MULTISCALE ANALYSIS FOR INTERFACIAL FRACTURES OF DUCTILE THIN FILM/CERAMIC SUBSTRATE SYSTEMS

Yueguang Wei, Haifeng Zhao and Siqi Shu

LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China

ABSTRACT

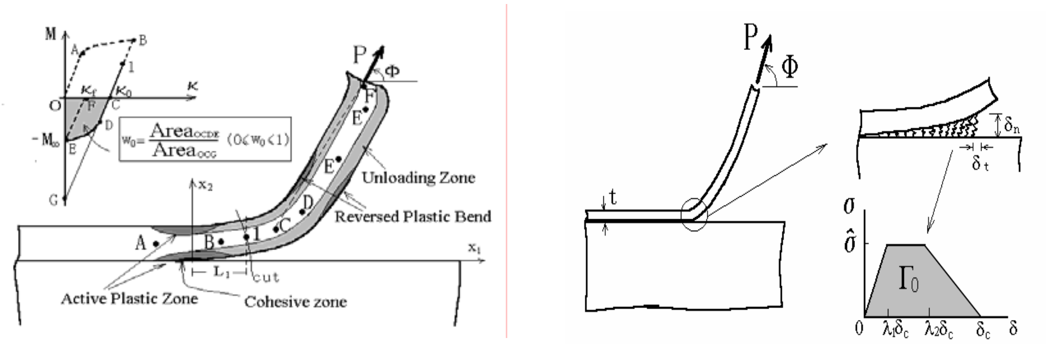
In this paper, both the cohesive zone/nonlinear bending model and the cohesive zone/plane strain elastic-plastic FE analysis model are adopted for analyzing the thin film nonlinear peeling process. Characteristics of the energy release rate are analyzed and presented. The analysis results based on both models are used to predict peeling experiment of copper thin film on the ceramic interface. Through prediction and analyses, one found that for the same experimental result, the effective simulations can be obtained based on both models, however, different material parameters are corresponded. It implies that two models are suitable for different scales. Combining the results based on both models, size effects of thin film delamination are characterized.

1 INTRODUCTION

With its particular characteristics, thin film has been widely applied to the surface and interfacial engineering areas. The material behaviors of the thin film systems mainly depend on the interfacial adhesion property (strength) between the thin film and substrate. In order to evaluate the adhesion behaviors, a simple test method, peel test, was presented and designed in fifty years ago [1]. Due to the good advantages of the test method, such as simply operating, the test method has been widely applying to many research regions [2-4]. Specifically, when both the thin film and substrate are elastic materials, the interfacial adhesion toughness can be obtained through directly measuring peeling force in peel test. However, with development of the research and application, it has been noted that when thin film is a ductile material, the measured peeling force is often much larger than the interfacial adhesion toughness. The phenomenon is come from the plastic dissipation due to plastic loading and unloading deformation of the thin film. In order to model the peeling force (or energy release rate) increase due to plastic dissipation, Kim and his collaborators [5,6] presented a bending model to predict the plastic dissipation during the process of the thin film peeling. Within the following decade after bending model was presented, most analyses related to the ductile thin film peeling adopted the bending model of Kim et al, e.g., [7,8]. However, Wei and Hutchinson [9] adopted a different method from that of Kim et al in analyzing the elastic-plastic thin film peeling problems. In their analysis, the thin film delamination process was simulated by using the two-dimensional elastic-plastic finite element method (FEM), except the detached part of thin film, which was described still by bending model. They obtained a different result from that based on the bending model, qualitatively and quantitatively. In the present research, in order to explore the connection of bending model solution with elastic-plastic FEM solution, both the cohesive zone/nonlinear bending model and the cohesive zone/plane strain elastic-plastic FE analysis model are adopted for analyzing the thin film nonlinear peeling process. By comparing the both model results, a primary connection of both the bending model and the two-dimensional FE analysis model is obtained. Furthermore, a multiscale model for the interfacial fractures of the ductile thin film/ceramic substrate systems will be presented.

2 BENDING MODELS AND DELAMINATING CRITERIA IN PEEL TEST

Delaminating process of elastic-plastic thin film in peel test can be described by figure 1(a). The thin film undergoes the delamination and plastically loading and unloading process under the act of the peel force P along some direction angle Φ. The cross-section of the thin film is from a stressing-free state to the loading and unloading processes, as described by OABCDEF, in sketch figure 1(a).



(a). Peel test (b). ($\Gamma_0, \hat{\sigma}$) criterion

Figure 1: Peel test sketch figure (a) and the cohesive zone simplified model (b).

The process of the ductile thin film peeled and delaminated along substrate interface can be characterized by the double-parameter criterion (for elastic delamination case, single-parameter criterion is needed). Two independent parameters are needed to characterize the main characters here, the interfacial adhesion property and the plastic dissipation of the system. In the present research, a double-parameter criterion, i.e. the cohesive zone model will be used for describing the elastic-plastic peeling process, which is described in figure 1 (b). The independent parameters of the model are $(\Gamma_0, \hat{\sigma})$, where Γ_0 is the interfacial adhesion toughness, $\hat{\sigma}$ is the interfacial separation strength. Another parameter of the model- relative separation displacement at the tip, $\delta_c = \sqrt{\delta_{tc}^2 + \delta_{nc}^2}$ can be expressed with $(\Gamma_0, \hat{\sigma})$. For the thin film peeling process, the relation between the peeling force P per unit width of thin film (or energy release rate of system) and the interfacial adhesion toughness, as well as the geometrical and physical parameters of thin film and substrate is usually concerned by investigators. Under steady-state delamination condition, the relation can be written as:

$$P(1-\cos\Phi) = \Gamma_0 \quad \text{(elastic)}; \quad P(1-\cos\Phi) = \Gamma_0 + \Gamma^P \quad \text{(elastic-plastic)} \tag{1}$$

where Γ^P is the plastic dissipation. Based on the stress-strain analysis for thin film bending model, one can obtain the fundamental relations of the thin film undergoing the nonlinear bending, furthermore, one can also obtain the plastic dissipation Γ^P, as given in next section. On the other hand, through plane strain elastic-plastic FE analysis for thin film peeling process, one can also obtain the plastic dissipation through numerical calculations.

3 FUNDAMENTAL RELATIONS

Kim and Aravas [5] derived the fundamental relations for thin film peeling process based on the bending model for thin film under the incompressible conditions ($\nu = 1/2$). The rigorous derivation based on the general case of the compressible elastic-plastic conditions is given by Wei and Hutchinson [10]. The relations of moment and curvature respectively for elastic, plastic and unloading cases can be dictated as follows:

$$\frac{M}{M_0}=\frac{2\kappa}{3\kappa_e}\,;\quad \frac{M}{M_0}=\{\frac{2}{3}-\frac{2}{N+2}\gamma\}\frac{1}{(\kappa/\kappa_e)^2}+\frac{2}{N+2}\gamma(\frac{\kappa}{\kappa_e})^N\,;\quad \frac{M}{M_0}=\frac{2}{3}\frac{\kappa-\kappa_0}{\kappa_e}\,, \quad (2)$$

and curvature relation: $\kappa=\sqrt{[1-\cos(\Phi-\theta)]\frac{2P}{B}+(1-w_0)\kappa_0^2}\,,\ \ \theta_B\approx\theta_{tip}\le\theta\le\theta_C\,.$ (3)

where $M_0=\frac{3}{2}M_e$ is the limit bending moment for elastic-perfectly plastic material; M_e and κ_e are the elastic limit moment and elastic limit curvature, respectively,

$$M_e=\tfrac{2}{3}M_0=\frac{\sigma_Y t^2}{6\sqrt{1-\nu+\nu^2}}\,,\quad \kappa_e==\frac{2(1-\nu^2)\sigma_Y}{Et\sqrt{1-\nu+\nu^2}}\,,$$

$$\gamma=2\sqrt{\tfrac{1}{3}(1-\nu+\nu^2)}^{\,1-N}(1-\nu)^N \quad (4)$$

$B=Et^3/12(1-\nu^2)$ is the bending modulus; w_0 ($0\le w_0\le 1$) is defined in figure 1(a) which characterizes the inversely plastic behavior (or Bauschinger effect); θ_{tip} is the crack tip slope angle at thin film delamination; N is material strain hardening exponent. For incompressible material $\nu=0.5$ and $\gamma=1$, expression (2) comes to the result of Kim and Aravas [5].
Suppose that substrate is rigid or Young's modulus of substrate is much larger than that of thin film, by means of formulas (2) ($M-\kappa$ relations in sketch of figure 1(a)), one can obtain the plastic dissipation relation through calculating the area within the circuit OABCDEO under $M-\kappa$ curve,

$$\Gamma^P=\tfrac{1}{2}M_e\kappa_e-\tfrac{1}{2}M_B(\kappa_B-\kappa_0)+(\frac{2}{3}-\frac{2}{N+2}\gamma)M_0(\kappa_e-\frac{\kappa_e^2}{\kappa_B})$$

$$+(2\gamma/(N+1)(N+2))M_0(\kappa_B^{N+1}/\kappa_e^N-\kappa_e)+\tfrac{1}{2}B\kappa_0^2 w_0 \quad (5)$$

When Wei-Hutchinson model is adopted, i.e. the total problem of the thin film peeling is divided into two sub-problems, referring to figure 1(a). Considering a section 1 at which the thin film is cut off, on the right side of the section 1, thin film peeling is still treated with the nonlinear bending model, on the left side of the section 1, thin film peeling and the substrate deformation is analyzed by using the plane strain FE analysis model based on the conventional elastic-plastic flow theory,

$$\dot{\sigma}_{ij}=D_{ijkl}\dot{\varepsilon}_{kl} \quad (6)$$

where elastic-plastic modulus tensor can be expressed by

$$D_{ijkl}=\frac{E}{1+\nu}\left\{\delta_{ik}\delta_{jl}+\frac{\nu}{1-2\nu}\delta_{ij}\delta_{kl}-\frac{(3/2)\Omega}{[1+(2/3)(1+\nu)H/E]\sigma_e^2}\sigma'_{ij}\sigma'_{kl}\right\} \quad (7)$$

where σ'_{ij} is devitoric stress, $\sigma_e = \sqrt{3\sigma'_{ij}\sigma'_{ij}/2}$ is effective stress, Ω =1 for plastic case, otherwise Ω =0. H is plastically hardening modulus and for strain hardening exponential materials

$$H = E\left\{(1/N)\left(\sigma_e/\sigma_Y\right)^{1/N-1} - 1\right\}^{-1} \tag{8}$$

For thin film steady-state delamination with velocity V along x_1-reverse direction

$$(\dot{\sigma}_{ij}, \dot{\varepsilon}_{ij}) = V\left(\frac{\partial \sigma_{ij}}{\partial x_1}, \frac{\partial \varepsilon_{ij}}{\partial x_1}\right), \tag{9}$$

one has the constitutive equation $\partial\sigma_{ij}/\partial x_1 = D_{ijkl}\partial\varepsilon_{kl}/\partial x_1$ (10)

For both the cohesive zone/nonlinear bending model and the cohesive zone/plane strain elastic-plastic FE analysis model, the parameter relation of the normalized energy release rate with independent parameters can be written as

$$P(1-\cos\Phi)/\Gamma_0 = f_1(E/\sigma_Y,\ \hat{\sigma}/\sigma_Y,\ N,\ \nu,\ t/\delta_c,\ w_0,\ \Phi) \tag{11}$$

Alternatively, above solution form can be expressed through introducing a length parameter which is taking as the length normalizing quantity, one has

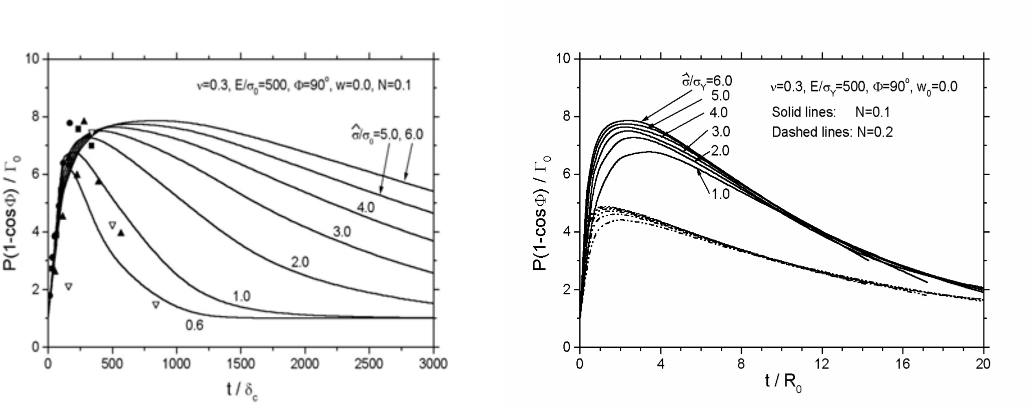
$$P(1-\cos\Phi) = f_2(E/\sigma_Y,\ \hat{\sigma}/\sigma_Y,\ N,\ \nu,\ t/R_0,\ w_0,\ \Phi) \tag{12}$$

where
$$R_0 = E\Gamma_0/3\pi(1-\nu^2)\sigma_Y^2 \tag{13}$$

is the introduced length parameter, characterizing the plastic zone size near the crack tip in small scale yielding fracture. One can easily set up a relationship between δ_c and R_0 by calculating the shadow zone area of figure 1(b) and by using the definition of R_0 in (13).

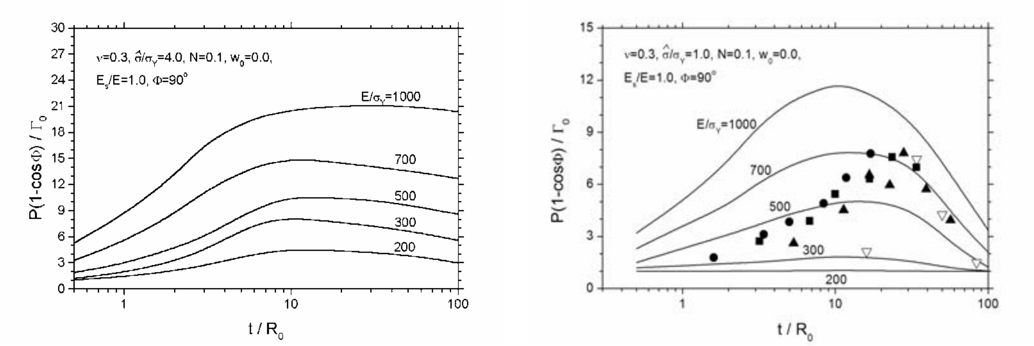
4 MODEL SOLUTIONS AND COMPARISON WITH EXPERIMENTS

Figure 2(a) and (b) show the relationships between the normalized peel force (energy release rate) and the normalized thin film thickness based on the cohesive zone/bending model. From figure 2, the peel forces increase sharply with increasing film thickness when film thickness is very small, and obtain the maximum values quickly, then decrease as film thickness increases. Figure 3(a) and (b) show the relationship between the normalized peel forces with the normalized film thickness based on the cohesive zone/plane strain elastic-plastic FE analysis model for the cases of the high and weak separation strength, respectively. Comparing with bending model, similarly, the results based on the plane strain elastic-plastic FE analysis model display a maximum value, however the normalized film thickness at the maximum point is much larger than that of bending model. Figure 4 shows the experimental results of peel force relation with thin film thickness for the Cu/ceramic system and for four different interfacial treatments. Comparisons of model results with the experimental results show in figure 2(a) and figure 3(b).



(a) (b)

Figure 2: Results based on the cohesive zone/bending model. (a) The separation displacement is taken as the normalizing length quantity. Compare modeling results with experimental results[11]. (b) R_0 is taken as the normalizing quantity.



(a) (b)

Figure 3: Results based on the cohesive zone/plane strain elastic-plastic FE analysis model. (a) For high separation strength case and (b) for weak separation strength case and comparing modeling results with experimental results[11].

5 DISCUSSIONS AND CONCLUSIONS

In last section, the solutions based on the cohesive zone/bending model and the cohesive zone/plane strain elastic-plastic FE analysis model have been calculated and compared with an experimental results. From analyses, different length parameter values of R_0 were corresponded on both model results if both model results are considered reliably. R_0 value of bending model is obviously larger than that of the FE analysis model. From (13), the larger R_0 value corresponds to the larger interface fracture toughness Γ_0. This implies that the bending model corresponds to the larger cohesive zone size, and therefore implies that the bending model is most suitable for a large scale thin film peeling problem. Comparably, the plane strain elastic-plastic FE analysis model is most suitable for a small scale thin film peeling problem. Thinkably, strain gradient plasticity theory[12] will correspond to the smallest Γ_0 value and is suitable for a micron scale thin film peeling problem.

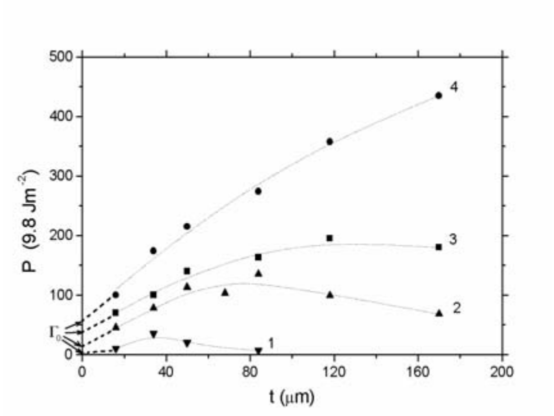


Figure 4: Experimental results of the peel force variation with film thickness t from [11] for Cu thin film delamination along ceramic substrate for four different interfacial treatments.

Through analyses for thin film peeling problems based on the bending model and the FE analysis model and comparison with experimental results, the following conclusions are obtained. (1) Adopting the bending model and considering the crack tip opening displacement as the normalizing quantity, the effects of the interface separation strength on the curves of energy release rate can be separated clearly. (2) Adopting the plane strain elastic-plastic FE analysis model can effectively model the thin film peeling experimental result, however the corresponding material parameter values are different from those of the bending model. (3) The different modeling results based on both models describe that they are suitable for different scale peeling problem.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (Grant No. 19925211), and jointly supported by "Bai Ren Plan" of Chinese Academy of Sciences.

References

1. Spies G.J. (1953). *J. Aircraft Eng.*, 25, 64.
2. Feliu-Baez R, Lockhart H.E., Burgess G. (2001). *Packaging Tech. Sci.*, 14, 63.
3. Choi J.W., Oh T.S. (2001). *J. Adhe. Sci. Tech.*, 15, 139.
4. Asai H., Iwase N., Suga T. (2001). *IEEE Trans. on Adv. Packaging*, 24, 104.
5. Kim K.S., Aravas N. (1988). *Int. J. Solids Struct.*, 24, 417.
6. Kim J., Kim K.S., Kim Y.H. (1989). *J. Adhe. Sci. Tech.*, 3, 175.
7. Kinloch A.J., Lau C.C., Williams J.G. (1994). *Int. J. Fracture*, 66, 45.
8. Moidu A.K., Sinclair A.N., Spelt J.K. (1998). *J. Testing Evalu.*, 26, 247.
9. Wei Y., Hutchinson J.W. (1998). *Int. J. Fracture*, 93, 315.
10. Wei Y., Hutchinson J.W. (2003). In *Encyclopedia of Comprehensive Structural Integrity*, 8, eds. Gerberich W.W. and Yang W., Chapter 5, Elsevier Science Publisher, 181.
11. Park, Y.B., Park, I.S., Yu, J.(1999). *Mater. Sci. Engin.* A266, 261.
12. Fleck N.A., Hutchinson J.W.(1997). *Adv. Appl. Mech.* 33, 295.