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ON THE DECOHESION OF RESIDUALLY STRESSED THIN FILMS

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Abstract—The propagation of cracks in a brittle substrate, as motivated by residual stress in the film, is analyzed. The results are used to predict trends in film decohesion with film thickness, residual stress, elastic properties and substrate toughness. The analysis is based on separate determinations of the strain energy release rate and mode I/modeII stress intensities for substrate cracks parallel to the interface. Experiments are performed on a system consisting of thin films bonded to SiO_2 substrates. Comparison between theory and experiment provides knowledge of the crack growth criterion and of trends in decohesion resistance.

Résumé—Nous analysons la propagation des fissures dans un support fragile, provoquée par une contrainte résiduelle dans le film. Nous utilisons les résultats pour prévoir la tendance du film à la décohésion selon l'épaisseur du film, la contrainte résiduelle, les propriétés élastiques et la dureté du support. Cette analyse est basée sur des déterminations séparées de la vitesse de libération de l'énergie de déformation et des valeurs de la contrainte de mode I ou II pour les fissures du support parallèles à l'interface. Nous utilisons pour nos expériences un système constitué de films minces liés à des supports de SiO_2. La comparaison entre la théorie et l'expérience permet de déterminer le critère de croissance des fissures, et la tendance à la résistance à la décohésion.

Zusammenfassung—Die von Restspannungen im Film ausgelöste Ausbreitung eines Risses in einem spröden Substrat wird analysiert. Mit den Ergebnissen werden die Tendenzen der Filmablösung in Abhängigkeit von Filmdicke, Restspannung, elastischen Eigenschaften und Substratzähigkeit vorausgesagt. Die Analyse beruht auf der getrennten Bestimmung der Rate, mit der die Verzerrungsenergie freigesetzt wird, und der Mode I/Mode II-Spannungsintensitäten für Substratrisse parallel zur Grenzfläche. Experimente werden an einem System dünner Filme auf SiO_2-Substraten ausgeführt. Aus dem Vergleich von Theorie und Experiment folgen ein Kriterium für Rißwachstum und die Tendenzen im Widerstand gegen Ablösung.

1. INTRODUCTION

Residually stressed thin films are susceptible to decohesion from substrates. The decohesion mechanism depends on the sign of the residual stress (tensile or compressive) and on the presence of a stress gradient. When the stress in the film is compressive, decohesion involves buckling above an initial interface separation, followed by delamination and eventual spalling [1]. When the film is in residual tension, decohesion can initiate preferentially at specimen edges and propagate inward [2]. Substrate spalling from films in residual tension has long been of interest. Rayleigh reported in a 1917 edition of *Engineering* [3], that small spalls occurred from the surface of a glass plate coated with a thin gelatine film. The magnitude of residual stress involved and the crack paths that led to spalling were of interest to Rayleigh. More recent experimental observations [2, 4] suggest that the cracks have a strong tendency to extend into the substrate (when brittle) and propagate parallel to the interface. Typically, the crack evolves into a trajectory a few film thicknesses beneath the interface creating a spall that incorporates the film and a portion of the underlying substrate. Furthermore, edge initiated decohesion is found to become more probable as the film thickness increases [2, 4]. The present article addresses some of the fundamental mechanics involved in edge decohesion, consistent with the crack trajectory and film thickness observations.

The basis for the analysis performed in this article, and the associated interpretation, involves fracture in edge-loaded plates [5]. Superposition principles indicate that generalized edge loading generates stress intensities exactly analogous to residual stress intensities (Fig. 1)†. The decohesion problem may thus be simulated by considering the behavior of edge loaded plates. Previous studies [5] revealed that in a *homogeneous* plate containing a sub-surface crack, steady-state mode I and II stress intensities develop,

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†Note that, at step (b) in Fig. 1, a crack either in the interface or in the substrate has no effect on the stresses and thus causes no stress intensification. The stress intensity thus derives entirely from step (c).

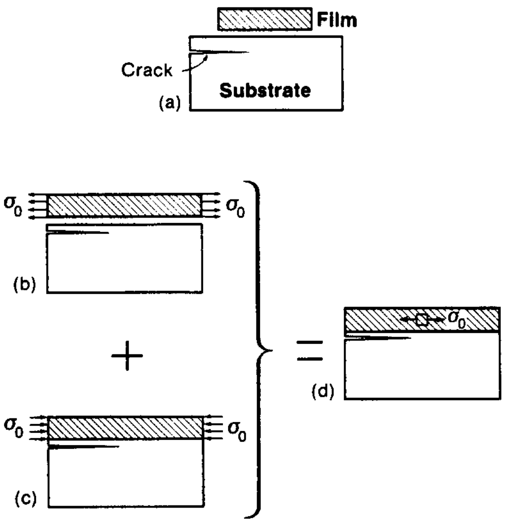

Fig. 1. A procedure for evaluating stresses and stress intensities in residually stressed systems, revealing equivalence with the edge loaded configuration: (a) unconstrained strain, (b) uniform stressing, (c) relaxation, (d) equivalent thermally stressed condition.

given by

$$K_{\rm I} = 0.43Pd^{-1/2} + 1.9Md^{-3/2}$$

$$K_{\rm II} = 0.56Pd^{-1/2} - 1.5Md^{-3/2} \qquad (1)$$

where P is the edge load, M the edge moment, d the crack depth (Fig. 2), and $K_{\rm I}$ and $K_{\rm II}$ are the mode I and mode II stress intensities, respectively. Furthermore, by systematically varying P and M on cracks having various depths, it was demonstrated that cracks tend to propagate into a trajectory with $K_{\rm II} = 0$, at a characteristic depth;

$$d^* = 2.7M/P. \qquad (2)$$

This behavior was rationalized by noting that the shear associated with the $K_{\rm II}$ component of the crack tip field continually deflects cracks until the $K_{\rm II} = 0$ condition is achieved. The present analysis extends the previous studies by considering bimaterial systems typical of practical thin film devices. Stress gradient effects are also considered and comparisons are made between plane strain and axisymmetric decohesion geometries. Combinations of analytical and numerical procedures are used to obtain the solutions. Analytical methods provide asymptotic limits for semi-infinite substrates. Complementary numerical solutions explore effects of substrate thickness, crack size and the influence of axisymmetric geometries.

The crack growth solutions are compared with crack trajectory observations obtained for a system consisting of thin films diffusion bonded to SiO_2 substrates. Implications for the adhesion of thin films are then discussed.

2. NUMERICAL PROCEDURES

Numerical computations were performed for thin films and substrates having plane and axisymmetric geometries. Initially, the trends were explored by examining a substrate 20 times the film thickness, and by constraining the lower surface of the substrate to remain planar, in order to facilitate comparisons with the analytical results for which the ratio of the substrate to film thickness, ξ, is infinite. In subsequent calculations, bending was allowed, as appropriate to the behavior of unsupported bimaterial devices, and the ratio of the substrate to film thickness, ξ, was varied between 3 and 150 to assess the effect of finite geometry.

The film was assigned a larger thermal expansion coefficient than the substrate, such that a uniform temperature decrease resulted in a residual tension of σ_0 in the film. Specifically, the thermal expansion coefficient of the substrate, α_s, was taken as zero, while that of the film, $\alpha_f > 0$. The ratio of Young's modulus of the film, E_f, to that of the substrate, E_s, was allowed to range between 0.1 and 10, while the film and substrate were assumed to have equal Poisson's ratio, $\nu = 0.3$. In some cases, edge cracks of length, a, were incorporated into the substrate, parallel to the interface and at a depth, between 1/2 to 6 times the film thickness (Fig. 2).

A finite element program† was used to determine stresses, strain energy release rates, and stress

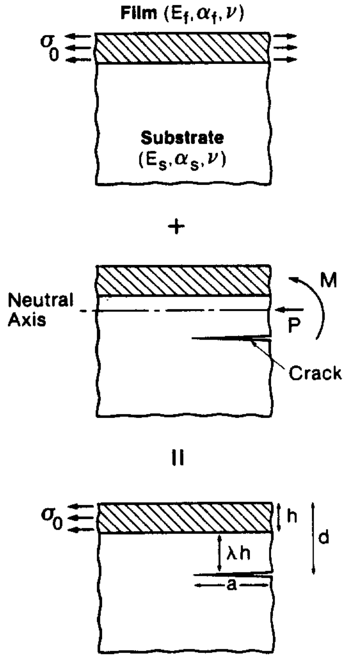

Fig. 2. Specimen and crack geometry used for analysis, indicating the equivalent force P and moment M.

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