

# SPECTRAL SCHEME FOR ANALYSIS OF DYNAMIC DELAMINATION OF A THIN FILM

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## ABSTRACT

We present a spectral scheme specially developed to simulate the delamination of thin films subjected to dynamic anti-plane shear loading conditions. The numerical scheme is based on an exact spectral representation of the elastodynamic relations between the interface traction stress, the interface displacement and the transient traction applied along the surface of the thin film. The formulation incorporates the contribution from all the wave reflections taking place in the film and the effect of the material mismatch between the film and the substrate, both of which are assumed to be linearly elastic. Its implementation involves an explicit time stepping scheme with, for each time step, the use of Fast Fourier Transform (FFT) to link the spatial and spectral domains, and the computation of a convolution over the past displacement and stresses history. A low-pass filter is also used in order to improve the stability of the method without affecting the precision of the results. We apply the developed scheme to thin film delamination problems involving non-propagating and propagating interface cracks. In the non-propagating case, special focus is placed on extracting the time-dependent stress intensity factor and on relating its evolution to the complex wave reflection events taking place in the thin film. In the propagating crack problem, we investigate the effect of the wave reflections off the film surface on the subsonic and intersonic crack motion.

## 1 INTRODUCTION

Thin film applications are increasingly prevalent in engineering applications, and interfacial adhesion is a critical parameter governing the mechanical behavior and reliability of a thin film on a substrate. Understanding the possible initiation and propagation of interface flaws is therefore important in the design of such structures. Among the various techniques used to investigate the interfacial strength of thin film structures, the recently introduced laser-induced delamination method (Wang *et al.* [1,2]) presents the advantage of not involving any contact with the thin film and therefore provides an attractive alternative to more conventional tests such as the peel or indentation tests.

The analysis supporting the dynamic delamination tests has so far relied on 1-D wave propagation (Wang *et al.* [1,2]). However, the one-dimensionality of the stress solution breaks down in the presence of a pre-existing flaw along the interface or as soon as the initial failure takes place, and more advanced tools are thus needed. One of the most successful additions to the list of numerical schemes for dynamic fracture simulations, the spectral formulation has been shown (Geubelle and Breitenfeld [3]) and (Breitenfeld and Geubelle [4]) to be very efficient to tackle fundamental dynamic fracture events taking place along the interface between two semi-infinite media. Our objective in this project is to develop and implement a spectral formulation for the thin film delamination problem. In this initial “feasibility study”, we consider the simpler mode III problem, the case of the transient anti-plane shear loading of the film/substrate system.

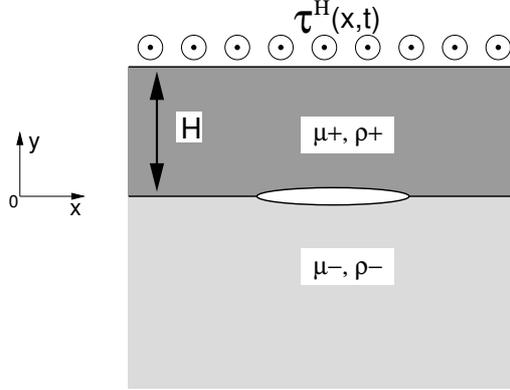


Figure 1: Geometry of the mode III interface fracture problem.

## 2 SPECTRAL FORMULATION

As shown in Figure 1, the problem at hand involves a dynamic fracture event that takes place at the interface between a semi-infinite substrate and a thin film of thickness  $H$  loaded along its external boundary ( $y = H$ ) by an arbitrary space- and time-dependent anti-plane shear traction  $\tau^H(x, t)$ . Both materials are assumed to be linearly elastic (with shear modulus  $\mu$  and density  $\rho$ ) and to have an infinite width. Inside both domains, the only non-vanishing displacement component  $u_z(x, y, t)$  satisfies the scalar wave equation

$$c_s^2(u_{z,xx} + u_{z,yy}) = \ddot{u}_z, \quad \text{with} \quad c_s = \sqrt{\frac{\mu}{\rho}}. \quad (1)$$

Taking a Fourier transform with respect to  $x$  and a Laplace transform with respect to time yields

$$\hat{\Omega}_{,yy} = q^2 \alpha_s^2 \hat{\Omega}, \quad \text{where} \quad \alpha_s = \sqrt{1 + \frac{p^2}{q^2 c_s^2}}. \quad (2)$$

In eqn (2),  $q$  denotes the spectral mode number, and  $p$  the Laplace domain variable.

The general solution of this equation is

$$\hat{\Omega}(y; p, q) = A(p, q)e^{|q|\alpha_s y} + B(p, q)e^{-|q|\alpha_s y}. \quad (3)$$

Using eqn (3), we can express the displacement  $u^\pm(x, t)$  and the traction stress  $\tau(x, t)$  along the interface in terms of  $A$  and  $B$ . These constants can then be determined by introducing an additional boundary condition in each domain. In the substrate, the solution must vanish when  $y \rightarrow -\infty$  and can be expressed in the space and time domain as

$$\tau^-(x, t) - \frac{\mu^-}{c_s^-} \dot{u}^-(x, t) = f^-(x, t), \quad (4)$$

where the convolution term is expressed in the Fourier domain as

$$F^-(t; q) = \mu^- |q| \int_{-\infty}^t C_\infty(|q|c_s^- t') U^-(t - t'; q) |q|c_s^- dt'. \quad (5)$$

The convolution kernel is given by  $C_\infty(T) = J_1(T)/T$ , with  $J_1$  denoting the Bessel function of the first kind and is plotted in Figure 2.

In the thin film, the boundary condition along the upper surface of the thin film yields

$$\left(1 + e^{-2\alpha_s^+ a}\right) \hat{T}^+ = \mu^+ |q| \alpha_s^+ \left(e^{-2\alpha_s^+ a} - 1\right) \hat{U}^+ + 2e^{-\alpha_s^+ a} \hat{T}^H, \quad (6)$$

where  $a = |q|H$ , and  $\hat{T}^H$  denotes the Laplace/Fourier transform of the applied traction  $\tau^H(x, t)$ . Back in the time and real space domain, this relation becomes

$$\begin{aligned} \frac{\mu^+}{c_s^+} \dot{u}^+(x, t) + \tau^+(x, t) = & \frac{\mu^+}{c_s^+} \dot{u}^+(x, t - 2\frac{H}{c_s^+}) + f^+(x, t) \\ & - \tau^+(x, t - 2\frac{H}{c_s^+}) - g^+(x, t) \\ & + 2\tau^H(x, t - \frac{H}{c_s^+}) + h^+(x, t) \end{aligned} \quad (7)$$

$$\doteq l^+(x, t).$$

The convolution terms are given in the Fourier domain by (see (Hendrickx [5]) for more details)

$$\begin{aligned} F^+(t; q) = & -\mu^+ |q| a U^+\left(t - 2\frac{H}{c_s^+}; q\right) + \mu^+ |q| \int_0^t \left\{ C_3(|q|c_s^+ t') - C_\infty(|q|c_s^+ t') \right\} U^+(t - t'; q) |q| c_s^+ dt', \\ G^+(t; q) = & -\int_0^t D_3(|q|c_s^+ t') T^+(t - t'; q) |q| c_s^+ dt', \\ H^+(t; q) = & -\int_0^t E_3(|q|c_s^+ t') T^H(t - t'; q) |q| c_s^+ dt'. \end{aligned} \quad (8)$$

One of the convolution kernels entering eqn (8) is presented in Figure 2 for two values of the non-dimensional mode number  $a$ , showing the effect of the wave reflection off the thin film surface at  $T = 2a$ .

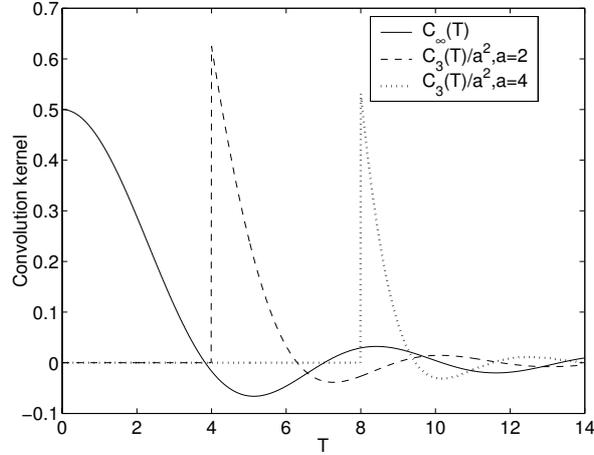


Figure 2: Convolution kernels  $C_\infty(T)$  and  $C_3(T)$  entering the spectral formulation.

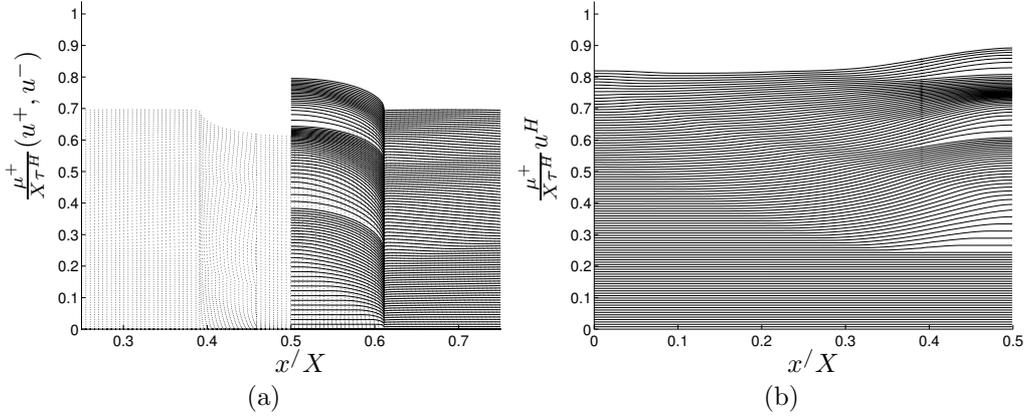


Figure 3: Evolution between  $t = 0$  and  $t = 6.5H / c_s^+$  of the displacements at the interface  $u^+(x, t)$  (solid curves) and  $u^-(x, t)$  (dotted curves) (left) and along the surface of the thin film  $u^H(x, t)$  (right). The time interval between the curves is  $H / 16c_s^+$ .

To model the dynamic failure of the interface, the elastodynamic relations (4) and (7) are combined with a cohesive failure model in which the interface strength  $\tau_{sr}$  is expressed as a prescribed function of the slip  $\delta(x, t) = u^+(x, t) - u^-(x, t)$  and, in the case of a rate-dependent failure response, of the slip rate. In the region where the interface traction stress is below the failure strength, interface continuity conditions are imposed. An explicit scheme is then used to integrate the interface velocity history to obtain the displacement jump. To assess the precision and stability of the numerical scheme, we have performed a modal analysis involving the dynamic response of a single spectral mode. This analysis has shown that, under certain conditions, the higher spectral modes may become unstable. This instability can however be resolved by adopting a conventional first-order low-pass filter on  $l^+(x, t)$ .

### 3 NON-PROPAGATING CRACK

We consider here the dynamic response of a non-propagating crack located between a substrate of fused silica ( $\mu^- = 30.8 \text{ GPa}$ ,  $\rho^- = 2200 \text{ kg/m}^3$ ,  $c_s^- = 3741 \text{ m/s}$ ) and an aluminium thin film ( $\mu^+ = 26.0 \text{ GPa}$ ,  $\rho^+ = 2710 \text{ kg/m}^3$ ,  $c_s^+ = 3097 \text{ m/s}$ ), the material system investigated in the experiments described in (Wang *et al.* [1]). The external loading along the film is a step function in time:  $\tau^H(x, t) = \tau_0^H H(t)$ . Figure 3 shows the evolution of the displacement along the interface, and along the surface of the thin film. This latter result is obtained through a similar spectral formulation described in (Hendrickx [5]).

To characterize the near-tip stress field, we compute the time-dependent stress intensity factor (SIF)  $K_{III}(t)$  defined as

$$\lim_{x \rightarrow x_c} \tau(x, t) = \frac{K_{III}(t)}{\sqrt{2\pi|x - x_c|}}. \quad (9)$$

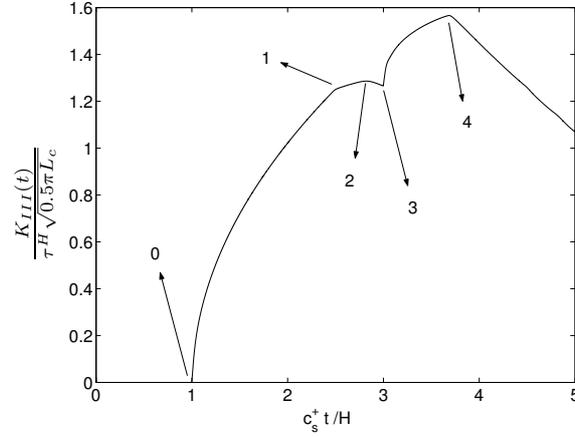


Figure 4: Evolution of the stress intensity factor  $K_{III}(t)$  defined by eqn (9).

In this relation,  $|x - x_c|$  denotes the distance to the crack tip. As can be observed in Figure 4, the evolution of the SIF is characterized by angular points corresponding to the arrival of waves at the crack tips. To each angular point - except to the first one, which corresponds to the initial plane wave reaching the interface - corresponds a motion of elastodynamic waves along the crack surfaces or in the thin film, as schematically shown in Figure 5. The association between these angular points and the different possible paths followed by the wave is done comparing the time at which the angular point occur and the length of the path. Some example of this correspondence are shown Table 1.

Table 1: Correspondence between angular points of Figure 4 and the paths shown in Figure 5.

Angular point	0	1	2	3	4
Path	O	OC	OB	OA	OD

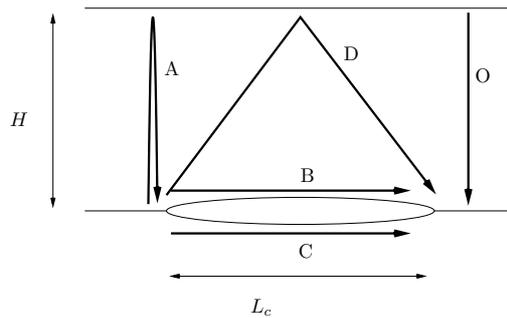


Figure 5: Wave trajectories for the non-moving crack problem.

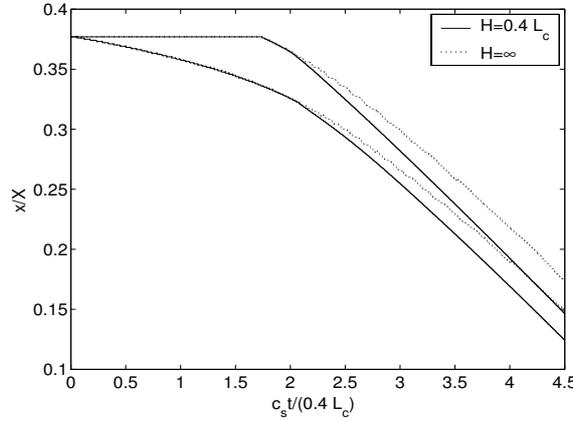


Figure 6: Comparison of the evolution of the crack and cohesive zone tips for a finite and infinite film thickness, showing an acceleration of the propagation due to the wave reflection of the wave on the surface ( $t = 0$  corresponds here to the arrival of the initial shear wave on the interface).

#### 4 PROPAGATING CRACK

To demonstrate the ability of the numerical scheme to capture the spontaneous delamination of thin films, we consider now the propagation of a crack of original length  $L_c = 250\mu\text{m}$  at an interface of initial strength  $\tau_{str0} = 500\text{MPa}$  and critical separation  $\delta_c = 0.96\mu\text{m}$  between the same materials as in Section 3. Figure 6 shows the evolution of the crack tip (the crack is the zone where  $\delta \geq \delta_c$ ) and cohesive zone tip (the cohesive zone is where  $\delta_c > \delta > 0$ ) locations for a simulation on a length  $X = 1\text{mm}$ . We analyze here the influence on the crack propagation of the waves coming from the crack and reflected off the surface. To study this, we compare the dynamic response in the case of a finite ( $H = 100\mu\text{m}$ ) and an infinite thickness for the thin film. As shown Figure 6, the waves reflected on the surface and coming back on the fracture plane accelerate the propagation of the crack. As expected, before the first reflection, the evolutions are totally identical.

#### ACKNOWLEDGEMENTS

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