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Numerical Determination of Driving Force for Cracks in Multi-Layered Systems

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Abstract

This work investigates the driving force or energy release rate of three types of cracks commonly encountered in multi-layered systems, namely surface, channelling and interfacial cracks. The cracks are driven by thermal stresses resulting from dissimilar thermal properties of each layer in the system. Two-dimensional finite element models are developed, enabling the energy release rate for each type of crack in the multi-layered system to be determined. It is found that several parameters including layer thicknesses, system profiles, material elastic properties and thermal loads, influence the energy release rate, and therefore determine the onset of cracking.

1. Introduction

In a large number of engineering applications, individual components are exposed to local loading conditions which can vary greatly with location. In such cases, the use of dissimilar materials including metals and ceramics in the form of multi-layered systems may be required. The choice of materials and the multilayer configuration are often designed primarily according to functional requirements. However, such systems must also preserve their structural integrity during manufacture and service.

The fracture behaviour of a multi-layered system is strongly influenced by various factors, such as its stress distribution, the relative stiffness of each layer and the fracture toughness of its constituents and interfaces. Areas where the fracture behaviour of multi-layered systems is of interest include high-temperature protective coatings, thin film-substrate systems for electronic packages and ceramic layered structures for solid oxide fuel cell applications [1].

A common cause of fracture in multi-layered systems is the presence of excessively high residual stresses. A multilayer is usually sintered together at high temperatures. Upon cooling to room temperature, residual stresses develop due to the fact that the materials have different thermal expansion coefficients and elastic properties. Other causes of fracture include thermal gradients [2-3] and thermal shock loadings [4-5]. The most widely used and simplest layered structure is a film-substrate bimaterial system. Cracking patterns commonly observed in such structures are surface cracks, channelling cracks, interfacial cracks, substrate cracks and substrate spalling [6-8]. In a fracture mechanics-based approach, each crack will grow when its driving force or energy release rate reaches the fracture toughness of the relevant material or interface.

Analytical solutions for energy release rates for various cracks in a bi-layered system have been derived and presented [9-11]. However, in order to study energy release rates for cracks within multi-layered systems, numerical approach has to be used. This is due to the fact that it involves several parameters, all contributing to the energy release rates of the cracks within the multi-layered systems. Such parameters include geometrical parameter such as the crack size and the thickness of each layer, as well as the material properties of each layer.

This work studies the energy release rate of surface, channeling and interfacial cracks in mutli-layered systems by using finite element analysis (FEA). The difficulty encountered in the FEA often lies in designing and constructing the mesh for the model. It is time-consuming and a new mesh usually has to be constructed when changing the location of the cracks within the model. This work makes use of a user-defined subroutine available within the FE package [12], enabling the changes of crack location to be modelled efficiently. The influences of the geometrical parameter and the material properties on energy release rates are also investigated.

2. Finite Element Models of Surface Cracks

A two-dimensional finite element model for a surface crack within a multi-layered system was constructed. The system consists of a multi-layered film of total thickness h and a substrate of thickness H. The multi-layered film can be made up of layers of different materials of various thicknesses. The substrate thickness is taken to be 10 times the film thickness for efficiency of the model. It was found that beyond this value the results are shown to be thickness independent. The surface crack has the depth a where $0 \le a \le h$. Due to symmetry, only one half of the cracked system represented by the length L was modelled. Sensitivity studies revealed the effects of crack interaction to be negligible once $L > H$. Therefore, the value of $L = H$ will be used throughout this work. The geometry for the FE model and a typical mesh for a 2-D surface crack are shown in Figure 1.

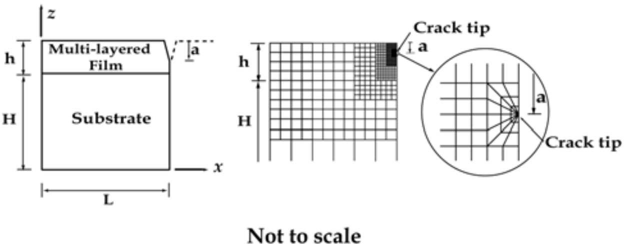

Figure 1: Geometry for the FE model and a typical FE mesh for a 2-D surface crack in the multi-layered system

Periodic and symmetric boundary conditions are prescribed on the plane $x = 0$, and $x = L$, respectively. The plane $z = 0$ is also constrained from bending as in most applications, the substrate is often much thicker than the films, thus resulting in no bending of the systems. Second-order isoparametric plane strain elements are used. The elements around the crack tip are focused on the crack tip with one edge of each element collapses to zero length. This work assumes linear elastic behaviour of the film materials, therefore a $1/\sqrt{r}$ singularity at the crack tip is required. This is done in the finite element by placing the mid-side nodes of the edges radiating out from the crack tip of each of the elements attached to the crack tip at one-quarter of the distance from the crack tip to the other node of the edge. The model is loaded thermally by imposing a temperature decrease representing the cooling down from sintering to room temperature.

Since the multi-layered film can consist of several layers, each having its own elastic properties and thickness, a user-defined subroutine was developed to specify the properties variation throughout the film. The subroutine prescribes the varying properties at the integration point of each element according to the film profile. This allows multi-layered systems of different film profile to be modelled efficiently.

The resulting energy release rates are given in terms of J-integral evaluated from the contours surrounding the crack tip, since in the case of linear elastic material response, the energy release rate for a surface crack extension, G_{sc}, is equal to the J-integral around the crack tip [13]. Four contour integrals were used and path independence of the results were checked by ensuring that the discrepancy of the J-integral evaluated from each contour was less than 5%.

3. Finite Element Models of Interfacial Cracks

A similar model to that described in Section 2 was constructed to study the energy release rates of interfacial cracks within a multi-layered system. The system consists of a substrate of thickness H and a multi-layered film of total thickness h. An interfacial crack of length a can be located between the film and the substrate or within the multi-layered film itself. It was reported that for a crack length longer than few times the film thickness, a steady state is reached and the energy release rate no longer depends on the crack length [14-15]. In this work, it is assumed that a is 5 times the total film thickness. The substrate thickness H is 10 times h as the FE results were found to be unchanged for $H > 10h$. The length L is chosen to be 20 times h, in order to avoid any edge effects. The geometry for the model and the FE mesh used in finding energy release rates of interfacial cracks are shown in Figure 2.

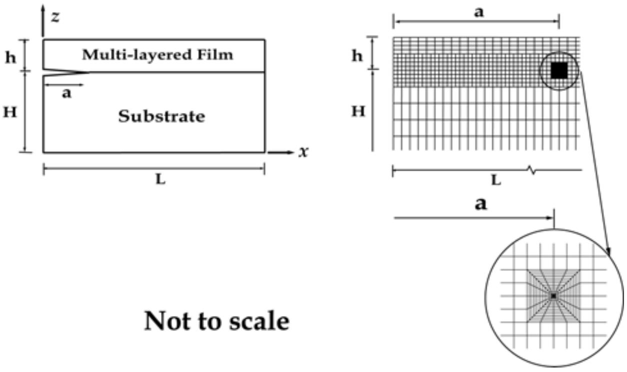

Figure 2: Geometry for the FE model and a typical FE mesh for a 2-D interfacial crack within the multi-layered system

The plane $x = L$ and $z = 0$ are constrained to move in the x and z direction, respectively. Similarly to the FE models for the surface crack, second-order isoparametric plane strain elements are used and the elements around the crack tip are focused on the crack tip with one edge of each element collapses to zero length. A $1/\sqrt{r}$ singularity at the crack tip is prescribed onto the model. The material variation within the multi-layered film is achieved via a user-defined subroutine described previously. The model is also loaded thermally by imposing a temperature decrease representing the cooling down from sintering to room temperature.

The resulting interfacial energy release rates are obtained from the FE simulation in terms of J-integral evaluated from the contours surrounding the crack tip. The mesh around the crack tip is refined such that the variation of the J-integral computed from each contour is less than 5%. Typically, fourteen contour integrals are used in the model and the average value is calculated. For an elastic problem, the energy release rate of the interfacial crack, G_i, is equal to the value of the J-integral around the crack tip.

Since interfacial cracking is of mixed mode in nature, the mode mixity also has to be evaluated. The mode of interfacial crack extension can be extracted from FE models by fitting the near-tip crack displacements to the near-tip crack opening and crack sliding displacements given by [16]

$$\delta_2 + i\delta_1 = \frac{8(K_1 + iK_2)}{E^*}\left(\frac{r}{2\pi}\right)^{1/2} \tag{1}$$

Here $E^* = \left(\frac{1}{2\overline{E}_1} + \frac{1}{2\overline{E}_2}\right)^{-1}$, where $\overline{E}_1$ and $\overline{E}_2$ are plane strain Young's moduli of the two materials forming the interface and K_1 and K_2 are the stress intensity factors of the mode I and mode II, respectively. Once δ_1 and δ_2 values are calculated from nodal displacements from the FE models and substituted in to the above equation, the complex K is solved, then the phase angle defining the mode mixity is found from

$$\psi = \tan^{-1}(K_2 / K_1)\ . \tag{2}$$

4. Energy Release Rates for Surface, Channelling and Interfacial Cracks

In order to evaluate the energy release rates of the various crack types described previously, we consider an arbitrary multi-layered system having the Dundurs parameter [17], $D_\alpha = -0.9$ and the film having greater thermal expansion coefficient than that of the substrate. This represents a system of a compliant film subjected to tensile residual stresses on a stiff substrate, which is typical of a structure used in various applications.

The accuracy of the FE model for the surface cracks was first checked by assuming the film to be homogeneous, and evaluating the energy release rate for cracks of various depth. The results were compared with analytical solutions based on the work on the bi-layered system by Beuth [9]. Good agreement was found throughout. Then the effects of crack size and film thickness on surface crack energy release rate were investigated. Figure 3 shows normalised energy release rate $G_{sc}/\sigma^2\overline{E}$ for a surface crack of various depth in a homogeneous film of different thickness. It can be seen that G_{sc} increases with increasing crack size until it reaches the maximum value at a location close but not reaching the film-substrate interface. It then drops once the crack gets closer to the interface. Greater energy release rate was obtained in the system with thicker film.

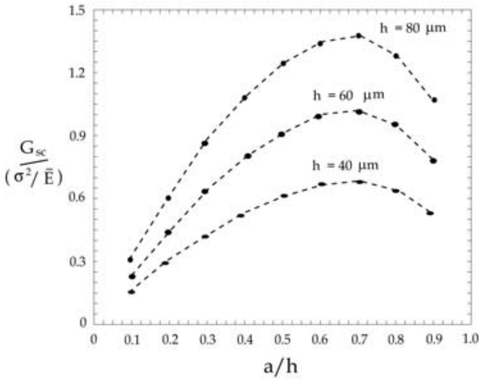

Figure 3: Normalised surface crack energy release rate against normalised crack length in homogeneous films of different thickness

However, one can reduce the surface crack energy release rate by using a multi-layered film of step-wise properties. This can be seen in Figure 4, where the surface crack energy release rates of films with different configurations are compared with the maximum of that of the homogeneous film. It was found that by inserting extra layers, having intermediate thermal expansion coefficient between that of the film and the substrate, in a bimaterial system, could substantially reduce the overall energy release rate. As can be seen from Figure 4 that the three-layered film alleviates energy release rates more effectively than the two-layered film. The most beneficial film is when it is made of a functionally graded material (FGM) having smooth transition of the thermal expansion coefficient at the film-substrate interface.

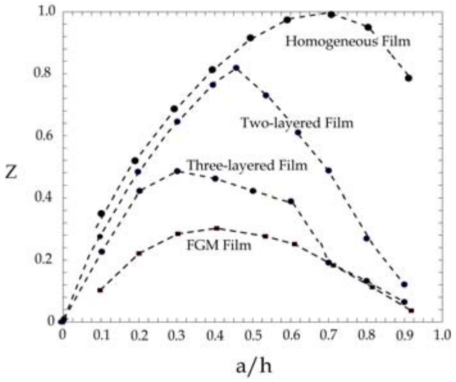

Figure 4: Normalised surface crack energy release rates in multi-layered systems with different film profile

Finite element modelling of a 3-D crack channelling across the film in a multi-layered system is highly complicated. Defining the shape of the crack front at each stage of crack growth such that the crack remains in a steady state poses great difficulty. However, the channelling crack energy release rate, G_{cc}, is often lower than G_{sc} and can be found using the relationship [9]

$$G_{cc} = \frac{1}{a}\int_0^a G_{sc}(a)da \qquad (3)$$

Therefore, the G_{cc} values can be evaluated numerically from the G_{sc} curves shown in Figure 4. This is shown in Figure 5.

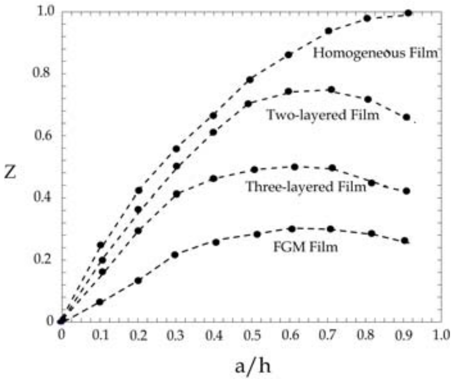

Figure 5: Normalised channelling crack energy release rate in multi-layered systems with different film profiles

In order to study the interfacial cracking within the multi-layered systems, the accuracy of the FE models and the technique used to extract the mode mixity was first tested. This was done by comparing the analytical and numerical energy release rates and mode mixity for an interfacial crack in a bimaterial system. The analytical solutions for G_i and ψ were obtained following the work of Suo and Hutchinson [10]. Good agreement was found and the same material systems as those used in studying surface cracks were investigated, i.e. the systems with homogeneous, two and three-layered and an FGM films. Interfacial energy release rates and mode mixity for all the interfaces within each multi-layered system were evaluated following the procedure described in Section 3. Film 1 is the layer adjacent to the substrate and Film 2 and Film 3 are the next layers stacking towards the free surface, respectively. The results are tabulated in Table 1.

Table 1: Interfacial energy release rates and mode mixitiy for multi-layered systems with different film profiles

Film type	G_i and ψ (in bracket) at the interfaces between		
	Substrate–Film1	Film 1 – Film 2	Film 2 - Film 3
Homogeneous	32.3 (46°)	N/A	N/A
Two-layered	19.4 (5°)	26.1 (33°)	N/A
Three-layered	12.3 (0°)	10.5 (33°)	8.3 (40°)
FGM	7.8 (0°)	N/A	N/A

It can be seen that interfacial energy release rates at the film-substrate interface is reduced when using intermediate layers and is the smallest when an FGM film is used. This is because the FGM film eliminates the abrupt interface where stress concentration leading to cracking occurs. When cracking within the film paralleling to the interface is concerned, it is reported that such cracks tends to have less energy release rates than those at the interfaces [15]. Therefore it will be assumed that such cracking is less likely than the interfacial ones.

Knowing the energy release rates of competing fracture modes within the multi-layered systems, one can predict whether cracking will occur or not under certain conditions by comparing it to the material fracture toughness. Surface and channelling cracks within the film will occur when their energy release rates reach the film fracture toughness. In some applications, it is not possible to measure the crack size to thickness ratio (a/h) of the film. For such cases, it is usually admissible to estimate the a/h values according to the quality of the film. Alternatively, conservative criterion can be used and the film is assumed to contain the worst flaws where energy release rate is at its highest.

Interfacial cracking will occur when the corresponding energy release rate reaches the interfacial fracture toughness of the two materials forming the interface. Note that interfacial fracture toughness depends on the mode of loading, so appropriate values must be used in the comparison.

5. Conclusions

This work studies the fracture behaviour commonly found in multi-layered systems as a result of thermal residual stresses during manufacture. Numerical approach using finite element analysis was pursued. Finite element models were constructed and user-defined subroutines were developed to determine the driving force or energy release rates for surface and interfacial cracks. Solutions for channelling cracks were derived from those of the surface cracks. It was found that the energy release rates increase with increasing film thickness. However, by using multi-layered films with step-wise properties can substantially help alleviating the crack driving force for all three types of cracks considered here.

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