MULTI-SCALE CHARACTERIZATIONS FOR DUCTILE THIN FILM DELAMINATION

YUEGUANG WEI[1] and GUANSHUI XU[2]
[1]*LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China*
[2]*Department of Mechanical Engineering, University of California at Riverside, CA 92521*

1. Introduction

The interfacial fracture behavior of a structured material, such as a thin film/substrate system, is governed by processes occurring over a diverse range of length scales. Most models of the fracture processes, however, usually focus on the process at a limited range of length scales. Continuum models based on elastic, elastic-plastic, and recently developed strain gradient constitutive relations are appropriate for the analysis of the macro-/microscopic mechanical response of solids, but they do not accurately represent the underlying fundamental deformation mechanism of crystal defects such as nucleation and motion of discrete dislocations and slip of grain boundaries. On the other hand, the discrete/continuum models, such as the discrete dislocation theory, may be capable of accounting for the fundamental dislocation mechanisms in the deformation and fracture process, but at the present stage of the development, this kind of model is limited to the consideration of nominally elastic behavior (i.e., relatively small or non-existent dislocation densities) at very small scale. The multiple-scale approaches toward materials modeling have led to a wealth of understanding of materials mechanical behavior within each domain of model's applicability. However, it is still of central importance to address the linkage between the models at the different length scales in order to develop mechanism based modeling of mechanical behavior of materials.

In this paper, we generalize our previous multiscale model (Wei and Xu, 2005) that is built upon the elastic-plastic and strain gradient models for plastic deformation at the macro-scale and the discrete dislocation for plastic deformation at the submicron scale

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to an analysis for the thin film delamination. In our model, we attempt to establish the linkage between these two models to address the large disparity between the relevant length scales involved in the ductile thin film delaminating processes at the interfacial crack tip.

For the macroscale analysis model for ductile thin film delamination, we shall use a two-parameter criterion to characterize the ductile fracture process as usually for elastic-plastic fracture analyses (Betegon and Hancock, 1991; O'Dowd and Shih, 1991; Xia et al., 1993; Tvergaard and Hutchinson, 1993; Wei and Wang, 1995a; 1995b). The two-parameter criterion adopted here will be a modified elastic-core model (or dislocation-free zone model, or called SSV model, refs. Suo et al., 1993 and Beltz et al., 1996). The ductile thin film will be treated with a strain gradient plasticity material (Fleck and Hutchinson, 1997; Gao et al., 1999), while the substrate is an elastic material. On the discrete dislocation model, there have been many researches related with the subject (Rice and Thomson, 1974; Lin and Thomson, 1986; Rice, 1992; Hsia et al., 1994; Xu and Argon, 1995; 1997; Wang, 1998; Mao and Li, 1999; Yang et al., 2001). We shall investigate dislocation shielding effect on the thin film delamination considering an elasticity mixed mode K-field including several discrete dislocations. The K-field and its radius will be related to the macroscopic crack-tip fracture toughness.

2. Model Descriptions

A linkage model for the thin film delamination is presented, as shown in figure 1. The entire description of thin film delamination should consist of both the macroscopic interface fracture process and the microscopic interface fracture process. These interface fracture characteristics can be described by using the continuum model and the discrete dislocation model, respectively, as sketched in figures 1(a), 1(b) and 1(c). Figure 1(a) and 1(b) are the thin film peeling macroscale model and delaminating macroscale model, respectively. Both macroscale models corresponding to the scale level which is larger than a micron or a sub-micron can be characterized using the conventional continuum model, i.e., the conventional elastic-plastic theory or the strain gradient theory. In this scale, with increasing loading there exist three regions around the interface crack tip: the elastic zone far away from the tip, the strain gradient dominated zone very near the crack tip and the plastic zone between the elastic zone and the strain gradient zone. In order to describe the multi-scale problem clearly, an elastic core model, or a modified SSV model is adopted here, as shown in figure 1(a) and 1(b). This model is an improvement on the conventional SSV model (Suo et al., 1993), which supposed that near the growing crack tip and the crack surface a dislocation-free zone strip exists with an infinite length. In the elastic core model or the modified SSV model, an elastic core

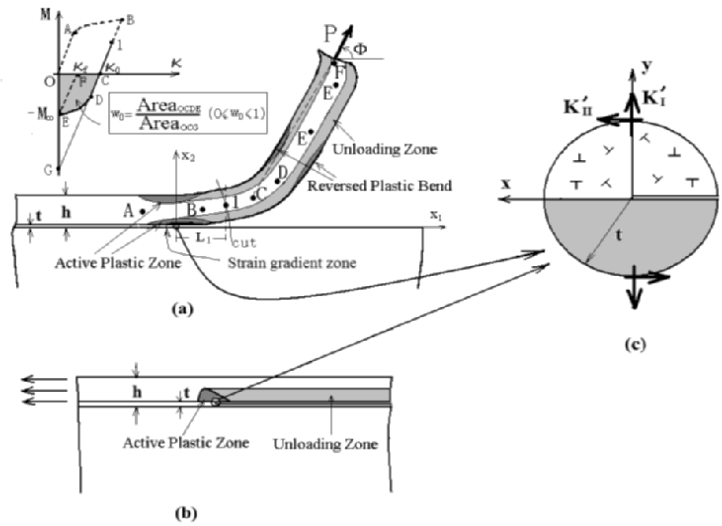

Figure 1. Multi-scale model for thin film delemination.

always surrounds crack tip during crack advance. Under steady-state crack growth condition, a semi-infinite elastic strip around the crack surface is left behind the crack tip. The radius of the elastic core (or thickness of the elastic layer), **t**, can be taken as a model parameter (Wei and Hutchinson, 1997, 1999). Within a much small scale which is smaller than a micron or sub-micron, the interface fracture behaviors will be predicted by using the discrete dislocation theory, as shown in Figure 1(c). With increasing load, dislocation nucleates and emits from the crack tip, and discrete dislocations exist (keep in equilibrium) within the region. The key problems are noted here: what is the discrete dislocation number in equilibrium or in limit equilibrium? What is the effective size of the discrete dislocation region, t? In addition, what are the macro-/microscale linkage conditions, i.e., the outer boundary conditions of the discrete dislocation model, or the inner boundary conditions of the continuum model? A treatment in the present study, the macroscopic analysis results will be taken as the outer boundary conditions for microscopic problem. The key point is to determine the intersection radius between microscopic problem and macroscopic problem. We shall study the problems in the present research.

3. Thin Film Delaminating (peeling) Analysis Using the Continuum Model

Specifically, we shall focus our attention on the thin film peeling analyses, and corresponding model has been given in figure 1(a). Using the modified SSV model and the mechanism-based strain gradient (MSG) plasticity flow theory (Gao et al., 1999; Huang et al., 2000), the relations of the normalized total energy release rate (or the normalized peel force) with the material parameters and the model parameter under steady-state delamination of thin film can be written through dimensional analysis,

$$\frac{P(1-\cos\Phi)}{G_0'} = f\left(\frac{E}{\sigma_Y}, \nu, N, \frac{h}{R_0}, \frac{l}{R_0}, \frac{R_0}{t}\right) \tag{1}$$

Where the length parameter l describes the strain gradient effect, t is the elastic core size, or intersection radius of microscopic with macroscopic fields to be determined; a length parameter R_0 is defined as follows

$$R_0 = \frac{EG_0'}{3\pi(1-\nu^2)\sigma_Y^2} \tag{2}$$

which is the plastic zone size in small scale yielding. G_0' is the macroscopic fracture toughness at tip. E is the Young's modulus and ν is Poisson's ratio. For simplicity, we consider that the Young's modulus and Poisson's ratio of substrate material are the same as those of thin film. Other parameters are defined in figure 1(a). Through finite element numerical simulation by using the MSG strain gradient theory, the detailed parameter relation (1) is given in figure 2 for several parameter values. The numerical process is similar to that by Wei et al. (2004). From figure 2, the variation of the normalized energy release rate is very sensitive to the elastic core size and length parameter R_0. For the typical metal materials, the value of R_0 is about one micron. Therefore, when elastic core size of the macroscopic model is taken as around submicron, the normalized energy release rate is much sensitive to the value of the elastic core size.

In order to determine the remote boundary condition for microscopic fracture analysis, the macro-scale crack tip solution is equivalently expressed into a standard interface K-field,

$$G_0' = \tfrac{1}{2}(1-\beta_D^2)\left(\frac{1-\nu^2}{E} + \frac{1-\nu_s^2}{E_s}\right)(K_I'^2 + K_{II}'^2) \tag{3}$$

$$\tan\Psi = \frac{\sigma_{12}}{\sigma_{22}} = \frac{\mathrm{Im}[(K_I' + iK_{II}')L_0^{i\varepsilon}]}{\mathrm{Re}[(K_I' + iK_{II}')L_0^{i\varepsilon}]} \tag{4}$$

where Ψ is the mode mixity, L_0 is a reference length, and

$$\sigma_{22} + i\sigma_{12} = (K_I' + iK_{II}')(2\pi r)^{-1/2} r^{-\varepsilon} \tag{5}$$

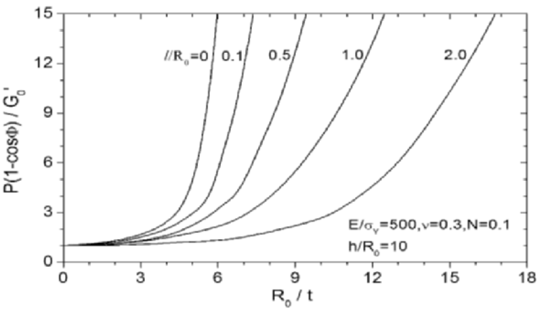

Figure 2. Macron scale model solution of the normalized energy release rate vs. thin film thickness.

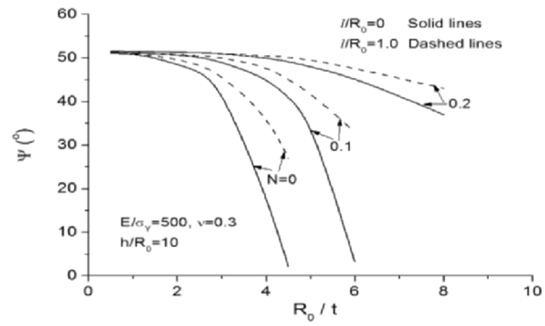

Figure 3. Variation of mode mixity with normalized thin film thickness.

$$\varepsilon = \tfrac{1}{2}\ln\left(\frac{1-\beta_D}{1+\beta_D}\right), \quad \beta_D = \tfrac{1}{2}\frac{\mu(1-2\nu_s) - \mu_s(1-2\nu)}{\mu(1-\nu_s) + \mu_s(1-\nu)} \tag{6}$$

For $E_s = E$ and $\nu_s = \nu$, then $\beta_D = 0$ and $\varepsilon = 0$, one has

$$G_0' = \frac{(1-\nu^2)(K_I'^2 + K_{II}'^2)}{E}, \quad \tan\Psi = \frac{K_{II}'}{K_I'} \tag{7}$$

The mode mixity variation with other parameters is calculated and the result is shown in figure 3. From figure 3, the mode mixity tends to mode I case with increasing the value of R_0 / t. Especially for conventional metals which are with weak hardening property. Therefore, we can approximately consider a Mode I crack field $(K_I', K_{II}' << K_I')$ exerted on the remote boundary of the micron scale model (the elastic interface fracture including discrete dislocations).

4. Fracture Analyses using the Discrete Dislocation Model

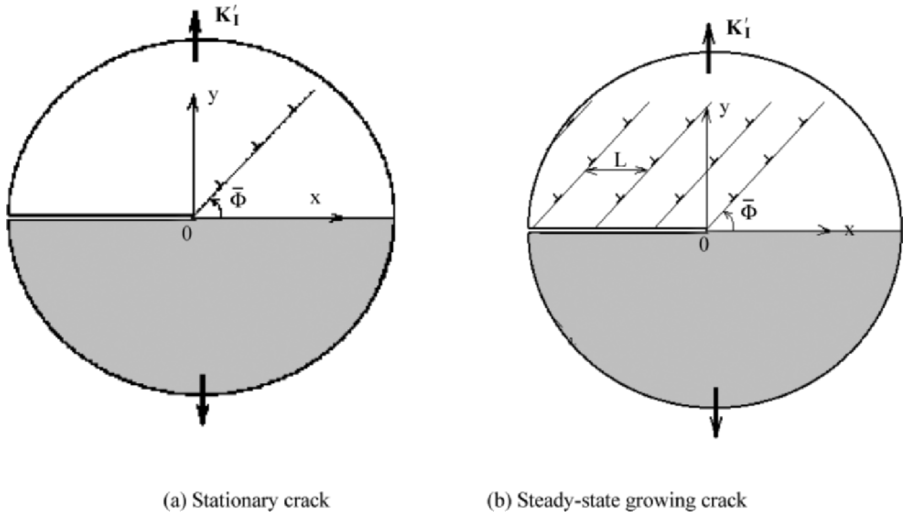

Figure 4. Dislocation slip models for interface crack.

As discussed above, the macroscopic fracture process is accompanied by a microscopic fracture process within the submicron zone near the crack tip. For the microscopic fracture analysis, the discrete dislocation theory is adopted here. The simplification model has been presented previously, as shown in figure 1(c), and as discussed above, we shall approximately consider a mode I field exerted on the remote boundary. The problem is characterized by figure 4 (a) and (b) for stationary and steady-state crack growing, respectively. The continuum solutions discussed above, a K_I' field, can be obtained based on the strain gradient theory and formula (7). The key problem here is how to properly select the radius of the outer boundary, t. The t value will be determined through bridging the continuum result with the micro-scale analysis result after the discrete dislocation analysis. In order to analyze crack growth behavior in micro-scale influenced by the discrete dislocations, as usual, a typical kind of the discrete dislocation arrangements will be considered, as shown in figure 4 (a), or (b). The possibility of putting the greatest numbers of dislocations within the region $0 < r < t$, will be investigated (corresponding to the limit equilibrium state for each dislocation), where r is polar coordinate. The arrangement of the discrete dislocations is according to the dislocation equilibrium status: $-1 \le f_d / f_d^c \le 1$, where f_d is dislocation force, $f_d^c = \sigma_f b$ is referred to as the lattice frictional resistance, σ_f and b are the critical shear strength along the slip plane and Burgers vector, respectively. For $f_d = f_d^c$, dislocation is in the limit equilibrium state. The limit equilibrium state will be considered in the present research. It is worth noting that Lin and Thomson (1986) obtained the dislocation force formulations and the dislocation shielding effect formulations (solutions), so we can directly base on the Lin and Thomson's formulations to analyze the interaction of crack with discrete dislocations.

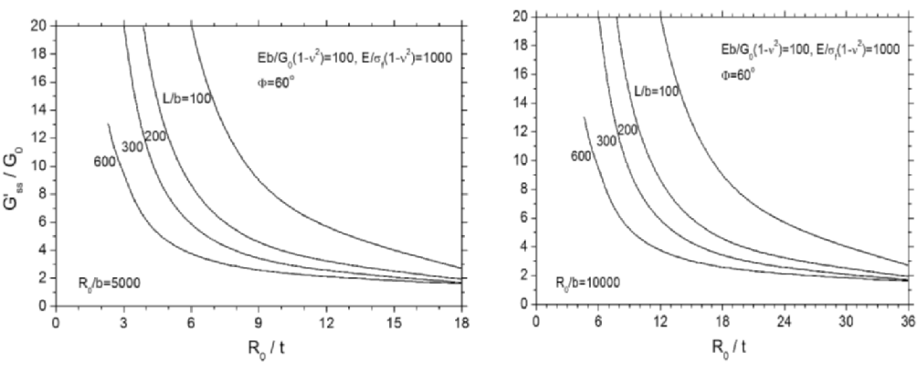

Figure 5. Ratio of the macron crack tip toughness to the micron crack tip toughness.

The macroscopic fracture solutions for crack steady-state growth have analyzed and obtained in section 3. Here we shall focus our attention on the microscopic fracture analysis. We have considered the possibility of existing discrete dislocations along a slip plane within the submicron scale in above sections. Let’s further investigate the existing possibility of dislocation distributed pattern as crack grows under the steady-state condition, i.e., investigate whether the dislocation pattern can be kept around the crack surface, accompanied by the new slip plane produced near crack tip (see figure 4(b)).

Here suppose that the space between slip planes is equal to L. There exists a question: what is the size of the slip plane space L? According to the experimental observation and measurement by Mao and Evans (1997), L is about 1 micron, or submicron. By calculating the dislocation forces for each dislocation or the dislocation pattern, one can examine the stability of the dislocation pattern (figure 4(b)), i.e., check whether or not $| f_d / f_d^c | \leq 1$ is met as crack grows. After the condition has been confirmed, we obtain several results about toughness ratio. Figures 5(a) and (b) show the toughness ratio variations with the normalized elastic core radius, t, for several normalized material parameters $Eb / G_0 (1 - \nu^2)$, R_0 / b, L / b, $E / \sigma_f (1 - \nu^2)$. The toughness ratio $G'_{ss} / G_0 = G'_0 / G_0$ describes the ratio of the macroscopic crack tip toughness to the micron crack tip toughness.

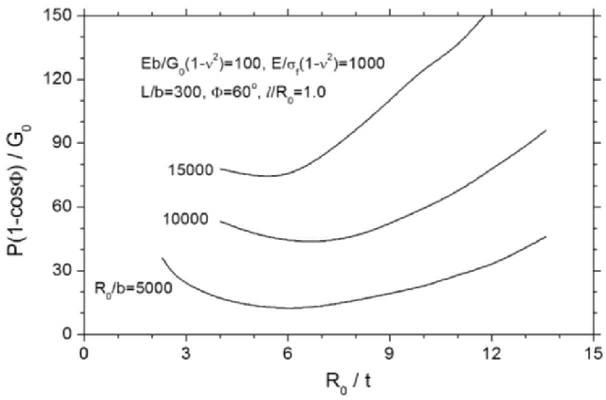

Figure 6. Total energy release rate normalized by the micron scale crack tip toughness vs. the normalized “elastic core” size. There exists the stationary value region.

5. The selection of “elastic core” size

We can directly calculate the energy release rate changing with the selection of the “elastic core” size t for the steady-state delamination. By increasing the discrete dislocation number along a slip plane, the corresponding “elastic core” size increases. From Figure 5, the toughness ratio from microscopic theory increases with increasing the “elastic core” size, however, it is just inverse feature from macroscopic theory (from figure 2). In order to conveniently compare both microscopic and macroscopic cases, the results shown in figure 5 and figure 2 will be used to plot the normalized total energy release rate:

$$\frac{P(1-\cos\Phi)}{G_0} = \frac{P(1-\cos\Phi)}{G'_{ss}}\frac{G'_{ss}}{G_0} = \frac{P(1-\cos\Phi)}{G'_0}\frac{G'_{ss}}{G_0} \tag{8}$$

where $G'_0 = G'_{ss}$ from present analysis. Figure 6 shows the normalized total energy release rate varying with the "elastic core" size for three parameter values of R_0 / b. Curves in figure 6 are come from both microscopic analysis results and macroscopic analysis results shown in figure 2 and figure 5 by using formula (8). From figure 6, around the value, $R_0 / t \approx 6$, the variation of the total energy release rate takes stationary value, or insensitive to the selection of t value, so the proper selection of the elastic core size is about $t \approx R_0 / 6$. For conventional metal materials, $R_0 \approx 1\mu$m, so the elastic core size is at about submicron scale.

6. Conclusion

A complete delaminating process for ductile thin film has been presented in the present research. The macroscopic delaminating process has been analyzed based on the strain gradient plasticity theory. The thin film delaminating characteristics, such as the interface fracture toughness, the plastically shielding effect etc. have been investigated. By using the discrete dislocation theory, microscopic fracture process has been analyzed, and a bridging model has been developed. In the bridging model, the macroscopic fracture solution (equivalent interface K field) has been taken as the outer boundary condition of the microscopic fracture problem. The shielding effect of discrete dislocations on the crack growth has been studied. The selection of the elastic core size t, the intersection radius between macron scale and micron scale, has been determined from a stationary value theorem that the total energy release rate should take the stationary value. According to present analysis, we have obtain elastic core size $t \approx R_0 / 6$, in submicron level.

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