analytical mechanical model for delamination with straight edges

In this section, a mechanical model for delamination with straight edges is developed analytically based on the PECs hypothesis to explain several aspects of thin-film spallation failure including nucleation, stable and unstable growth, size of spallation and final kinking off. Fig. 1 shows a rectangular thin film-substrate composite material system with a through-width interface delamination of width b and of length $2R_B$. The delamination tips or the edges of the bubble are denoted by the label 'B'. The thickness of the film h is assumed so small that only in-plane residual stresses are induced in it before delamination; and the thickness of the substrate is assumed so large that it has negligible global deformation, such as bending, extension or twisting, due to residual stresses in the film. Both the film and substrate materials are assumed to be homogeneous and isotropic. The film material has Young's modulus E and Poisson's ratio ν.

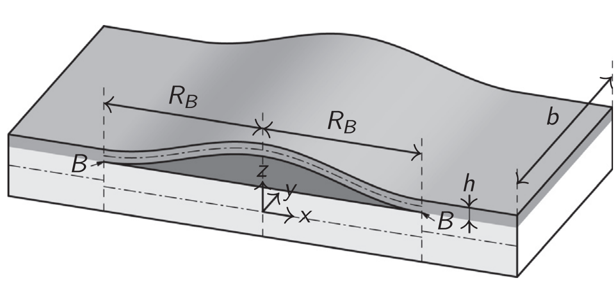

Fig. 1. A delamination bubble with straight edges.

In general, a uniaxial uniform residual stress (i.e. $\sigma_x = \sigma_0$, $\sigma_y = 0$, $\tau_{xy} = 0$) is achieved for a long film strip with the width of the film less than twice the thickness, and a plane stress model is suitable. Conversely, a biaxial uniform residual stress (i.e. $\sigma_x = \sigma_0, \sigma_y = \sigma_0$, $\tau_{xy} = 0$) is achieved when both the width and length of the film are larger than twenty times the thickness [21,22], and a plane strain model is suitable.

2.1. Nucleation of a delamination bubble, bubble energy and total energy release rate

According to the PECs hypothesis, the nucleation of PEC-driven delamination is caused by pockets of tensile stress and shear stress, with the former being dominant [9,10], on and around the interface. The details are unclear and are not considered in the present work. Once a delamination has nucleated, the strain energy of the stresses is freed and becomes the bottom surface energy of the delamination, the surface energy of the substrate underneath the bubble, and part of the strain energy in the delaminated bubble. Note that the term 'delamination bubble' is used here to differentiate it from 'delamination buckle' as the length of the bubble $2R_B$ at this stage is far shorter than the critical buckling length. In order to calculate the strain energy in the bubble, its shape is approximated to be sinusoidal and represented by

$$w(x) = \frac{A}{2}\left[1 + \cos\left(\frac{\pi x}{R_B}\right)\right] \quad (1)$$

with w representing the upward deflection and A the amplitude, as shown in Fig. 2. Clamped edge conditions at $x = \pm R_B$ are assumed

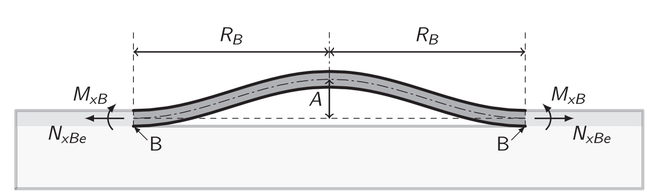

Fig. 2. Free-body diagram of a delamination bubble's oxide film.

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