A computational fracture mechanics study of buckling in thin film systems

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Chapter 1

Introduction

1.1 Flexible displays

A flexible display is a flat panel display on a thin, flexible substrate. Thin film is the keyword for making a display that is flexible during usage and can be rolled for storage. A possible application for a flexible display is an E-reader, a monochrome paperlike display as can be seen in figure 1.1. Such displays use electronic ink in an active matrix, and can be read like paper. Important features of the E-reader are high readability during daylight without the need for a backlight, resulting in low power consumption. Other applications of flexible displays are full-color screens for moving images in telecom devices or, in the automotive industry, for instance a curved display on the dashboard of a car, or an extractable screen for a cellular phone with a display size larger than the phone.

![Rollable E-reader (Polymer Vision)](image)

1.2 Layers and buckling

The substrate of the display can be made of polymer for an electrophoretic (monochrome) display or metal for an organic light-emitting device (OLED). The top layer is a transparent conductive hard coat, for instance indium tin oxide (ITO). It protects the display from scratches, fingerprints or dust and at the same time allows one to apply a voltage across the thickness of the display. Polymer barrier layers are necessary to protect the organic layers in the active matrix from moisture.

All of these layers have different thermal and mechanical properties. The display can be regarded as a compliant layer structure with a thin but very stiff top layer. During the deposition of the top layer in the manufacturing process the device is cooled down from the elevated process temperature. Through the difference in thermal expansion coefficient between the layers, biaxial
compressive stress is introduced in the adhesive interface. While using the device additional stresses due to bending act on the interface. As a consequence, buckling delamination is a common failure mode observed in flexible displays. The delamination is initiated by imperfections in the interface, i.e. small regions where the adhesion between the layers is lower. The outer layer can then buckle away from the substrate due to compressive stress. When subjected to extra stresses, from bending for instance, these delaminated regions can grow. Cracking can also occur when the layers are subjected to tensile stress, see figure 1.2.

![Compressive buckling](image)

Figure 1.2: Failure from buckling delamination and tensile cracking, Timmermans [22]

1.3 Straight sided and telephone cord buckling

A failure mode that is frequently observed in multi-layer systems with a stiff top layer is telephone cord buckling [1, 7, 15]. An example of telephone cord buckling is shown in figure 1.3. Through literature study it is understood that only in limited conditions, at a low stress state, straight sided buckles are observed. For high stress states the telephone cord buckle morphology is preferred over straight sided buckling. The straight sided buckle transitions to a telephone cord buckle. More energy is expected to be released through buckling if the buckle advances along a curved path instead of linearly [11].

![Telephone cord buckling](image)

Figure 1.3: Telephone cord buckling, Moon [15]

At the edge of the buckle the interface between film and substrate experiences both normal and shear stresses. The interface toughness is dependent on the magnitude of the stress and the relation between the normal and shear component. A detailed description of the stress state along the front and the edge of the buckle, taking the elastic mismatch between the layers into account, and its influence on the interface toughness, is not available yet. Through numerical analysis by means of finite element method (FEM), we can come to a better understanding of the mechanics of the telephone cord buckle. A FEM model with reliable results can be of great help for predicting the stress state at the crack front and interface failure.
1.4 Objective

The objective for this study is to characterize the telephone cord buckling morphology and predict interface failure by 3D FEM analysis, taking substrate compliance and mode mixity into account. In describing the buckle morphology, the stress state around the crack front is of crucial importance. Linear elastic fracture mechanics is used in this study and the transition between the bonded and delaminated parts of the film is treated as an interface crack. In a FEM approach the stress state around the crack front can be observed for various loading conditions.

1.5 Structure of this report

The structure of this report is as follows. In chapter 2 a brief overview of linear elastic fracture mechanics is given for bulk fracture and interface fracture. Some numerical procedures that are needed to calculate the stress intensities are presented. In chapter 3 fracture problems with simple geometries and well known analytical solutions are compared with FEM models. The reliability of the solution can be validated. In chapter 4 the buckling phenomenon is described in further detail, starting with a brief overview of literature in this area. The buckle morphology is investigated with the influence of the substrate compliance and mode mixity taken into account. An example of a buckle modeled in a FEM analysis is shown in figure 1.4.

Figure 1.4: A straight sided buckle analyzed by FEM
Chapter 2

Fracture mechanics theory

2.1 Bulk fracture mechanics

When a defect or crack exists in a material, it may be desirable to predict under which loads the crack will grow. Three different classes of crack propagation criteria exist; energy, stress and deformation criteria. Energy criteria such as the energy balance of Griffith, have a global character and predict crack growth based on the global loading of the material. A stress criterion has a more local character as it predicts growth based on the stress state around the crack tip. A deformation criterion is based on the deformation at the tip or in the crack [19].

In this study linear elastic fracture mechanics (LEFM) is being used. All loads acting on a crack can be decomposed in three different crack loading modes, as shown in figure 2.1. Mode I is the opening mode where the crack faces are separated by opening, mode II is the sliding mode where the crack faces are subjected to in-plane sliding, and mode III is an out of plane tearing mode. A combination of mode I, II and III loading is called mode-mixity. In this study we will focus on mode I and II as it has been shown that mode III has a very small contribution to the fracture criterion for the problems of interest in this report [11].

Figure 2.1: The three fracture modes distinguished in LEFM

For the growth of the crack, over a distance $da$, small compared to the sample size, we can write the following energy balance. The difference between the change in supplied mechanical energy $U_e$ and the change in internal elastic energy $U_i$, when the crack grows by an infinitesimal distance $da$, equals the dissipated energy $U_a$ by crack growth over the small distance $da$.

$$\frac{dU_e}{da} - \frac{dU_i}{da} = \frac{dU_a}{da}$$

(2.1)

The crack propagation is assumed to be slow, there is no kinetic energy in the system, the temperature is constant and there is no dissipation except for the energy dissipated by the fracture. When the energy available for dissipation is divided by the sample thickness $B$ we get the energy release rate $G$ per unit area.
\[ G = \frac{1}{B} \left( \frac{dU_e}{da} - \frac{dU_i}{da} \right) \] (2.2)

In describing the deformation and the stress state around the crack tip a coordinate system is defined as in figure 2.2a. The origin is situated in the tip with the crack lying in the negative \( x \)-direction. The cylindrical coordinates \( \theta \) and \( r \) are the angle measured from the positive \( x \)-axis and the distance from the crack tip respectively. The crack is a discontinuity in the material, implying singular stresses around the crack tip, figure 2.2b. While approaching the tip along the line \( \theta = 0 \) the stress increases as \( \sigma_{ij} \sim \frac{1}{\sqrt{2\pi r}} \) \[19\].

![Figure 2.2: a) Conventions at the crack tip, b) Stress distribution at a crack tip](image)

The intensity of these singular stress fields is characterized by the stress intensity factors (SIFs) \( K_I \) and \( K_{II} \) for opening and shear mode respectively. In complex notation, which will prove useful later on, these stresses for \( \theta = 0 \) are related to the SIFs as:

\[ \sigma_{22} + i\sigma_{12} = \frac{K_I + iK_{II}}{\sqrt{2\pi r}} \] (2.3)

For mode I loading of the crack, \( \sigma_{12} = 0 \), there is no shear component and \( K_{II} = 0 \). The stress fields for mode I loading are symmetric around the \( x \)-axis, while the fields for mode II loading are anti-symmetric. The energy release rate \( G \) is related to the SIFs by:

\[ G = \frac{(K_I^2 + K_{II}^2)}{E} \] (2.4)

where \( E \) equals \( E \) in plane stress and \( E/(1 - \nu^2) \) in plane strain and \( E, \nu \) denote the Young’s modulus and Poisson’s ratio of the material respectively. The argument of the complex SIF \( K = K_I + K_{II} \) is called the mode angle and represents the relative amount of mode II to mode I loading, with a mode angle \( \psi = 0^\circ \) corresponding to pure mode I loading:

\[ \psi = \tan^{-1} \left( \frac{K_{II}}{K_I} \right) \] (2.5)

The crack opening behind the crack tip, \( \delta \), can be shown to be related to the SIFs close to the tip, via:

\[ \delta_y + i\delta_x = \frac{8(K_I + iK_{II})}{E/(1-\nu^2)} \sqrt{\frac{r}{2\pi}} \] (2.6)

\( \delta \) represents the distance between the two corresponding points on the crack faces, \( \delta_i(r) = u_i(r,\theta=\pi) - u_i(r,\theta=-\pi) \). The displacements \( \delta_x \) and \( \delta_y \) are shown schematically in figure 2.3.
2.2 Interface fracture mechanics

2.2.1 Stress intensity factors

When two layers of different materials are attached to each other there is an elastic mismatch at the interface. Assume that a crack is present in the interface. The stress singularity around the tip is now determined by the geometric discontinuity of the crack and by the elastic discontinuity over the interface. The first analytical solution for this case was given by Williams [25]. Because of the elastic mismatch some shear stress will be present even under pure mode I load and there will always be a mixed mode stress state. The SIFs, which now characterize the stress singularity, are denoted as $K_1$ and $K_2$ and are related to the stress state along the interface ($\theta = 0$) ahead of the tip by:

$$\sigma_{yy} + i\sigma_{xy} = \frac{(K_1 + iK_2)\nu^\epsilon}{\sqrt{2\pi r}}$$  \hspace{1cm} (2.7)

where $\epsilon$ is a parameter which characterizes the elastic mismatch as defined below. The consequence of (2.7) is that, in front of the crack, $\theta = 0$, the stresses in the vicinity of the crack become infinitely large and change sign with an increasing frequency while approaching the tip. The dimension of the complex SIF is $\sigma \sqrt{E/L}$. $K_1$ and $K_2$ reduce to $K_I$ and $K_{II}$ when $\epsilon = 0$. The bimaterial constant $\epsilon$ is a real constant and a measure for the oscillatory character of the stress state around the tip. The singular stress fields are oscillatory in form and of order $r^\lambda$ with $\lambda = -1/2 + i\epsilon$, see figure 2.4. The constant $\epsilon$ is defined as:

$$\epsilon = \frac{1}{2\pi} \ln \left[ \left( \frac{\kappa_1 - 1}{\mu_1} \right) / \left( \frac{\kappa_2 - 1}{\mu_2} \right) \right]$$

$$= \frac{1}{2\pi} \ln \left[ \left( \frac{1 - \beta}{1 + \beta} \right) \right]$$  \hspace{1cm} (2.8)

The Kolosov constants $\kappa_i$ in (2.8) are $\kappa_i = 3 - 4\nu_i$ in plane strain, $\kappa_i = (3 - \nu_i)/(1 + \nu_i)$ in plane stress; furthermore $\mu_i = E_i/(1 + \nu_i)$. The Dundurs’ parameter $\beta$ is a measure of the in-plane bulk moduli, and is zero when the two materials are equal:

$$\beta = \frac{\mu_1(\kappa_2 - 1) - \mu_2(\kappa_1 - 1)}{\mu_1(\kappa_2 + 1) + \mu_2(\kappa_1 + 1)}$$  \hspace{1cm} (2.9)

Similar to (2.6) the CODs can be written as:

$$\delta_y + i\delta_x = \frac{8(K_1 + iK_2)}{(1 + 2i\epsilon) \cosh(\pi\epsilon)E^*} \sqrt{\frac{r}{2\pi}} r^{i\epsilon}$$  \hspace{1cm} (2.10)

where $E^* = \frac{2E_1E_2}{E_1 + E_2}$ and $E^*_i = \frac{E_i}{(1 - \nu_i)}$ for plane strain. When the stress intensity factors are known, similar to (2.4), the energy release rate can easily be calculated:

$$G = \frac{(1 - \beta^2)}{E^*} (K_1^2 + K_2^2)$$  \hspace{1cm} (2.11)
2.2.2 Mode angle and reference length

The stress on the interface has an oscillatory character, see (2.7). As a consequence, the amount of normal to shear traction varies with the distance from the crack tip. This has to be taken into account in the determination of the mode angle. An arbitrarily chosen reference length \( l \) has to be set for this purpose. Based on the complex stress intensity factor \( K = K_1 + iK_2 \), the mode angle can then be determined using [10]:

\[
\psi = \arg(Kl^\varepsilon) = \tan^{-1} \left[ \frac{\text{Im}(Kl^\varepsilon)}{\text{Re}(Kl^\varepsilon)} \right] \tag{2.12}
\]

In the case of a crack in a uniform material, \( \varepsilon = 0 \), we have \( l^\varepsilon = 1 \) and (2.12) reduces to (2.5). The choice of a reference length for a bimaterial interface is subject to a lot of discussion. A logical choice is to take a reference length larger than the zone dominated by large stress fluctuations. A characteristic size of the specimen, such as the crack length or thickness of the film can be used to study the mixed mode character of the crack, independent of material behavior. To study the fracture behavior a material based reference length can be chosen, such as the size of the plastic zone. The choice is here of secondary importance, since a mode angle determined for a reference length \( l_1 \) can easily be transferred into the mode angle for length \( l_2 \):

\[
\psi_2 = \psi_1 + \varepsilon \ln(l_2/l_1) \tag{2.13}
\]

In interface fracture mechanics, the interface toughness \( \Gamma \) is not a constant value but depends on the mode angle, as discussed by Cao and Evans [5]. Therefore, for an interface both \( G \) and \( \psi \) are required to predict crack propagation. An interface toughness \( \Gamma(\psi) \) dependent on the mode mixity is introduced. This \( \Gamma(\psi) \) can be split in the toughness in mode I loading \( G_I^c \) and a function of the mode angle \( f(\psi) \).

\[
\Gamma(\psi) = G_I^c f(\psi) \tag{2.14}
\]

For \( f(\psi) \) we take [10]:

\[
f(\psi) = [1 + \tan^2(\psi)] \tag{2.15}
\]

In brittle fracture \( \lambda = 1 \) and the interface toughness is constant for the range of mode mixity. For \( \lambda = 0 \) the interface only fails in pure mode I loading. Cordill et al. [7] give some experimental values for Tungsten and Platinum layers on \( SiO_2 \) substrates. \( G_I^c \) ranges from 0.2 to 0.5 \( J/m^2 \), and \( \lambda \) is about 0.3. For \( \lambda = 0.3 \) the function \( f(\psi) \) is shown in figure 2.5. For pure sliding mode, \( \psi = +\pi/2 \), the interface is more than 4.5 times tougher compared to pure opening mode, where \( \psi = 0 \). As \( \Gamma \) is of the same dimension as \( G \), the dimensionless value of \( G/\Gamma(\psi) \) will be chosen later as a crack propagation parameter.
2.2.3 Contact zone

The linear elastic fracture mechanics solutions found for bimaterial interfaces predict interpenetration of the crack faces near the crack tip. Due to the oscillatory behavior of the stresses near the crack tip, with stresses increasing in frequency and amplitude while approaching the tip, the crack surfaces will wrinkle. Although physically not feasible, this implies interpenetration of the materials close to the tip [9]. The materials would more likely contact each other and deform. The solution to an analytical model of the crack would be wrong and this was seen as a reason to reject it. However, if the length over which this contact occurs is very small compared to the crack length, the analysis may provide accurate SIFs for the near-tip field [17]. The region between the crack tip and the largest distance from the tip where contact is made is called the contact zone.

An estimation of the contact zone size can be made by finding the largest $r$ for which the opening gap $\delta_y$ from the crack opening displacements (2.10) equals zero [17]:

$$
Re \left[ \frac{(K_1 + iK_2)r^{i\epsilon}}{(1 + 2i\epsilon)} \right] = 0 \quad (2.16)
$$

A contact zone size for a crack between dissimilar plates is derived in Appendix A. A more general derivation can be made by assuming that $|\epsilon| < 1$ and $K_1 > 0$. The complex number between the brackets lies in the right half of the complex plane. Approaching the tip at $r = 0$ the sign of $\epsilon$ determines if the imaginary axis is approached at $\frac{\pi}{2}$ or $-\frac{\pi}{2}$. Both cases can be captured in the following expression for the contact radius:

$$
r_c = \exp \left[ -\frac{1}{\epsilon} \left( \text{sign}(\epsilon) \frac{\pi}{2} + \tan^{-1} \left( \frac{K_2 - 2\epsilon K_1}{K_1 + 2\epsilon K_2} \right) \right) \right] \quad (2.17)
$$

With (2.17) an estimation of the contact zone size for all cracks between dissimilar media can be made, when the SIFs and $\epsilon$ are known.

2.3 Finite element fracture mechanics

Exact solutions to crack problems are limited to simple geometries and boundary conditions. For complex geometries an analytical calculation of the stress intensity factors may not be feasible. Numerical methods such as the finite element method (FEM) can then be a helpful tool.

2.3.1 Quarter point elements

For a two-dimensional or axi-symmetric analysis 8-noded quadratic elements are widely used. The quadratic interpolation functions can describe a (bi-)linear stress field, in contrast with linear elements that can only describe constant stresses. The nodes numbered 1-4 are placed at the corners. The nodes with numbers 5-8 should normally be placed halfway the element sides; when
not placed in the middle this may lead to a singularity in the stiffness matrix. Barsoum [4] proposed to place the nodes on the edges adjacent to the crack tip at \( l/4 \), instead of \( l/2 \), where \( l \) is the element edge length, see figure 2.6. The thus introduced singularity in the stress field matches the \( r^\lambda \) singularity, for uniform materials \( \lambda = -\frac{1}{2} \), expected at the crack tip.

![Figure 2.6: A quadratic and a quarter point element, node 1 is the crack tip](image)

This property of quarter point elements holds for 8-noded elements and for 6-noded elements generated by collapsing the 1-4 side of an 8-noded element, i.e. the so-called collapsed triangular element, see figure 2.7a. Barsoum [4] showed that this element has superior results in crack analysis, when placed around the crack with the quarter point nodes facing the crack tip and forming a focused crack tip mesh as sketched in figure 2.7b.

![Figure 2.7: a) Collapsed triangular element, b) Focused cracktip mesh with collapsed quarter point elements](image)

For bimaterial cracks \( \lambda \neq -\frac{1}{2} \) and the quarter point elements do not exactly describe the oscillatory singularity at the crack tip, as observed by Abdel Wahab et al. [24] and in the following chapter.

### 2.3.2 Computation of the stress intensity factors

There are three different types of computational methods for SIF evaluation: displacement methods, stress methods and integral or energy methods. The computation of the SIFs in the finite element program MSC Marc is not accurate for bimaterial interfaces. Because of the ease of implementation a displacement method is considered here. The opening displacements of the opposite crack faces are collected from the output of the FEM model using a Fortran subroutine. This routine collects the nodal displacements from a pre-defined set of nodes close to the crack tip from which the stress intensity factors can be calculated. For this purpose equation (2.10) is rewritten as:

\[
K_1 + iK_2 = \frac{(\delta_y + i\delta_x)(1 + 2i\varepsilon)\cosh(\pi\varepsilon)E^*}{8\sqrt{\pi^3}\varepsilon}\quad (2.18)
\]
In the next chapter several benchmark problems are solved using this method and the results are compared with analytical solutions. They are used to validate the crack opening displacement (COD) method to study the dependency of material mismatch, mode angle and mesh size. The Fortran subroutine is further explained in Appendix B.

2.3.3 Extrapolation techniques

The relation between the SIFs and the displacements given by (2.18) is only valid close to the crack tip. If the singularity at the crack tip is not well described by the elements, the solution \( \lim_{r \to 0} K(r) \) is not exact. The curve of \( K(r) \) shows a constant slope with increasing \( r \). A linear extrapolation technique can be used from two arbitrary distances \( r_i \) and \( r_j \) behind the crack tip, see figure 2.8. Extrapolating this slope to \( r = 0 \) using

\[
K^* = \frac{r_j}{r_j - r_i} K(r_i) - \frac{r_i}{r_j - r_i} K(r_j)
\]  

(2.19)
gives an accurate estimation of the SIFs. This simple linear extrapolation in combination with crack opening displacements was first proposed by Chan et al. [6]. More recently Xuan et al. [27] used extrapolation with linear triangular elements, comparing the estimation of the SIFs for coarse and fine meshes.

![Figure 2.8: Extrapolation of the stress intensity factors at the crack tip](image)

Another estimation technique was proposed by Matos et al. [14]. In linear elastic fracture mechanics the path independent J-integral is equal to the energy release rate \( G \). Matos therefore proposed to determine the distance \( r \) where \( G(r) \) from the COD method, using (2.11) and (2.18), agrees with the J-integral. It is expected that \( K(r) \) at this distance \( r \) is a good estimate.
Chapter 3

Benchmark problems

3.1 Crack in an infinite homogeneous plate

3.1.1 Problem description

First a benchmark of a plate with a center crack is considered. A plate of uniform material is subjected to far-field uniaxial tension as shown in figure 3.1. A crack is present in the center of the plate at an angle $\theta$ with respect to the plane normal to the loading direction.

![Figure 3.1: Crack in an infinite homogeneous plate](image)

The dimensions of the plate are large compared to the crack length $2a$, so a uniform, far-field stress can be assumed. For the angle $\theta = 0^\circ$ the crack is subjected to pure opening mode. A wide range of mode-mixity is covered while varying $\theta$ between $0^\circ \leq \theta < 90^\circ$. Sih et al. [20] presented the exact solution for the stress intensities of this problem:

$$
K_I = \sigma \sqrt{\pi a \cos^2 \theta}, \quad K_{II} = \sigma \sqrt{\pi a \sin \theta \cos \theta}
$$

(3.1)

This problem has been modeled with the FEM program MSC Marc. The size of the plate is chosen to be 10x10 m, and the cracklength $2a$ is 1m. The model uses the assumption of plane strain in the thickness direction. To investigate the dependency of the COD method on the element size, three different mesh sizes are chosen. Around the crack tips collapsed elements are used in a focused mesh according to figure 2.7. To determine the influence of the element type a comparison is made between a model using 4 node linear elements and one using 8 node quadratic elements. For the latter also a model was made with quarter point elements around the crack tips as described earlier.
3.1.2 Results

In figure 3.2 stress intensity results, determined with (2.18) are shown for three different mesh sizes. The element sizes near the cracktip are 0.0125, 0.025 and 0.05 m. The angle of the crack is $\theta = 15^\circ$, while the far field stress $\sigma_{yy}$ is 1 kPa. The horizontal axis of the diagrams represents the normalized distance from the cracktip $r/2a$. The vertical axis shows the stress intensity factors $K_I$ and $K_{II}$ normalized to the exact solution according to (3.1), which for the given loading equals $K_I = 1169.4 N/m^{1.3}$ and $K_{II} = 313.3 N/m^{1.5}$.

![Figure 3.2: Normalized stress intensities as function of the distance to the cracktip for $\theta = 15^\circ$ as obtained using linear elements, ordinary quadratic elements and quarter point quadratic elements; three different element sizes have been used](image)

For the linear elements, while approaching the crack tip, $K_I$ becomes more accurate apart from the three nodes closest to the tip. A significant mesh-dependency is observed. The smallest element size gives the best results, approaching the analytical solution to within 5.5%. This indicates that the displacement field around the crack tip is described better by a fine mesh. The solution for $K_{II}$ is, compared to $K_I$, closer to the analytical solution. Because of the small crack angle only a small amount of shear is present. Here also the smallest element size provides the best results, for the highest value it is almost exact. Linear elements probably are best used with a very fine mesh. These results are on par with Xuan [27] and extrapolation will improve the accuracy.

The results for quadratic elements are shown in the middle row in figure 3.2. The same conclusions as for linear elements can be drawn here; the $K_I$ accuracy increases for smaller element size and the
highest value is the best; $K_{II}$ is almost exact close to the tip. Particularly $K_I$, however, suddenly becomes less accurate within the elements nearest to the tip. The quarter point elements pick up the singularity around the crack tip more accurately than the standard elements. The SIF results from different mesh sizes vary only marginally and are exact, or at least within 1% from the exact solution, close to the crack tip. The sudden drop observed for the other element types at the tip is no longer present for the crack tip elements. The quarter point elements thus provide the best solution for the crack in an infinite plate.

![Graph](image)

Figure 3.3: Mode angle dependency with quarter point elements

The angle of the crack with respect to the positive $x$-axis was varied to $15^\circ$, $30^\circ$ and $45^\circ$, and figure 3.3 shows the SIFs [N/m$^{1.5}$] for these different angles. The horizontal solid lines represent the analytical values from (3.1). As expected, $K_I$ is highest for a small crack angle. For a crack angle of $45^\circ$ the values of $K_I$ and $K_{II}$ are equal. The curves have a constant slope. At the node closest to the crack tip the $K_I$ and $K_{II}$ are very accurate, within 1% error. It can be concluded that the quarter point elements are very accurate at the node closest to the crack tip, using moderate mesh sizes and with different mode angles in homogeneous materials.

### 3.2 Interface crack in an infinite plate

#### 3.2.1 Problem description

A similar benchmark to the infinite homogeneous plate was presented by Rice [18], but here the plate consists of two semi infinite parts with an isolated crack in the interface. The upper half-plane, $y > 0$, is occupied by a material with elastic properties $E_1$ and $\nu_1$, the lower half-plane, $y < 0$, by a material with $E_2$ and $\nu_2$, see figure 3.4. The plate is loaded by stresses $\sigma_{xx}^\infty$ and $\sigma_{xy}^\infty$ applied at infinity. The interface of the two materials lies along the $x$-axis and it has a small crack of length $2a$. The origin of the orthogonal coordinate system is situated in the right hand crack tip. The solution for the right hand tip was found by Rice [17, 18]:

![Graph](image)
\[ K_1 + iK_2 = (\sigma_{yy}^\infty + i\sigma_{xy}^\infty) (1 + 2i\varepsilon) (\pi a)^{1/2} (2a)^{-i\varepsilon} \quad (3.2) \]

**3.2.2 Boundary conditions**

We will consider the bimaterial plate with uniform farfield normal stress \( \sigma_{yy}^\infty \) only. Due to the elastic mismatch between the two materials the horizontal stress \( \sigma_{xx} \) will generally be discontinuous across the bond line \( y = 0 \). A distinction should be made between \( (\sigma_{xx}^\infty)_1 \) and \( (\sigma_{xx}^\infty)_2 \). The analytical solution requires continuity of the strain \( \varepsilon_{xx} \) along the interface [18]:

\[ (\varepsilon_{xx})_1 = (\varepsilon_{xx})_2 \quad (3.3) \]

In a FEM simulation this relation can be met by requiring that all nodes on each vertical edge of the plate have the same horizontal displacement. Sukumar [21] even constrained the edges in \( x \)-direction. Another way to meet this requirement is to apply opposing stresses on the vertical edges, \( (\sigma_{xx})_1^\infty \) at \( y > 0 \) and \( (\sigma_{xx})_2^\infty \) at \( y < 0 \), as used by Agrawal [2]. An extra boundary condition is therefore necessary. For plane strain conditions, Rice [18] gives this condition as:

\[ (\sigma_{xx})_2^\infty = \frac{E_2}{E_1} \left( \frac{1 - \nu_2^2}{1 - \nu_1^2} \right) (\sigma_{xx})_1^\infty + \left[ \frac{\nu_2}{1 - \nu_2} - \frac{E_2}{E_1} \frac{\nu_1(1 + \nu_1)}{1 - \nu_1^2} \right] \sigma_{yy}^\infty \quad (3.4) \]

In (3.4) the two stresses \( (\sigma_{xx})_1^\infty \) and \( (\sigma_{xx})_2^\infty \) are unknown so one has to be chosen. In Agrawal [2] \( (\sigma_{xx})_1^\infty \) is chosen to be zero. Simulations show that similar conditions can be obtained without these extra boundary conditions, by making the plate much wider than it is high. Figure 3.5 shows the accuracy of the energy release rate solution as a function of the height-width relation.

Using the symmetry with respect to the \( y \)-axis, the FEM model used here occupies the right half of the plate and the nodal displacements at the right hand edge are linked in \( x \)-direction, to meet (3.3). Quarter point, collapsed elements were used around the crack tip.

**3.2.3 Results**

The FEM model was made using four different material combinations. The plate dimensions are \( 400 \times 400 \text{mm} \) and the half crack width \( a \) is \( 5 \text{mm} \). The applied load \( \sigma_{yy}^\infty \) is \( 100 \text{MPa} \). The material properties and the corresponding analytical SIFs from (3.2) are shown in table 3.1. The contact zone size for this benchmark is very small compared to the element size, as shown in appendix A.

In figure 3.6 the results are shown for three different mesh sizes using the same material properties, for which the elastic mismatch equals 40. The element sizes at the crack tip are \( 15.6 \times 10^{-3} \text{mm} \), \( 31.25 \times 10^{-3} \text{mm} \) and \( 62.5 \times 10^{-3} \text{mm} \). The graphs show the results for the SIFs,
Figure 3.5: Effect of specimen aspect ratio on the computed $G$, normalized by the exact value $G_a$, for an interface crack in an infinite plate.

![Graph showing the effect of specimen aspect ratio on the computed $G$, normalized by the exact value $G_a$.]

Figure 3.6: Computed SIFs, energy release rate and mode angle as a function of the distance to the crack tip for a mismatch of $E_1/E_2 = 40$; the results have been obtained for three different element sizes and have been normalized using the analytical values of table 3.1.

![Graphs showing the computed SIFs, energy release rate, and mode angle as a function of the distance to the crack tip for different element sizes.

Table 3.1: Material properties and analytical SIFs

<table>
<thead>
<tr>
<th>Mismatch</th>
<th>$E_1$ [GPa]</th>
<th>$E_2$ [GPa]</th>
<th>$\nu_1$</th>
<th>$\nu_2$</th>
<th>$\varepsilon$</th>
<th>$K_1$</th>
<th>$K_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.01</td>
<td>200</td>
<td>198</td>
<td>0.25</td>
<td>0.25</td>
<td>-5.33e-4</td>
<td>1.26e7</td>
<td>-4.41e4</td>
</tr>
<tr>
<td>3</td>
<td>206.84</td>
<td>68.948</td>
<td>0.3</td>
<td>0.22</td>
<td>-0.0656</td>
<td>1.15e7</td>
<td>-5.30e6</td>
</tr>
<tr>
<td>40</td>
<td>200</td>
<td>5</td>
<td>0.25</td>
<td>0.25</td>
<td>-0.1045</td>
<td>9.90e6</td>
<td>-8.13e6</td>
</tr>
<tr>
<td>100</td>
<td>200</td>
<td>2</td>
<td>0.25</td>
<td>0.25</td>
<td>-0.1080</td>
<td>9.73e6</td>
<td>-8.36e6</td>
</tr>
</tbody>
</table>

Table 3.1: Material properties and analytical SIFs
energy release rate and mode angle. The horizontal axis represents the dimensionless distance from the crack tip; the vertical axis is normalized to the analytical solution. For the mode angle $\psi$ a reference length of $2a$ was used. In each of the diagrams, the node closest to the crack tip shows a large deviation from the rest of the curve. This behavior was also seen with non quarter point elements in the homogenous plate in figure 3.2, indicating that the stress singularity in an interface is not exactly described by the quarter point elements. Mesh refinement does give results closer to the analytical value but the inaccurate value at the first node persists. For all mesh sizes the maximum value of $G(r)$ seems to give the best estimate. Extrapolation from the straight segment may provide more accuracy but is not necessary as the maximum value for all meshes lies within an error of 1%.

Figure 3.7: Computed normalized energy release rate for the interface crack using different values of the elastic mismatch

In figure 3.7 energy release rate is shown for four different material combinations. The mesh size at the crack tip is $31.25 \cdot 10^{-3} \text{mm}$. The material combination with mismatch 1.01 is close to the homogeneous situation. The energy release rate is almost exact in the node closest to the crack tip, as would be be expected for the truly homogeneous material. Increasing the mismatch between the materials introduces an increasing error in this node because the quarter point elements no longer provide the right description of the singularity. However, the energy release rate at some elements away from the tip and the constant slope seem to be unaffected.

<table>
<thead>
<tr>
<th>Mismatch</th>
<th>mesh size [\text{mm}]</th>
<th>$G_{\text{analytical}} [\text{N/m}]$</th>
<th>$J$ Marc [\text{N/m}]</th>
<th>Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.01</td>
<td>31.25</td>
<td>740.03</td>
<td>740.81</td>
<td>0.105</td>
</tr>
<tr>
<td>3</td>
<td>31.25</td>
<td>1394.1</td>
<td>1395.5</td>
<td>0.100</td>
</tr>
<tr>
<td>40</td>
<td>15.6</td>
<td>14170</td>
<td>14179</td>
<td>0.063</td>
</tr>
<tr>
<td></td>
<td>31.25</td>
<td>14170</td>
<td>14183</td>
<td>0.092</td>
</tr>
<tr>
<td>100</td>
<td>31.25</td>
<td>34763</td>
<td>34793</td>
<td>0.086</td>
</tr>
</tbody>
</table>

Table 3.2: Accuracy of FEM output by contour integral evaluation

Table 3.2 compares the $J$-integral from the FEM output with the analytical solution combining
(3.2) and (2.11). The FEM model does describe the interface crack well. The errors in the J-
integral values are much smaller than those in the $G$ computed from the COD, as shown in figure
3.6. This shows that the values computed via the COD are more sensitive to the inability of
the quarter point elements to pick up the proper singularity than the $J$-integral method. Figure
3.8 shows that quarter point elements still do a better job for interface fracture problems than
ordinary quadratic or linear elements.

![Figure 3.8: Computed energy release rate for linear, quadratic and quarter point elements, using
a mismatch of 40](image)

### 3.3 Penny-shaped crack

#### 3.3.1 Problem description

In the next benchmark problem we consider two dissimilar materials that are connected by an
interface lying in the $x$–$y$ plane, except for a circular area $r < a$. This crack is axisymmetric
around the $z$-axis, with the origin placed in the center of the crack. The size of the elastic half-
spaces are large compared to the radius of the crack $a$. When subjected to a far field stress $\sigma_{zz}$
the crack surface remains traction free, $\sigma_{zz} = 0$. The solution for the stresses around the crack
was obtained by Willis [26] and the stress intensity factors are given by Kassir and Bregman [12]:

$$K_1 + iK_2 = 2\sigma_{zz}\sqrt{a}\frac{\Gamma(2 + i\varepsilon)}{\Gamma(1 + i\varepsilon)}(2a)^{-i\varepsilon}$$

(3.5)

Note that Kassir and Bregman use a different definition of the stress intensity factors from
the one used here, as they use an extra $1/\sqrt{\pi}$ factor in their definition of the SIFs. In (3.5) the
$\text{Gamma function}$ is used, which is defined as:

$$\Gamma(z) = \int_{0}^{\infty} t^{z-1}e^{-t}dt$$

(3.6)

![Figure 3.9: A penny-shaped crack](image)
3.3.2 Results using an axisymmetric and a 3D model

The model of the bimaterial interface problem in an infinite plate of section 3.2 has been used as a basis for the penny-shaped crack problem. Mesh size, loading and crackwidth $a$ are the same, with the exception that for the penny-shaped crack axisymmetric elements were used. A second model using 3D elements was made, covering a quarter of the geometry, see figure 3.9. The mismatch is 40, half crack width $a$ is $5\,mm$ and the domain size is $400\times400\,mm$. The far edges are constrained in radial direction. The element size at the crack tip is $62.5\,\mu m$. The far field stress $\sigma_{zz}$ is $100\,MPa$.

![Energy release rate and mode angle comparison](image)

Figure 3.10: Energy release rate and mode angle, a comparison between axisymmetric and 3D penny-shaped crack

Figure 3.10 shows a comparison between the results of the axisymmetric and the 3D model. The energy release rate from the COD method is divided by the analytical value, $G_a = 5761.1\,N/m$. The results are very similar to those of the plane strain problem as given in figure 3.6. The quarter point element thus gives comparable results for both plane strain, axisymmetric and 3D problems.
3.4 Semi-infinite interface crack in a bilayer

3.4.1 Problem description

Liechti and Chai [13] presented a plane strain, bimaterial interfacial specimen as an experimental geometry covering a large range of the mode mixity $\psi$. It consists of two layers of dissimilar materials, $E_1$, $\nu_1$, thickness $h$ and $E_2$, $\nu_2$, thickness $H$, see figure 3.11. The elastic material properties for both layers can be chosen arbitrarily. A crack with semi-infinite length is present along the bonding line. The bottom layer is rigidly clamped, the top layer is rigidly gripped and can be subjected to displacements in $x$- and $y$-direction. A vertical displacement $V$ subjects the crack to an opening load, a horizontal displacement $U$ to a shear load. By combining these displacements different modes can be chosen, varying from pure opening mode to pure shear mode.

![Figure 3.11: Crack in a bimaterial interface](image)

The analytical solution for the stress intensity factors of this semi-infinite crack is provided by Hutchinson and Suo [10]:

$$K = h^{-1/2} e^{i\omega} \left( \frac{E^*}{1 - \beta^2} \right)^{1/2} \left[ \frac{V}{\sqrt{2}} \left( \frac{h}{E_1} + \frac{H}{E_2} \right)^{-1/2} + i \frac{U}{\sqrt{2}} \left( \frac{h}{\mu_1} + \frac{H}{\mu_2} \right)^{-1/2} \right]$$

(3.7)

where $E^* = \frac{2E_1E_2}{E_1+E_2}$, $E_i = \frac{2\mu_i(1-\nu_i)}{1-2\nu_i}$ and $\omega$ is a real quantity depending on $\mu_1/\mu_2$, $\nu_1$, $\nu_2$ and $h/H$ [10]. The mode angle is provided by Liechti and Chai [13], for a reference length equal to the layer thickness $h = H$:

$$\psi = \tan^{-1} \left( \frac{Im[Kh^{i\varepsilon}]}{Re[Kh^{i\varepsilon}]} \right)$$

(3.8)

This benchmark was simulated with a Marc FEM model. Simulations were performed with two material combinations and three loading conditions. The layer thicknesses were chosen equal, $h = H = 1m$. The total length along the $x$-direction is $50m$, the length of the crack is $25m$, i.e. well beyond the $L > 2h$ condition of Liechti and Chai [13]. The material properties used are shown in table 3.3. The opening mode was applied by a displacement $V = 10^{-3}m$, the sliding mode by a displacement $U = 10^{-3}m$, and the combined opening and sliding mode by both values simultaneously. To avoid interpenetration of the materials the MSC Marc contact option is used.

<table>
<thead>
<tr>
<th>mismatch</th>
<th>$E_1$</th>
<th>$E_2$</th>
<th>$\nu_{1,2}$</th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>$\varepsilon$</th>
<th>$\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10000</td>
<td>10000</td>
<td>0.33</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0°</td>
</tr>
<tr>
<td>10</td>
<td>10000</td>
<td>1000</td>
<td>0.33</td>
<td>0.8182</td>
<td>0.2076</td>
<td>-0.0671</td>
<td>-13.6°</td>
</tr>
</tbody>
</table>

Table 3.3: Material properties semi-infinite interface crack
3.4.2 Results

Figure 3.12 shows the normalized SIFs for a semi-infinite crack in a homogenous material, mismatch 1, for three loading conditions. The graphs have a constant slope and the SIFs at the node closest to the crack tip are the most accurate. This was also seen earlier in figure 3.2 for quarter point elements used for cracks with homogeneous materials.

![Normalized SIFs for a semi-infinite crack in a homogenous material](image1)

Figure 3.12: Computed, normalized SIFs for the semi-infinite crack in a homogeneous material

Figure 3.13 shows the normalized SIFs and mode angle for a material combination with a mismatch of 10. The difference with the analytical solution is larger than for the previous benchmarks. A reason could be that the boundary conditions for this problem are close to the crack. For opening and combined loading $K_1$ and $K_2$ are most accurate close to the crack tip, with reasonable error, see table 3.4. The error in $K_2$ is the largest. Evaluating the contact zone size given by equation (2.17) gives for opening $r_c = 1.4209 \cdot 10^{-11} m$, opening and sliding $r_c = 1.4952 \cdot 10^{-8} m$ and sliding $r_c = 0.2119 m$. For the sliding mode load the contact area is therefore almost of the same order of magnitude as the thickness $h$, so the stress field given by the analytical solution can be considered inaccurate.

![Normalized SIFs and mode angle for a material combination with a mismatch of 10](image2)

Figure 3.13: Computed SIFs and mode angle for the semi-infinite crack in an interface, for a mismatch of 10

The FEM model does seem to represent the benchmark problem well if the energy release rate is observed. The contour integral $J$ from the FEM output agrees well with the analytical solution,
Table 3.4: Stress intensity factors for the semi-infinite interface crack, for a mismatch of 10

<table>
<thead>
<tr>
<th></th>
<th>Analytical</th>
<th>COD</th>
<th>Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Opening</td>
<td>$K_1$</td>
<td>1.1647</td>
<td>1.1494</td>
</tr>
<tr>
<td></td>
<td>$K_2$</td>
<td>-0.2818</td>
<td>-0.2951</td>
</tr>
<tr>
<td>Opening &amp; sliding</td>
<td>$K_1$</td>
<td>1.3067</td>
<td>1.2855</td>
</tr>
<tr>
<td></td>
<td>$K_2$</td>
<td>0.3049</td>
<td>0.2910</td>
</tr>
<tr>
<td>Sliding</td>
<td>$K_1$</td>
<td>0.1419</td>
<td>0.2463</td>
</tr>
<tr>
<td></td>
<td>$K_2$</td>
<td>0.5867</td>
<td>0.5411</td>
</tr>
</tbody>
</table>

Table 3.5: Energy release rate for the semi-infinite interface crack, for a mismatch of 10, as computed by different methods

<table>
<thead>
<tr>
<th></th>
<th>$G_{\text{analytical}}$</th>
<th>$J_{\text{Marc}}$</th>
<th>$G_{\text{COD}}$</th>
<th>$G_{\text{COD}}$ Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Opening</td>
<td>6.7348e-4</td>
<td>6.7289e-4</td>
<td>6.6041e-4</td>
<td>-1.94</td>
</tr>
<tr>
<td>Opening &amp; sliding</td>
<td>8.4436e-4</td>
<td>8.4436e-4</td>
<td>8.1471e-4</td>
<td>-3.64</td>
</tr>
<tr>
<td>Sliding</td>
<td>1.7088e-4</td>
<td>1.7088e-4</td>
<td>1.6579e-4</td>
<td>-5.09</td>
</tr>
</tbody>
</table>

as can be seen in table 3.5.
Chapter 4

Buckling delamination

4.1 Literature

In buckling driven delamination of thin films the interface between the film and substrate fails and the film bends away from the substrate to relax its compressive stress. The buckling starts when a critical externally applied stress is reached in the case of classical Euler buckling. The height of the buckle increases with increasing stress. When the debonded area grows, the buckle becomes wider or longer and more energy is released. The delamination front can be regarded as an interface crack in the spirit of the previous chapters. The interface strength is strongly dependent on the mode mixity and, in fact, interfaces are typically tougher in mode II than in mode I loading. The buckle morphology influences the loading of the crack tip, i.e. the mode angle, and therefore the geometry of the buckle is of importance in predicting the preferred direction in which the buckle will grow. In this chapter we will discuss the transition between a straight sided buckle and a telephone cord buckle with a FEM model made for buckling in thin films. First a brief overview is given on research that can be found in literature regarding telephone cord buckling.

4.1.1 Straight-sided vs telephone cord buckles

In experiments long, straight buckles and curved, telephone cord like buckles are observed [1, 7, 15]. In plane strain or biaxial compression a straight buckle releases energy only in transversal direction, whereas the longitudinal compression remains present. This may induce secondary buckling phenomena such as telephone cord buckling. Audoly et al. [3] analyzed the stability of the straight sided buckle, suggesting that the residual stresses can induce symmetric or anti-symmetric secondary buckling. Above a certain Poisson ratio, \( \nu = 0.255 \), anti-symmetric secondary buckling, or telephone cord buckling, is the most likely to occur. Audoly et al. suggest that due to the secondary buckling of a straight sided blister, the undulations are transmitted to the tip, preventing straight propagation [3].

Moon et al. [15] investigated the residual stresses in telephone cord buckles. Diamond like carbon films on glass substrates showed telephone cord buckling after depositing the film. Samples were sliced using a focused ion beam (FIB) cutter and the profile was analyzed by atomic force microscopy (AFM). The difference in the profile of the buckle height before and after cutting was used to calculate the residual stresses in the buckled film. The profile and residual stresses in the telephone cord buckles are very close to analytical models of axisymmetrical buckles. The front of the telephone cord buckle is best described by a circular buckle with radius \( r = b \), bonded at the edge, while a unit segment along the length of the telephone cord buckle is best modeled by a circular buckle pinned at its center with radius \( r = 2b \). An example of a unit segment and a pinned buckle are given in figure 4.1. The energy release rate and mode mixity of these pinned and unpinned circular buckles were used to describe the telephone cord buckle morphology. It was concluded that at high stresses the interface toughness decreases due to the change in mode angle and straight buckling was not the preferred direction [15]. It has to be noted that the
energy release rates and mode angles for these circular buckles are constant because the models are axisymmetrical. This analysis therefore does not give a detailed description of these variables along the front.

Jensen and Sheinman [11] made a numerical analysis of a straight sided buckle, with a semi-circular front in a uniform material under biaxial compression. The energy release rate and mode angle were calculated along the straight sides and the front. It was found that at low stress states, $\sigma/\sigma_c < 5$, the front has a constant radius and the buckle advances in a straight line, leaving behind straight edges. Different elliptical shapes of the growing front where investigated and the circular shape has the least variation in the mode angle. A crack propagation criterium based on the mode I stress intensity factor was used. For $\sigma/\sigma_c > 2.5$ the mode I SIF along the front is higher than at the sides, indicating growth at the front. At high stresses the shape of the advancing front changes and the buckle is more likely to follow a curved path. In this way more elastic energy stored in the film is released. A maximum in the released energy was found when the radius of the telephone cord curve $R_0$ equals the buckle width $2b$. In this study a uniform material was used and the additional compliance of the substrate was thus not taken into account.

4.1.2 Substrate compliance

In flexible displays the top layer has the highest stiffness of all the layers, with a typical stiffness of 150 GPa. The energy released with a compliant substrate, typically 6.5 GPa, is higher than with a stiff substrate [8, 28]. Because its influence on the released energy and on the interface toughness through the mode angle, it is important to include the lower stiffness of the substrate in the buckling analysis.

Parry et al. [16] compared straight sided buckle profiles, measured using AFM, with a FEM model. Furthermore they extended the model for various substrate compliances, from a very stiff substrate, $\alpha = -1$, to a very compliant substrate, $\alpha = 0.98$. For a stiff substrate the film is clamped at the edges and there exists a very sharp transition between the stress in the bonded part of the film and stress in the relaxed, delaminated film. With a stiff film and a more compliant substrate this transition is much smoother [16]. The edge on which the strain is applied, in a FE model for instance, should be far away from this transition.

Hutchinson and Suo [10] showed that the average energy release rate for a stiff substrate is not limited and is proportional with $\varepsilon^2$. With this information, it is expected that the buckle width increases with the applied stress, and the buckle will spread sideways. The mode II component of the energy release rate also increases, and eventually reaches pure shear at some point, resulting in a stronger interface according to (2.14). This is seen as the main reason why straight sided buckles have characteristic widths, and tunnel at the tip instead of becoming wider. Cotterel and Chen [8] found for very compliant substrates, and high $b/h$ ratios, that there is a maximum in the average energy release rate. This indicates that for compliant substrates the sideways growth of the buckle is limited by the increase in mode mixity and by a maximum in the energy release rate.
4.2 Straight sided buckling

First we will consider a straight sided buckle to illustrate the buckling phenomenon. A straight sided buckle contains a straight sided part with constant width \(2b\) and a circular front with radius \(b\). A schematic representation can be seen in figure 4.2. The thickness of the film is denoted as \(h\). Bending of this thin film system can be represented by plane strain loading, cooling down by biaxial compression. The amount of elastic energy stored in the film is a measure of the energy released after buckling.

4.2.1 Plane strain loading

The energy stored in a plate in plane strain compression, \(\varepsilon_y = \varepsilon, \varepsilon_x = 0\) and \(\sigma_z = 0\), per unit of volume before buckling is:

\[
U_1 = \frac{1}{2} \frac{E}{1-\nu} \varepsilon^2 \tag{4.1}
\]

If the film can release all the elastic energy by buckling, there is no elastic energy left in the straight part far behind the front:

\[
U_2 = 0 \tag{4.2}
\]
\[ G_0 = (U_1 - U_2)h = \frac{E_f \varepsilon^2 h}{2(1 - \nu^2)} \quad (4.3) \]

For the straight sided part of a buckle, well behind the curved front, in steady state, the energy release rate was derived by Hutchinson and Suo [10]:

\[ G_{\text{side}} = G_0 \left( 1 - \frac{\sigma_c}{\sigma} \right) \left( 1 + 3 \frac{\sigma_c}{\sigma} \right) \quad (4.4) \]

with \( E_f \) and \( \nu_f \) the Young’s modulus and Poisson’s ratio of the film respectively. \( G_{\text{side}} \) has a peak at \( \sigma/\sigma_c = 3 \), and approaches \( G_0 \) for large stresses. The critical buckling stress, \( \sigma_c \), for Euler buckling in a clamped-clamped film:

\[ \sigma_c = \frac{\pi^2}{12} \frac{E_f}{(1 - \nu^2)} \left( \frac{h}{b} \right)^2 \quad (4.5) \]

In analogy the substrate should be much stiffer than the film, \( E_s \gg E_f \). The film thickness \( h \) is small compared to the buckle width \( b \), so \( h/b \ll 1 \). The accompanying critical buckling strain for plane strain conditions is:

\[ \varepsilon_c = \frac{\pi^2}{12} \left( \frac{h}{b} \right)^2 \quad (4.6) \]

### 4.2.2 Biaxial strain loading

Buckling occurring in flexible displays during the manufacturing process is mainly caused by the cooling down of the deposited film, causing biaxial stress. The energy per unit volume stored in a film or a plate under biaxial strain, \( \varepsilon_x = \varepsilon_y = \varepsilon \), \( \sigma_z = 0 \), is:

\[ U_1 = \frac{E}{1 - \nu} \varepsilon^2 \quad (4.7) \]

Buckling can release the transversal energy in the film, but the energy from the longitudinal strain, along the buckle, remains in the film, which makes the residual energy:

\[ U_2 = \frac{E \varepsilon^2}{2} \quad (4.8) \]

![Figure 4.4: Plate subjected to a compressive biaxial strain \( \varepsilon \), before 1) and after 2) buckling](image)

The maximum energy per unit area available for buckling is therefore calculated from \( U_1 - U_2 \):

\[ G^*_0 = \frac{(1 + \nu)}{2} \frac{E \varepsilon^2 h}{1 - \nu} \quad (4.9) \]
The critical buckling stress for biaxial stress is equal to the case of plane strain. The critical buckling strain is therefore lower than in plane strain:

\[ \varepsilon_c^* = \frac{\pi^2}{12} \frac{1}{1 + \nu} \left( \frac{h}{b} \right)^2 \]  

(4.10)

### 4.2.3 The circular front

Hutchinson and Suo [10] showed that the energy release rate is not constant along the buckle. The average, steady state energy release rate along the curved front is:

\[ G_{ss} = G_0 \left(1 - \frac{\sigma_c}{\sigma} \right)^2 \]  

(4.11)

The energy released at the front is lower than at the sides, \( G_{ss} < G_{side} \) for all \( \sigma/\sigma_c \), which implies that the crack will grow along the sides rather than at the front, and the buckle width \( b \) will increase. However, experiments show that buckles are of characteristic width and grow along the curved front in a straight or telephone cord like way [1]. It appears that the mode mixity is of importance, as the interface toughness is dependent of the energy release rate and the mode angle [10]. Note that the above derivation for the curved front and the straight sides is true for a clamped-clamped plate or a film on a rigid substrate, but in flexible displays, other multilayer systems and coatings, the top layer is typically stiffer than the substrate, changing the mode mixity and influencing the propagation. Also \( G_{ss} \) is a value averaged over the front, and does not give a detailed description of the energy release rate along the front. A FE model can provide a detailed description of the energy release rate and the mode angle along the front.

### 4.3 FE model of a straight sided buckle

In this section a FE model is compared with the analytical solution for the straight sided part mentioned previously, \( G_{side} \). As choices have to be made regarding film and substrate thickness, material properties and buckle width, these values are chosen equal to those from the experiments performed by Abdallah et al. [1]. They observed telephone cord buckling in Si\(_3\)N\(_4\) layers, \( E_f = 150\) GPa, \( \nu_f = 0.3 \) with a layer thickness of 400nm. The substrate is a hard coat, \( E_s = 6.5\) GPa, \( \nu_s = 0.3 \), with thickness 3\( \mu \)m. The Dundur’s parameter \( \alpha \) is 0.92. After oxygen plasma treatment telephone cord patterns were observed. The average width of the buckles was 31\( \mu \)m.

To initiate the out of plane buckling, elements in the debonded part of the film are raised from the substrate. The size of this initial flaw is 0.5% of the film thickness at \( y = 0 \) and zero just outside the crack tip mesh. The elements at the tip are collapsed quarter point elements with sides of 25nm, and the half crack tip mesh size is 1/4th of the film thickness. The three dimensional elements are forming a film and substrate combination, which is shown in figure 4.5. The strain is gradually increased until the maximum of 10\( \varepsilon_c \) is reached.

![Figure 4.5: FE model of the straight part of a buckle](image)

According to Parry et al. [16] the in-plane size of the bonded part of the film should be sufficiently large to avoid influence on the buckling mode because the edge must be far away from
the stress singularity at the tip. The FE models that are used in this study have an in plane size of $10b$.

4.3.1 Straight sided buckling, numerical validation

In this section a FE model of the straight sided part is used to validate the results with the theory from the previous section. Symmetry with respect to the $y$-axis is assumed. The load in incrementally applied at the far edge, $y = 10b$. Figure 4.6 shows the energy release rate as a function of the applied strain, for a straight sided buckle in plane strain and in a biaxial strain state. The substrate has the same elastic properties as the film, $E_s = E_f = 150\text{GPa}$. This can be regarded as a relatively stiff substrate [8]. In the left hand graph it is clearly seen that more energy is released in a biaxially stressed film. The difference almost disappears when the energy release rate is divided by $G_0$ from (4.3) or (4.9) and the strain by $(4.6)$ or $(4.10)$ from the previous section, as can be seen in the right diagram.

![Figure 4.6: Energy release rate for a straight sided buckle in a homogeneous crack, for plane strain or biaxial strain](image)

In figure 4.7 the influence of the substrate compliance on the energy release rate is shown for plane strain. As the normalized solutions for plane strain and biaxial stress coincide, only plane strain is used here. The energy release rate and the strain are normalized with $\varepsilon_c$ and $G_0$ from (4.3) and (4.6). The top layer is a Si$_3$N$_4$ layer, $E_f = 150\text{GPa}$, $\nu_f = 0.3$. The material properties of the substrate were varied to investigate the influence on the buckling. The energy release rate for the compliant substrate, $E_s = 6.5\text{GPa}$, is the highest in the graph. This was also found by Cotterell and Chen [8], as well as Yu and Hutchinson [28]. The peak lies just before $\varepsilon/\varepsilon_c = 3$ because the film on a compliant substrate starts buckling earlier, due to the rotation and displacement at the buckle edge. For the substrate with elastic properties equal to the film, less energy is released compared to the more compliant substrate. It is very close to the case of a stiff substrate, where the Young’s modulus of the substrate is taken 100 times stiffer than the film. That solution is almost equal to the analytical $G_{side}$ from (4.4). From $\varepsilon/\varepsilon_c > 2$ contact occurs between the film and substrate near the crack tip. This contact shields the crack tip as mentioned by Cotterell and Chen [8] and the Euler buckling theory is not valid anymore. From $\varepsilon/\varepsilon_c > 4$ the FEM solution starts to differ from $G_{side}$.

4.3.2 Interface behavior in straight sided buckling

To illustrate the influence of substrate compliance on mode mixity and interface strength, a comparison between a crack with a compliant substrate, and one with a relatively stiff, $E_s = E_f$, substrate is made. With a stiffer substrate the results would be influenced by contact close to the crack tip. For determining the mode angle a choice has to be made regarding the reference length. Here the film thickness is chosen as a reference length, in section 4.6 the influence of this choice is
debated. The interface toughness $\Gamma$ is derived with (2.14). For the fracture toughness parameters $G_i^c = 0.3\, J/m^2$ and $\lambda = 0.3$ are chosen.

The comparison is shown in figure 4.8. From the top left graph it can be seen that for a compliant substrate, the energy released by buckling is more than twice as high as for a film on a stiffer substrate. The mode angle at the crack tip, shown in the top right graph, is closer to mode I, and consequently the interface strength $\Gamma$ in the bottom left graph is lower. For the stiff substrate there is contact with the film at strains higher than $9\varepsilon_c$ as the mode angle reaches $\pi/2$. The bottom right graph shows the energy release rate $G$ divided by the interface strength $\Gamma$. The crack in the more compliant substrate is 3 times more likely to propagate than with a stiffer substrate. This shows that the maximum energy release rate is not sufficient but that the mode angle is also important for the prediction of crack propagation.

In figure 4.9 the buckle height is shown for the same simulations as in figure 4.8. The height of the delamination in the middle of the buckle, at $y = 0$, is divided by the film thickness $h$. Buckling starts at $\varepsilon = \varepsilon_c$. The film on a compliant substrate shows a larger deformation.

For a compliant substrate more energy is released through buckling of the film. In figure 4.10 the strains in a compliant and a stiff substrate are shown along the path $0 < y < 3b$. Far away from the crack, which lies at $y/b = 1$, the strain in the stiff substrate is equal to the applied load, $10\varepsilon_c$. In the debonded part the substrate is compressed more by the applied strain, as the debonded film does not contribute to the load distribution. If the substrate is compliant, this compression is much larger. The weak substrate must distribute the entire load and experiences a larger deformation.

### 4.4 FE model of straight sided buckle with a circular front

In this section the FEM model is expanded to a 3D representation of a delaminated buckle, including a straight side and a circular front, according to figure 4.2. The length of the straight sided part is $3b$ and the front is a half circle with constant radius. With this model the fracture parameters along the entire front can be determined. In the former section the solution for the straight sided part was presented. With a 3D model, including the front, a good estimation can be made of the location along the edge where a buckle will grow. For the interface fracture parameters, $G_i^c = 0.3\, J/m^2$ and $\lambda = 0.3$ are chosen. Buckling delamination in a flexible display is mostly occurring during the manufacturing process from cooling down and by bending the device during usage. They can be represented as biaxial compression and as compression in plane strain respectively. As shown in the previous section, the stress states have no influence on the straight sided part, but differences may be found at the front.

The origin of the orthogonal coordinate system lies in the center of the circular front, the
Figure 4.8: Fracture parameters for compliant and stiff substrate, for straight sided buckle in plane strain

Figure 4.9: Buckle height of buckle with stiff and compliant substrate, for straight sided buckle in plane strain

straight sides are parallel to the $x$-axis and the interface lies at $z = 0$. An example of the FEM model is shown in figure 4.11. Symmetry is assumed for $y = 0$, and the strain is applied on the film and substrate at the far edges. $z$–displacement is restricted at $z = -H$. The film consists of 3400 quadratic elements, with 6 elements in thickness direction. The substrate, where the displacements are smaller, also contains 3400 quadratic elements, but spread over a larger thickness. To indicate the position along the edge of the buckle the angle $\theta$ is used. Straight ahead in the circular front $\theta = 0$, while $\theta = \pi/2$ represents the transition from the curved front to the straight side. Infinitely far behind the front $\theta$ approaches $\pi$. 
Figure 4.10: The $y y$–component of the total strain in the substrate, for a relatively stiff and a compliant substrate, the applied load is $10 \varepsilon_c$.

Figure 4.11: FE model of a buckle with straight side and circular front.

4.4.1 Plane strain results

In figure 4.12 the energy release rate $G$, mode angle $\psi$ and interface toughness $\Gamma$ for a buckle in a uniform material are shown for plane strain, with the strain applied in $y$-direction. The strain is increased incrementally to a maximum of $\varepsilon = 15 \varepsilon_c$. Because the mode angle shows large variations at low stresses, and the energy release rate is then still low, the first increments of the simulation are not shown. The graphs start at approximately $1.5 \varepsilon_c$. The top left diagram shows the energy release rate along the front for increasing strain. At high strains, approaching $\varepsilon = 15 \varepsilon_c$, the most energy is released at the circular front at $\theta = 0$. This may seem to contradict the assumption that $G_{ss} > G_{side}$, from (4.4) and (4.11), but $G_{ss}$ only gives an average energy release rate over the entire front, $0 < \theta < \pi/2$. Only a small part of the front has an energy release rate higher than that at the straight side. Far behind the front, at $\theta = 0.9 \pi$, the energy release rate $G$ is almost $1.5 N/m$, this is the same result as was shown earlier in figure 4.8 for the straight sided part. The top right diagram shows the mode angle. At the place of the highest energy release rate, the mode angle is closest to zero, implying a high mode I component. This leads to the lowest interface strength, $\Gamma$, in the bottom left graph. The energy release rate is highest at the front, and also the interface is expected to be the weakest there. There is no contact between the substrate and the film at $0 < \theta < \pi/4$. The buckle growth direction will possibly be straight ahead because the high value of energy release rate combined with a large mode I component. The buckle might become wider at low stresses, because the energy release rate is relatively high at the straight side, but at high stresses the crack will see a large mode II component and eventually pure shear. At $\theta = 0.9 \pi$ the mode angle drops below $-\pi/2$. The Mentat postprocessing shows a small penetration. In a model with a coarser mesh but with the same properties this effect was greater. According to the MSC Marc manual a lower order, linear element type is preferred in contact analysis. The quadratic element type used in this FE model however is more suited to the large bending deformations, and the quarter point elements are proven to be more accurate for the crack analysis.
Figure 4.12: Fracture parameters for a 3D FE model under plane strain, relatively stiff substrate, maximum applied strain is $15\varepsilon_c$.

For a substrate that is more compliant, $E_f = 150GPa$ and $E_s = 6.5GPa$, the results are shown in figure 4.13. The energy release rate is twice as high over almost the entire buckle. This was already shown for the straight side in figure 4.8. At the front the mode angle is closer to mode I, compared to the crack in a uniform material. At the transition from the front to the straight side the mode angle drops below $-\pi/2$ and only at high stresses there is compressive contact between $\pi/3 < \theta < \pi/2$. The mode angle $\psi$ there reaches $-0.6\pi$. The solution is not a smooth line there, which is seen amplified in the graph for $\Gamma$. An elastic mismatch between the materials worsens the results for contact. Because this occurs at the place where the interface toughness is high and the energy release rate is low, it does not influence the bottom right graph, which shows that the favorable propagation direction is still straight ahead. It can be concluded that for plane strain, for stiff and compliant substrates, straight sided buckling is preferred over telephone cord buckling.

4.4.2 Biaxial strain results

These simulations are repeated for biaxial strain. The crack propagation parameters for a buckle in a uniform material are shown in figure 4.14. This model is similar to the model used by Jensen and Sheinman [11], and consists of a symmetrical buckle, half width $b$, straight part $3b$, and a semi-circular front with radius $b$, in a uniform material under biaxial compression. The results are similar. The energy release rate is low at the front and the maximum lies between $0.55\pi < \theta < 0.6\pi$, just behind the front. Jensen and Sheinman [11] found for $\varepsilon/\varepsilon_c = 2$ that the maximum lies at $b/2$, $\theta = 0.65\pi$ behind the front. The energy release rate at the straight sided part is higher than at the front. The mode angle, however, is closer to mode II, so in spite of the higher energy release rate compared to the circular front, the buckle is not likely to become wider. Instead the buckle will grow at the transition part. The variation of the mode angle along the front and the straight side is much smaller than the variation of the energy release rate, as was concluded by Jensen and Sheinman [11]. The maximum strain Jensen and Sheinman used was $8\varepsilon_c$. Only at strains close to $10\varepsilon_c$ compressive contact is observed at the straight side. For strains above $10\varepsilon_c$ there was penetration of the substrate by the film over a large area, although the contact option op in the Marc program was enabled. These results are not reliable and the strains shown in figure 4.14 are therefore limited to $10\varepsilon_c$. 

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Figure 4.13: Fracture parameters for a 3D FE model under plane strain, maximum applied strain is $15\varepsilon_c$.

Figure 4.14: Fracture parameters for a biaxial strained 3D FE model, relatively stiff substrate, maximum applied strain is $10\varepsilon_c$.

For the more compliant substrate the results are shown in figure 4.15. The geometry, elastic properties and buckle width are chosen equal to experiments by Abdallah et al. [1]. The energy release rate for the straight side is equal or slightly larger than at the front for the entire range of applied strains. At $\varepsilon = 10\varepsilon_c$ both are about $3N/m$. The load was increased to $15\varepsilon_c$. For plane strain loading this did not change the trend in the energy release rate but rather showed contact over a wider area. For biaxial compression the profile of the normal displacement changed at higher stresses. The most energy is released at the front, but over a wider range than in plane strain, and the peak lies close to $\theta = \pi/4$, and not straight ahead like in plane strain. The mode
angle shows a large mode I component at the front, the straight sides are mostly loaded in mode II. The bottom right graph shows that the crack is most likely to propagate at the front, \( \theta = \pi/4 \), and not at the straight side. In literature on buckling in thin films the energy release rate \( G \) is regarded as the most important crack propagation parameter. If a certain value of \( \Gamma \) is reached the delamination can grow. The crack is now not assumed to propagate at the place of the highest energy release rate, because the interface is strong there. For biaxial stress the mode angle and the compliance of the substrate have shown to be of great importance in predicting the crack propagation.

![Diagram](image1)

Figure 4.15: Fracture parameters for a biaxial strained 3D FE model, maximum applied strain \( 15\varepsilon_c \).

These results can be made more visible by the normal displacement profile of the buckle. The contour bands of the displacement in \( z \)-direction of the film are shown in figure 4.16. If the \( z \)-displacement is regarded as an indication of mode I loading, it is easy to verify the conclusions from figure 4.15.

![Diagram](image2)

Figure 4.16: Contour bands of the displacement in \( z \)-direction for a buckle in a film with compliant substrate under biaxial straining, \( 15\varepsilon_c \).

In figure 4.17 for all \( \varepsilon/\varepsilon_c \) the angle is shown where the maximum value of \( G/\Gamma \) is present. For plane strain, \( G/\Gamma \) shifts from the straight side to \( \theta = 0 \) at \( \varepsilon = 3\varepsilon_c \), for both substrates. For strains below \( 3\varepsilon_c \) the maximum in \( G/\Gamma \) lies at the straight side. In biaxial compression the results are more interesting. For a stiff substrate it will approach \( \theta = \pi/2 \) for increasing strain. On a compliant substrate however, the maximum shifts to the front for strains above \( 4\varepsilon_c \), but at high strains, above \( 10\varepsilon_c \), it shifts back to \( \theta = \pi/4 \). Although this is only indicative because figure
4.17 only show the maximum value of $G/\Gamma$ and not the range with the highest values, it can be expected that telephone cord buckling will not occur in plane strain.

![Figure 4.17: Location of maximum $G/\Gamma$ for 3D FE model](image)

**4.5 Influence of buckle front shape**

**4.5.1 Elliptical shape**

In plane strain loading conditions, a crack is expected to grow along a straight line. To simulate this, the circular front of the mesh used previously is given an elliptical shape. Two sizes of a sharp front are made with the largest semi-axis along the assumed growth direction, 20% larger and two times larger than the circular radius. To avoid the contact problem the maximum load applied here is $10\varepsilon_c$. For plane strain the trend in $G$ and $\psi$ is not altered by the higher strains used earlier. The results at the end of the load, $\varepsilon = 10\varepsilon_c$, are shown combined in figure 4.18. For the comparison the buckle with a circular front is included and a blunt front is simulated with a 20% smaller radius in that direction. The energy release rate for the elliptical shape with radius 1.2$b$ differs very little from a circular shape. The mode angle is slightly higher at the front and lower behind the front. These changes are more clear for the elliptical shape with half-axis 2$b$. If the front is elongated there is no contact at the transition to the straight side, and $G$ and $\psi$ seem to be more smooth. The trend in $G$ and $\psi$ does not change much.

If we look at figure 4.19 we see that for biaxial compression the trend does change. The maximum in energy release rate shifts to $\theta = 0$, whereas the maximum that was first present at $\theta = \pi/4$, has decreased. For the largest part of the front, $0.1\pi < \theta < 0.45\pi$ the energy release rate was higher for the circular shape. The mode angle however is not affected much by the movement of the front. The maximum value for $G/\Gamma$ moves to $\theta = 0$.

For an elliptically shaped front and a stiff substrate the maximum in energy release rate is lower than for a circular front, as can be seen in figure 4.20. The maximum value for $G/\Gamma$ is also lower compared with the circular shape, but it is situated at $\theta = 0.35\pi$. It can be concluded that the shape of the front influences the energy release rate. The mode angle however is rather insensitive to a change in the shape.

**4.5.2 Asymmetric shape**

It is believed that telephone cord buckles grow from straight sided buckles. The straight sided buckle becomes unstable above a certain stress level. Audoly [3] suggests that residual stresses cause a secondary buckling mode that changes the profile of the buckle. This can be transferred to the front, changing the loading of the front and preventing straight propagation. In experiments Volinsky [23] observed that telephone cord buckles start as straight sided buckles. When a certain
Figure 4.18: Comparison of various shapes of the front, for plane strain, the applied load is $10\varepsilon_c$

length is reached it switches to a telephone cord buckle. Images were taken from the experiment, showing profiles of the different stages of the growing telephone cord buckle. These profiles are shown in figure 4.21.

In the FE model the first shape of this new front is made by moving the nodes at the front in radial direction. The magnitude is $B \sin(x/b\pi) \sin(y/b\pi)$ for $0 < \theta < \pi/2$, and $\frac{B}{b} \sin(x/b\pi) \sin(y/b\pi)$ for $-\pi/2 < \theta < 0$. For the factor $B$ two different values are used, $b/20$ and $b/15$. A schematic view of this new shape can be seen in figure 4.22.

In figure 4.23 the results are shown for this asymmetric front. The symmetric, circular front is included for comparison. The straight side is not shown. The energy release rate shows two peaks, at $\theta = -0.25\pi$ where the front is moved closer to the origin, and at $\theta = 0.15\pi$, where the front is extended. For a larger distortion, $B = b/15$, more energy is released at the part where the front is extended, though the difference is very small. The maximum energy release rate is lower

Figure 4.19: Comparison of a circular and an elliptical front, for biaxial strain, the applied load is $15\varepsilon_c$
Figure 4.20: Comparison of a circular and an elliptical front, for biaxial strain, stiff substrate, the applied load is $10\varepsilon_c$

Figure 4.21: Stages of the growing telephone cord buckle, Volinsky [23]

Figure 4.22: Distortion of the circular shape at the front of a straight sided buckle

compared to the circular form. This can also be seen in the figures 4.18 and 4.20. The mode angle is almost constant along the front, with a small bump at $\theta = 0.2\pi$. The maximum in the $G/\Gamma$ plot lies at $\theta = 0.15\pi$ and not at the angle of the maximum extension, $\theta = 0.25\pi$. The FE model used here does not allow for a greater distortion of the circular shape as neighboring elements would then turn inside out. Notwithstanding the small distortion of the shape of the front, the maximum in $G/\Gamma$ lies at the part where the front was extended.
Figure 4.23: Comparison of the fracture parameters for varying shapes of the asymmetric front, for biaxial strain; the applied load is $10\varepsilon_c$.

The contour bands of the normal displacement of the film at $15\varepsilon_c$ are shown in figure 4.24. Although the sides are straight, and there is only a small distortion at the front, the instability of the buckle profile is clear. For $0 < \theta < \pi/2$ the normal deflection of the film is higher than for $-\pi/2 < \theta < 0$. The change in the shape of the front, compared with figure 4.16 introduces the possibility for the straight sided part to relax some of the residual energy, described by (4.8). A secondary, non-symmetric buckling mode can be observed.

Figure 4.24: Contour bands of the displacement in $z$-direction for an asymmetric buckle in a film with compliant substrate under biaxial straining, $15\varepsilon_c$
4.6 Reference length

The influence of the mode angle on the interface toughness and the propagation of a crack is shown in the previous sections. The choice of the reference length is still unclear in literature. Two characteristic dimensions for the buckle are the thickness of the film \( h \) and the width of the crack \( 2b \). In figure 4.25 these are both used as reference lengths. The reference length has no influence on the energy release rate. As expected from (2.13) the mode angle shifts by \( \varepsilon \ln(l_2/l_1) \). This does change the prediction of the interface toughness \( \Gamma \). The front however is not affected much by the reference length, in the right hand graph it makes a vertical shift, but the trend remains the same.

![Graphs showing comparison between two reference lengths, \( l = h \) and \( l = 2b \), for biaxial strain; the applied load is \( 15\varepsilon_c \).](image)

Figure 4.25: Comparison between two reference lengths, \( l = h \) and \( l = 2b \), for biaxial strain; the applied load is \( 15\varepsilon_c \).
Chapter 5

Discussion

5.1 Conclusions

To study the buckling behavior of thin film systems the energy release rate and mode angle of the stress intensity factor are of great importance. The interface strength is strongly dependent on this mode angle so the value of the energy release rate is not sufficient for the prediction of telephone cord buckles.

To accurately determine these parameters a crack opening displacement method is used. The results of this method for FE simulations are validated with the analytical solution for simple geometries. A crack in an infinite homogeneous plate was perfectly described by collapsed quarter point elements. The stress intensity factors are best derived from the nodes that are near the crack tip. If the crack lies in an interface between two dissimilar media these crack tip elements did not exactly describe the oscillatory stress singularity. The difference with the exact value increases with the elastic mismatch between these materials. The SIFs are then best calculated at the second element next to the tip. This conclusion can also be made for an axisymmetric and a 3D penny shaped crack.

The amount of energy that is stored in the film that can be released by buckling, $G_0$, can be derived for plane strain and biaxial strain. This is compared with the energy released by the straight sided part of the buckle, for both stress states. The critical strain $\varepsilon_c$, that is necessary for the onset of buckling, can also be derived for both stress states. When the results are made dimensionless by dividing by $G_0$ and $\varepsilon_c$ they are equal for plane strain and biaxial strain.

For Euler buckling the edges must be clamped, but for most buckling driven delamination the substrate is compliant, and therefore will deform. This will lead to a higher energy release rate, and a mode angle that lies closer to mode I compared to a stiff substrate. The interface toughness is lower for stresses with a large mode I component. For high stresses the mode II component becomes larger and contact will take place between the film and the buckle. This is an important reason why buckles tend to tunnel rather than becoming wider.

For crack propagation prediction, the mode angle and the compliance of the substrate need to be taken into account [8]. A 3D FE model of a straight sided buckle with a circular front was made with the same dimensions and elastic properties as a buckle that was observed by Abdallah et al. [1]. This model was subjected to plane strain and biaxial compression. For plane strain the buckle is expected to grow in a straight line. This was found for a stiff and a compliant substrate. Extending the front by making the front elliptical did not change the trend in energy release rate or mode angle. In contrast to literature, where an average value of the energy release rate is assumed at a circular front, there is a local maximum in energy release rate at the front, higher than at the straight side.

In biaxial compression different results are observed. For a stiff substrate the maximum in energy release rate lies just behind the transition to the straight sided part. This was also found by Jensen and Sheinman [11]. The energy release rate is higher at the straight sided part compared
to the front. When the mode angle and interface strength are taken into account, the buckle is not likely to become wider. The energy release rate $G$ divided by the interface toughness $\Gamma$ is larger at the front, and the maximum lies just behind the front. For a compliant substrate this does not change much, but at high stresses the peak lies in the circular front, at approximately $\theta = \pi/4$. This can be an explanation for the start of telephone cord buckling.

An asymmetric model with a small distortion of the circular shape with a compliant substrate was subjected to biaxial compression. The highest energy release rate $G$ and $G/\Gamma$ can be seen at the part where the front is extended. The normal deflection of the film at the front agreed with the energy release rate. The asymmetry in the buckled film introduced secondary buckling in the straight sided part.

The choice of the reference length for the mode angle is shown to be of minor importance in predicting crack propagation. The shift in mode angle that is the result of choosing a different reference length is only significant in the interface strength where the energy release rate is low.

### 5.2 Recommendations

In this report the onset of telephone cord buckling is studied by static FEM analyses. A transient analysis of the crack propagation in an initially straight sided buckle, for instance with cohesive zone elements to simulate the interface adhesion, can give more insight and can validate the predictions from this report. In the experiments that were performed by Abdallah et al. [1] residual stresses from oxygen plasma treatment and stresses from bending the film cause telephone cord buckling. In further research this can be implemented. Performing experiments, with stiff films on compliant substrates that show straight sided and telephone cord buckles could be used to further validate the results.
Appendix A

Contact size estimate for infinite plate

For an interface crack between two semi-infinite plates with crack length $2a$, the SIFs are defined as [18]:

$$K_1 + iK_2 = Te^{i\Psi} (1 + 2i\varepsilon) (\pi a)^{1/2}(2a)^{-i\varepsilon}$$

(A.1)

where $\sigma_{yy}^\infty + i\sigma_{xy}^\infty = Te^{i\Psi}$, with $\Psi = \tan^{-1} \left( \frac{\sigma_{xy}^\infty}{\sigma_{yy}^\infty} \right)$. Substituting (A.1) into (2.16) will yield the contact zone size for this problem.

$$\text{Re} \left[ e^{i\Psi} \left( \frac{r}{2a} \right)^{i\varepsilon} \right] = 0$$

(A.2)

or

$$\cos \left( \Psi + \varepsilon \ln \left( \frac{r}{2a} \right) \right) = 0$$

(A.3)

Making the assumption that $\varepsilon > 0$, an estimation for the contact zone can be made as follows:

$$r_c = 2ae^{-(\Psi + \pi/2)/\varepsilon}$$

(A.4)

In the case of a negative $\varepsilon$ both $\varepsilon$ and $\Psi$ should be multiplied by -1, which is equivalent to swapping both materials.

More recent studies, like by Agrawal [2], show that this contact zone is actually very small, for most cases on the (sub-)atomic level. From (A.4) it can be understood that $r_c$ will be very small, unless $\Psi$ is close to $-\pi/2$. For the case of the interface crack in an infinite plate as used by Agrawal [2], with $E_1 = 200 \text{GPa}$, $E_2 = 5 \text{GPa}$, $\varepsilon = -0.1045$, crack length $2a = 10 \cdot 10^{-3}$ m, and subjected to vertical normal stress $\Psi = 0$, and a the contact zone is $r_c = 3 \cdot 10^{-6}$ m, which can be considered sufficiently small to be neglected.
Appendix B

User subroutine

The Fortran code in this Appendix can be used as a user subroutine in Marc FEM analysis to export nodal displacements to a text file. Node number, number of the accompanying tip, angle $\theta$, $r$, increment number, $x$–coordinate and the load case time are also exported. The text file can easily be imported into Matlab to calculate SIFs from these results. In the Marc file a set of nodes named ‘cracktipnodes’ must be defined, consisting of the crack tip nodes with corresponding node pairs. The global coordinate system should be defined as in section 4.4. The routine was written by O. van der Sluis from Philips Applied Technologies but for this study it is extended for 3D models.

c-----------------------------------------------------------------------
c Subroutines ubginc.f and uedinc.f are used to print out the
CTODs (crack tip opening displacements) of the nodes behind
the cracktip. Notice that the CTODs are defined as the difference
between matching crack nodes. These values can be used to
determine the fracture toughnesses: $K_1$, $K_2$, $K_3$ from which
the mode angle is determined.

Necessary input from .mud-file:
!!the set 'cracktipnodes' should be defined!!
In this set, the cracktipnode and the nodes behind the crack tip
are included.
The result is written to 'ctod.txt' and can be post-processed
directly with Matlab by load('ctod.txt');

IMPORTANT: current assumptions:
- one crack tip node (can be easily extended though)
- one set of nodes 'cracktipnodes', all lying at interface, $z=0$
- front starts at $y=0$

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Changes:
- extended for multiple crack tip nodes
- node pairs for 'crack opening displacement' method are
  automatically linked to corresponding tip
- crack opening displacements are calculated in local
  coordinate system

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subroutine ubginc(inc,incsub)
... dummy user subroutine which is called at the beginning of each increment

inc : increment number
incsub: sub-increment number

---

C Include some ] block to get nodal coordinates

---

C IMPLICIT REAL *8 (A-H, O-Z) I-N=integer
include '../common/implicit'
include '../common/dimen'
include '../common/spacevec'
include '../common/strvar'
include '../common/blnk' !for internal<->external node numbers

---

crknod Array of node numbers in crack (set cracktipnodes)
coor Array of crack node coordinates
crdtmp Auxiliary array of coordinates
cmatch Array of matching nodes in crack
crktip Array containing the crack tip/front nodes
nodset Name of node set in model (contains cracktip nodes)
ifound The number of matching crack node pairs
C (which equals the length of the CTOD-array in UEDINC)
crdtip Coordinates of all identified crack tip/front nodes
icrack Number of crack tip nodes = size of crktip array

dimension coord(500,3),crdtmp(3),crdtip(50,3),
* crdmatch(50,3)
integer crknod(500),match(500,2),crktip(50),logfnd,
* crknodb(500)
character*80 nodset

---

C Define common block for usage in UEDINC-subroutine.
C 'Match' and 'ifound' are included in this common block.
COMMON/olaf/match,ifound,crktip,crdtip,itip,coord

---

C Check the increment number: only perform this in inc. 0
IF (inc.GT.0) THEN
RETURN
ELSE
    nodset='cracktipnodes'
    CALL setinf(nodset,khava,crknod,ityp,numa)
    nodset='topnodes'
    CALL setinf(nodset,khavb,crknodb,itypb,numb)
    IF ((khava.EQ.0)) THEN
        WRITE(0,('NO CRACKTIPNODES-SET SPECIFIED -> ABORT!'))
        CALL quit(9999)
    ENDIF
    c
    WRITE(0,('\'\"\'khava\"\',IS)') khava
    WRITE(0,('\'\"\'numa\"\',I4)') numa
    WRITE(0,('\'\"\'numb\"\',I4)') numb
    c
    WRITE(0,('\'\"\'cracknodes\"\',100I6)') crknod
    IF ((khava.EQ.0)) THEN
        WRITE(0,('\'\"\'NO CRACKTIPNODES-SET SPECIFIED -> ABORT!\"\')
        CALL quit(9999)
    ENDIF
    c
    Determine corresponding nodes behind the crack tip
    c
    Retrieve coordinates of crack tip nodes
    jrdpre=0

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DO inodes=1,numa
  User internal node numbers as input using nodint
  CALL VECFTC(crdtmp,xord_d,ncrdmx,ncrd,
    * nodint(crknod(inodes)),jrdpre,2,1)
  DO idof=1,3
    coord(inodes,idof)=crdtmp(idof)
  ENDDO
ENDDO

DO inodes=1,numa
  WRITE(0,'(''Node: '', I5, '' coord: '', 3E13.5)')
    * crknod(inodes),coord(inodes,1),coord(inodes,2),
    * coord(inodes,3)
ENDDO
DO inodes=1,numb
  WRITE(0,'(''Topnode: '', I5)')
    * crknnodb(inodes)
ENDDO

c----------------------------------------------------
c Find matching/opposite nodes in crack
c----------------------------------------------------
epstol=2.d-7
ifound=0
icrack=0

DO inodes=1,numa
  DO jnodes=1,numa
    C Determine difference in coordinates if nodenumbers are
    C not equal. Also, prevent inverse results (e.g., node1&node10
    C and node10*node1) by demanding inodes < jnodes
    IF (inodes.NE.jnodes.AND.inodes.LT.jnodes) THEN
      deldis=SQRT((coord(inodes,1)-coord(jnodes,1))**2+
        * (coord(inodes,2)-coord(jnodes,2))**2)
      IF (deldis.LT.epstol) THEN
        ifound=ifound+1
        logfnd=1
        match(ifound,1)=crknod(inodes)
        match(ifound,2)=crknnod(jnodes)
        match(ifound,3)=coord(inodes,1)
        match(ifound,4)=coord(inodes,2)
        match(ifound,5)=coord(inodes,3)
      ENDIF
    ENDDO
  ENDDO
ENDDO
WRITE(0,'(''Found: '', I5)') ifound
C------------------------------------------------
C Finding single crack tips
C------------------------------------------------
itip=0
LOGFND=0 !indicates if corresponding node found
DO jnodes=1,numa
  IF (inodes.NE.jnodes) THEN
    deldis=SQRT((coord(inodes,1)-coord(jnodes,1))**2+
      * (coord(inodes,2)-coord(jnodes,2))**2)
    IF (deldis.LT.epstol) THEN
      ifound=ifound+1
      write(0,'(''ifound:'',i4)') ifound
    ENDIF
  ENDIF
ENDDO
WRITE(0,'(''Found: '', I5)') ifound

logfnd=1
ENDIF
ENDIF
ENDDO
IF (logfnd.NE.1) THEN !no corresponding nodes found -> cracktipnode
  itip=itip+1
  crktip(itip)=crknod(inodes)
  DO idof=1,3
      crdtip(itip,idof)=coord(inodes,idof)
  END
ENDDO
WRITE(0,'((''Cracktip: '',I5,'' coord: '', 3E13.5)') * crktip(itip),(crdtip(itip,idof),idof=1,3)
ENDIF
ENDDO
WRITE(0,'((''Found: '', I5)') itip
WRITE(0,'((''Cracktipnode'',50I5)') crktip
IF (ifound.LT.(numa-itip)/2.D0) THEN
  WRITE(0,'($''Found number of matching crack nodes '')')
  WRITE(0,'(''is not sufficient!! -> check!'')')
  WRITE(0,'('' Matching crack nodes:'')')
  WRITE(0,'('' Number of crack nodes: '',I5)') numa
  DO inodes=1,ifound
      WRITE(0,'(2I8)') match(inodes,1), match(inodes,2)
  ENDDO
ENDIF
return
end
C-----------------------------------------------------------------------
C
C subroutine uedinc(inc,incsub)
C implicit real*8 (a-h,o-z) dp
C dummy user subroutine that would get called at the end of each
C increment
C include '../common/creeps'
C include '../common/dimen'
C include '../common/spacevec'
C include '../common/strvar'
C include '../common/blnk' !for internal<->external node numbers
C-----------------------------------------------------------------------

dimension disp_a(3),disp_b(3),ctod(500,3),crd_0(3),
      * crdtip(50,3),disp_c(3),crd_a(3),
      * coord(500,3)
integer match(500,2),crktip(50),tipnu,crknodb(500)
character*80 filename

COMMON/olaf/match,ifound,crktip,crdtip,tipnu,crknodb
      * crknodb,numb

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Check the increment number: only perform this in the final increment

IF (inc.LT.1) THEN
  C This is the wrong increment
  RETURN
ELSE
  WRITE(0,(''Start subroutine UEDINC''))
ENDIF

DO inodes=1,ifound
  WRITE(0,'(''Start subroutine UEDINC'')')
  IF (match(inodes,1).EQ.crknodb(inodes2)) THEN
    itop=1
  ENDIF
  IF (itop.EQ.1) THEN
    ctod(inodes,1)=(disp_a(1)-disp_b(1))
    ctod(inodes,2)=(disp_a(2)-disp_b(2))
    ctod(inodes,3)=(disp_a(3)-disp_b(3))
  ELSE
    ctod(inodes,1)=(disp_b(1)-disp_a(1))
    ctod(inodes,2)=(disp_b(2)-disp_a(2))
    ctod(inodes,3)=(disp_b(3)-disp_a(3))
  ENDIF
ENDDO

GET coordinates with VECFTC (coordinates of node2 are equal...)
C Note: coordinates are initial coordinates!
CALL VECFTC(crd_0,xord_d,ncrdmx,ncrd,
  * nodint(match(inodes,1)),jrdpre,2,1)

*** Behind front, theta is positive ***
IF (crd_0(1).LT.-1.d-5) THEN
  IF (crd_0(2).GT.1.d-5) THEN
    r_0=SQRT((crdtip(itnr,1)-crd_0(1))**2+(crdtip(itnr,2)-crd_0(2))**2+(crdtip(itnr,3)-crd_0(3))**2)
    thtip=acos(crdtip(itnr,1)/r_0)
    SQR2(crdtip(itnr,1)**2+(crdtip(itnr,2)**2))
tipnu=crktip(itnr)
httipnu=httip
du=ctod(inodes,2)
dv=ctod(inodes,3)
du=ctod(inodes,1)
th=acos(crd_0(1)/SQRT(crd_0(1)**2+
   (crd_0(2)**2)))*crd_0(2)/SQRT(crd_0(2)**2)
ENDIF
ENDIF
ENDDO
ENDIF

** At the front, theta has sign (+1.d-6 don't devide by zero) **

ELSE
th=atan(crd_0(2)/(crd_0(1)+1.d-6))
DO itnr=1,itip
  IF (crdtip(itnr,1).GT.-1d-5) THEN
    thtip=atan(crdtip(itnr,2)/(crdtip(itnr,1)+1.d-6))
    IF (ABS(thtip-th).LT.2.d-2) THEN
      r_0=SQRT((crdtip(itnr,1)-crd_0(1))**2+
        (crdtip(itnr,2)-crd_0(2))**2+
        (crdtip(itnr,3)-crd_0(3))**2)
      c save tip
tipnu=crktip(itnr)
httipnu=httip
du=ctod(inodes,1)*cos(th)+ctod(inodes,2)*sin(th)
dv=ctod(inodes,3)
du=ctod(inodes,2)*cos(th)-ctod(inodes,1)*sin(th)
    ENDIF
  ENDIF
ENDDO
ENDIF

WRITE(21,'(2I7,6E13.5,1I5,2E13.5)') match(inodes,1), tipnu,
   * th,httipnu,du,dv,dw,r_0,
   * inc,
   * crd_0(1), cptim
ENDDO

return
end
Bibliography


