Thin Film Adhesion and Morphology of Graphene on Undulated Electronic Substrates

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# TABLE OF CONTENTS

TABLE OF CONTENTS ........................................................................................................... I

LIST OF FIGURES ................................................................................................................ V

LIST OF TABLES .................................................................................................................. X

ABSTRACT ........................................................................................................................ XI

ACKNOWLEDGEMENTS .................................................................................................. XIII

CHAPTER 1  INTRODUCTION ............................................................................................... 1

1.1  Introduction of adhesion .......................................................................................... 1
    1.1.1  Definition of adhesion ...................................................................................... 1
    1.1.2  Adhesion mechanisms .................................................................................... 3
    1.1.3  Adhesion effects ............................................................................................. 5

1.2  Review of solid adhesion ..................................................................................... 8
    1.2.1  Hertz contact theory ...................................................................................... 8
    1.2.2  JKR theory ...................................................................................................... 10
    1.2.3  DMT theory ..................................................................................................... 12
    1.2.4  Dugdale-Barenblatt-Maugis model ................................................................. 13
    1.2.5  Adhesion map for solids contact ..................................................................... 15
    1.2.6  Other adhesion models ................................................................................... 16

1.3  Review of thin film adhesion .............................................................................. 18
    1.3.1  Peel test ............................................................................................................ 19
    1.3.2  Blister test ....................................................................................................... 20
    1.3.3  Punch test ....................................................................................................... 23

1.4  Graphene and its adhesion property ................................................................. 24

1.5  Research objectives ............................................................................................ 28

1.6  Organization of the thesis .................................................................................... 29
CHAPTER 2  THIN FILM ADHESION IN THE LONG RANGE
INTERSURFACE FORCE .................................................................31

2.1  New Tabor parameter .................................................................31

2.2  Punch test model .................................................................37
  2.2.1 Rectangular film under pure stretching ..........................37
  2.2.2 Rectangular film under pure bending ............................53
  2.2.3 Circular film under pure stretching .................................55
  2.2.4 Circular film under pure bending ....................................58

2.3  Pressurized blister model ......................................................59
  2.3.1 Rectangular pressurized blister under pure stretching ..........................59
  2.3.2 Rectangular pressurized blister under pure bending ..............64
  2.3.3 Circular pressurized blister under pure stretching ..................65
  2.3.4 Circular pressurized blister under pure bending .....................69

2.4  Constrained blister model ......................................................70
  2.4.1 Circular constrained blister under pure stretching ...............70
  2.4.2 Circular constrained blister under pure bending .................75
  2.4.3 Rectangular constrained blister under pure stretching ..........76
  2.4.4 Rectangular constrained blister under pure bending ...............79
  2.4.5 Discussion ................................................................................79

2.5  New adhesion map for thin film ...........................................89

CHAPTER 3  HYSTERESIS OF LOADING AND UNLOADING A RIGID
PUNCH TO A CLAMPED MEMBRANE ........................................92

3.1  Rectangular film .................................................................92

3.2  Circular film .................................................................96

3.3  Discussion ................................................................................99

CHAPTER 4  MOLECULAR MECHANICS SIMULATION OF
GRAPHENE-GRAPHENE ADHESION ...........................................106

4.1  Molecular mechanics simulation method ..............................106
4.2 Young’ modulus and effective thickness of graphene .........................107
4.3 Adhesion energy of two graphene layers ..............................................116
4.4 Adhesion mechanics between graphene-substrate ..............................118
4.5 Adhesion mechanics between two graphene layers ............................130
4.6 Misorientation effect to the adhesion property of graphene ...............133

CHAPTER 5 GRAPHENE ON ELECTRONIC SUBSTRATES..............136
5.1 Introduction .......................................................................................136
5.2 Experiment .........................................................................................139
  5.2.1 Sample preparation ........................................................................139
  5.2.2 Blister formation ..........................................................................144
5.3 Model and Analysis ............................................................................150
5.4 Discussion ..........................................................................................155
5.5 Graphene on other substrate materials .............................................159

CHAPTER 6 CONCLUSION AND FUTURE WORK .....................161
6.1 Significant contributions and conclusions .........................................161
6.2 Future work .......................................................................................163

REFERENCES .........................................................................................166

APPENDIX 1: MATHEMATICA PROGRAM FOR RECTANGULAR PUNCH TEST MODEL UNDER PURE STRETCHING ........................................179

APPENDIX 2: MATHEMATICA PROGRAM FOR RECTANGULAR PUNCH TEST MODEL UNDER PURE BENDING ............................................183
LIST OF FIGURES

Figure 1.1 Adhesion between bodies of different size compared to gravity [1] ........................................... 2
Figure 1.2 Interaction energy between two surfaces described by DLVO theory [14]................................. 5
Figure 1.3 The epidermal electronics attach to the skin [19] ........................................................................ 7
Figure 1.4 Typical MEMS R-F switch [22]. (a) “ON” stage and (b) “OFF” stage................................. 7
Figure 1.5 Comparison of different adhesion models. Normal load $P$ is applied to compress two spheres. 9
Figure 1.6 Mechanical properties of different adhesion models. (a) Equilibrium relation between contact radius and the applied load. Either applied load or penetration depth equals zero at point A, B, M and N. Point C and D represent load-controlled and displacement-controlled pull-off respectively for JKR model. (b) Relation between the contact radius and penetration depth. Hertz and DMT have the same profile. (c) Equilibrium relation between applied load and penetration depth. ................................................................................................. 10
Figure 1.7 Relation between contact radius and applied load for various $\lambda$ [29] ........................................ 14
Figure 1.8 Lennard-Jones potential and the uniform disjoining pressure approximation ....................... 15
Figure 1.9 Adhesion map for the contact of elastic spheres [31] ............................................................... 16
Figure 1.10 Typical peel test [48] ............................................................................................................... 20
Figure 1.11 Blister models. (a) Standard pressurized blister. (b) Constrained blister. (c) Island blister. (d) Peninsular blister. The left part is the side view from the cross section of dash line and right part is the top view. The adhered regions and delaminated regions are shown in different colors.......................... 22
Figure 1.12 Punch test model ...................................................................................................................... 23
Figure 1.13 The world’s thinnest balloon [80] ............................................................................................ 25
Figure 1.14 Direct measurement of graphene adhesion using nano-particles [84] ..................................... 27
Figure 1.15 Probing mechanical properties of graphene using corrugated elastic substrate [91]........... 28
Figure 2.1 (a) Schematic of a clamped circular membrane adhered to a rigid substrate, (b) Schematic of half the membrane profile drawn in normalized coordinates ........................................................... 32
Figure 2.2 (a) Schematic of a clamped rectangular membrane adhered to a planar punch surface. (b) Drawing in normalized coordinates and variables .................................................................................................................................... 38
Figure 2.3 Membrane profile for fixed half contact length $c = 0.1$ and a range of disjoining pressure ....... 39
Figure 2.4 Mechanical response for a range of disjoining pressure .......................................................... 42
Figure 2.5 Energy as function of contact length for punch displacement $w_0 = 0.5 \gamma^{1/4}$ and a range of disjoining pressure ............................................................ 43
Figure 2.6 Total energy of the membrane-punch system for disjoining pressure ....................................... 44
Figure 2.7 Mechanical response for a range of disjoining pressure .......................................................... 47
Figure 2.8 Punch displacement as a function of half contact length for a range of disjoining pressure .... 49
Figure 2.9 Cohesive edge as a function of half contact length for a range of disjoining pressure .......... 50
Figure 2.10 Comparison of mechanical response, $F(w_0)$, between 1-D model (solid) and the 2-D axisymmetric membrane ...................................................................................................................... 52
Figure 2.11 Mechanical response of a clamped rectangular membrane under pure bending ............... 55
Figure 2.12 Mechanical response of a clamped circular membrane under pure stretching ............... 57
Figure 2.13 Mechanical response of a clamped circular membrane under pure bending ............... 57
Figure 2.14 (a) Schematic of a standard pressurized test. (b) Model drawn in normalized coordinates. .62
Figure 4.3 (a) A graphene sheet with the central atom pulled up and the periphery is clamped. The radius of the sheet is 35.1 Å. (b) Theoretical model of a clamped thin film with point load applied in the center.

Figure 4.4 Potential change as a function of central displacement. The data points are the simulation result and the solid curves with different color represent different pairs of Young’s modulus and thickness of graphene.

Figure 4.5 (a) Graphene sheet with different clamped regions in the center. The radius of the sheet is 35.1 Å. (b) Theoretical model of a clamped punch model.

Figure 4.6 Potential change as a function of central displacement. The data points are the simulation result and the solid curves with different color represent different clamped radius in the center.

Figure 4.7 Intersurface pressure as a function of separation between two graphene sheets. The black data points are from larger model with radius of 41 Å and the gray data points are from the smaller model with radius of 14.5 Å. The top inserted figure shows two graphene sheets with radius of 41 Å. The bottom inserted figure shows the surface potential as a function of graphene-graphene separation. The black points are from the larger model and the gray ones are from the smaller model.

Figure 4.8 (a) Side view of the graphene graphene adhesion model in molecular mechanics simulation. The top deformable graphene layer is clamped at the periphery. The bottom layer is fixed as a rigid substrate. The radius of the graphene membrane is 40 Å. (b) Continuum model of a clamped circular film adhered to a rigid substrate.

Figure 4.9 Central separation between two graphene sheets as a function of displacement. The inserted figure shows the deformed profile of the two sheets.

Figure 4.10 Applied force as a function of punch displacement. The results of JKR model DMT model are shown as the solid lines. The data points with different shapes are for different clamped regions.

Figure 4.11 (a) Side view of the graphene graphene adhesion model in molecular mechanics simulation. The top deformable graphene layer is clamped at the periphery. The bottom layer is fixed as a rigid substrate. The width of the graphene membrane is 85 Å. (b) Continuum model of a clamped rectangular film adhered to a rigid substrate.

Figure 4.12 Central separation between two graphene sheets as a function of displacement. The inserted figure shows the deformed profile of the two sheets.

Figure 4.13 Applied force as a function of punch displacement. The gray curve is the JKR model result and the black curve is the DMT model result. The data points with different shapes are for different clamped regions.

Figure 4.14 (a) Side view of the circular graphene-graphene adhesion model built in HyperChem. Two deformable graphene layers are clamped at the periphery. The radius of the graphene membrane is 40 Å. (b) Side view of the rectangular graphene-graphene adhesion model. The width of the graphene is 85 Å. (c) The theoretical model of two films adhesion.

Figure 4.15 The applied force as a function of central displacement. The circular data points are the simulation result of rectangular graphene-graphene model and the triangular shape is for circular graphene-graphene model.

Figure 4.16 Different moiré patterns are formed when two graphene sheets are twisted various angles.
Figure 4.17 (a) The intersurface force as a function of separation when two graphene sheets are twisted different angles. (b) The applied force as a function of punch displacement in the circular graphene adhesion model for different twisted angles ........................................................... 135

Figure 5.1 Illustration of nano pillars and graphene blisters ..................................................................................... 138

Figure 5.2 Graphene morphology is regulated by the intensity of the adhesion between the interface .... 139

Figure 5.3 Procedures for nano pillar fabrication ........................................................................................................... 140

Figure 5.4 Fabricated gold pillar patterns with height $w_0 = 60\pm 10$ nm, radius $R = 25$ nm and inter-pillar separation $H = 500$ nm. The bottom figure shows the zoom in region............................................ 141

Figure 5.5 Procedures for CVD grown graphene [140]. The top figures illustrates the experiment set up. The bottom one shows the operation parameters ................................................................. 142

Figure 5.6 Transfer process of CVD grown graphene ........................................................................................................... 144

Figure 5.7 Raman Spectra of graphene on gold. The position of G-band is around 1589 cm$^{-1}$ and 2D-band position is 2680 cm$^{-1}$. The intensity of 2D-band is more than two times of the G-band and this verifies the graphene to be single layer ................................................................. 145

Figure 5.8 SEM and AFM image of the graphene on gold pillars with 0.5 $\mu$m separation. (a) High-angle viewed SEM image, scale bar is 100 nm. (b) Top view of the same region in SEM. (c) High-angle viewed SEM image of the same region after the AFM scanning. Pillars A, B, and C were removed by the AFM tip. The blister D was destroyed by AFM tip. (d) AFM image of the same region ................................................................................................................................ 147

Figure 5.9 SEM and AFM image of the graphene on gold pillars with 0.5 $\mu$m separation in a different region. (a) High-angle viewed SEM image, scale bar is 100 nm. The radial corrugations of blisters are clear to see. (b) Top view of the same region in SEM. (c) High-angle viewed SEM image of the same region after the AFM scanning. Pillars L, M and N were destroyed by AFM tip during scanning. (d) AFM image of the same region ................................................................................................................................ 148

Figure 5.10 SEM and AFM image of the graphene on gold pillars with 0.5 $\mu$m separation in a different pattern region. (a) High-angle viewed SEM image, scale bar is 100 nm. The radial corrugations of blisters are clear to see. (b) Top view of the same region in SEM. (c) High-angle viewed SEM image of the same region after the AFM scanning. Pillar Q was destroyed by AFM tip during scanning. (d) AFM image of the same region ................................................................................................................................ 149

Figure 5.11 Schematic of two blister models. The parameters are defined as: $w_0$: the height of the pillar; $a$: radius of the blister; $H$: separation between two pillars ................................................................................................................................ 151

Figure 5.12 (a) Schematic of four blisters. The red spots represent four gold pillars. The gray region shows the quarter size of the delaminated region. The dash curves show the critical contact edges when the blisters begin to interact with one and another. The solid curves in the center show the contact edges after the blisters coalesce. (b) The dimensionless parameter as a function of the pillar height. The vertical axis is defined as ratio of the delaminated area to the original full contact area. $w_0$ is the height of the pillar. $w_0'$ is the critical height when the blisters begin to interact and $w_0''$ is the critical height when graphene snap off the substrate. 154

Figure 5.13 SEM image of graphene on pillars with separation of 1 $\mu$m. It is very difficult to form the expected blisters as previous with inter-pillar separation of 0.5 $\mu$m. Graphene was destroyed by the pillars and cracks can be seen around the pillars. The dark region is the shade after focusing on a smaller size under SEM. The edge of the graphene is clear to see ............................. 156

Figure 5.14 The radial and tangential stress of the blister as functions of radial distance [131]. $\beta_0$ is the initial residual stress ................................................................................................................................ 158
Figure 5.15 Graphene transferred to silicon dioxide substrate (a) and silicon nitride substrate (b). ........ 160
Figure 5.16 SEM image of copper nano particles trapped by graphene on the silicon dioxide substrate. 160
LIST OF TABLES

Table 2.1 Normalized coordinates and variables ....................................................................................... 33
Table 6.1 The prediction of the blisters shape .......................................................................................... 165
ABSTRACT

Adhesion is the interaction between dissimilar particles or surfaces, which has significant impacts in nanotechnology and life sciences, such as stability of microstructures, cell adhesion, and bacterial aggregation. In order to quantify adhesion, several theoretical models have been built from the pioneered work of Hertz contact theory to the Johnson-Kendall-Roberts (JKR), Derjaguin-Muller-Toporov (DMT), and Dugdale-Barenblatt-Maugis models. These celebrated contact mechanics models have been shown to be successful in a wide spectrum of metallic, ceramic and polymeric solid materials, and continue to make invaluable contributions in many branches of science and technology. However, these models inevitably break down in thin membranes, shells and microcapsules that exercise plate-bending and membrane-stretching and conform to the contact surface geometry.

Based on a thermodynamic energy balance method, this thesis constructs a framework to model the mechanical behavior of thin films under intersurface adhesion. Depending on the intersurface force magnitude and range, JKR limit and DMT limit are discussed. To account for the transition between these two limits, a new Tabor’s parameter in the context of thin films is derived to relate the membrane thickness and stiffness and the intersurface force magnitude and range. The models are demonstrated for several thin film delamination configurations including standard pressurized blister test, constrained blister test, and punch test for a membrane clamped at the periphery. The adhesion hysteresis of loading and unloading a rigid punch to a clamped membrane is discussed as well. The trends and graphs are useful in experimentally gauging the adhesion strength of thin film material and the associated intersurface force magnitude and
range, and are also helpful in formulating design criteria for micro- and nano- electromechanical systems (MEMS/NEMS) devices comprising voltage activated bridges such as RF-switches.

Graphene, being a monolayer of carbon atoms, possesses extreme mechanical and electrical properties and proves to be an indispensible conducting medium for next generation of micro electronics. The adhesion properties of graphene on electronic substrates hold the keys to high performance and long term reliability of electronics systems. Molecular mechanics simulation is implemented to explore the adhesion mechanics between two identical or misoriented graphene. Mechanical properties including elastic modulus, effective thickness and adhesion energy of two graphene layers are obtained. The simulation result is comparable with the continuum model. Experiments to study the adhesion properties between graphene and electronic substrates are conducted. The morphology of graphene on the substrates is found to be strongly related to the interfacial adhesion energy and geometrical properties of the undulated substrate surface. The results and trends obtained here set design guidelines for graphene based devices.
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Chapter 1 Introduction

1.1 Introduction of adhesion

1.1.1 Definition of adhesion

Generally, any attraction phenomenon between objects can be considered as adhesion, like the interaction between atoms to form molecules, stiction of dust on window glass to turn it opaque, attraction between two magnets, and even gravitational pull of an apple to the ground. There are four kinds of forces in nature: strong interaction, weak interaction, electromagnetic force and gravity. The first two forces act between neutrons, protons, electrons, and other elementary particles. They have a very short range of action, less than $10^{-5}$ nm, and belong to the domain of nuclear and high-energy physics and are beyond the scope of this thesis. The latter two forces working between atoms and molecules are effective over a larger range of distances, from subatomic to practically infinite distances, and govern the behavior of almost everything having nonzero mass. When jumping up, we always fall to the ground. It is the gravitational force between our body and the earth that prevents us jumping higher, not the adhesion between our feet and the ground. On the other hand, our body does not break to pieces during jumping. This is the contribution of intermolecular attraction which holds the cells, tissues and other components together. Adhesion seems to be dominant in some situations, whereas gravity plays a leading role in others. Kendall [1] compared these two forces as shown in Figure 1.1. In the macro world, gravitation shown as the solid line is several orders of magnitude larger than adhesion represented by dash line. The dominated force can explain many phenomenon in daily life, such as formation of atmosphere, dropping of a cannon ball after traveling a parabolic path, the movement of a satellite around the earth, et al. Such weak adhesion escapes our common
Though adhesion still exists, we cannot feel it when our finger touches the desk. But for some thin film materials, the adhesion effect is apparent. Weak adhesion can still cause a plastic wrap to adhere to our hand because of high flexibility of the film. More properties of thin film adhesion will be discussed later in this chapter. As the dimension goes to micrometer or even nanometer scale, gravitation is sufficiently weak to be neglected compared to adhesion. Figure 1.1 shows that the gravitational pull of a bacterium with 1 μm diameter is less than 1 pN while the adhesion force is around 1 μN. Movements of molecules and atoms are governed by such adhesion force without the effect of gravity being taken into account. That is why adhesion has significant impacts in nano-technology [2] and life sciences [3]. This multiscale effect is one of the fundamental issues in building MEMS and NEMS (Micro/Nano Electromechanical Systems). In biology, apposing cells adhere to form multicell aggregates and ultimately tissues. Such cell adhesion is mediated by interactions between receptors and ligands which provide not only physical linkage but also communication between cells and its environment [4-8]. In the present context, adhesion is the attraction exerted between particles or surfaces that originates from electromagnetic interactions excluding gravity.

Figure 1.1 Adhesion between bodies of different size compared to gravity [1]
1.1.2 Adhesion mechanisms

Adhesion can be caused by different mechanisms. Electrostatic adhesion is attributed to the transfer of electrons across the interface creating positive and negative charges that attract one another describing by the Coulomb’s law. The phenomena of animal fur sticking to a rubbed rubber balloon, as well as the attraction of a plastic wrap to our hand after removing from a package can be explained by such theory.

Another source for adhesion is mechanical interlocking. Materials in contact fill the voids or pores of the surfaces and lock-on mechanically to the substrate. Example includes the rubber bonding to the textiles and paper. The improved adhesion between polymer and glass or silicon substrates is attributed to the mechanical interlocking of polymer lobes diffused into pits on substrates [9, 10]. This mechanism requires that the substrate surface consist of a maze of peaks and valleys. The microroughness on the adhered surface can improve bond strength and durability.

van der Waals force is another distinct source for adhesion and is defined as the attractive forces between molecules. This is the most common type of attraction force to govern the movements of atoms and molecules. Three different forces are included in van der Waals force. Keesom force describes the attraction force between two permanent dipoles. Debye force is the interaction between a permanent dipole and a corresponding induced dipole. London dispersion force is the interaction between two instantaneously induced dipoles. As an example in the animal world, gecko foot adhesion has drawn interests from researchers [11-13]. Recent studies reveal that the specific adhesion property of gecko foot is strongly related to its remarkable aligned microscopic hairs which are splitted into nanometer size spatula at the end [11, 12].
These spatulas come in close contact with the surface to induce strong van der Waals forces to hold the gecko on the wall.

DLVO (Derjaguin, Landau, Verwey and Overbeek) theory combines van der Waals attraction with electrostatic repulsion and is widely used to explain adhesion in colloidal science. Stability of colloidal suspensions in a dielectric medium is determined by the sum of attractive van der Waals potential and repulsive electrostatic potential shown in Figure 1.2. Dilute electrolyte solution ((a)) with a long Debye length supplies strong electrostatic repulsion, which is much larger than the van der Waals attraction. The resulting potential provides repulsion and the colloids remain stable. More concentrated electrolyte solutions decrease the surface potential and particles come into stable equilibrium at secondary minimum shown as curve (b). For higher concentrated electrolyte solutions, the energy barrier will be much lower and even falls below 0 ((d)). The attraction force becomes dominant and the particles coagulate rapidly. As the electrolyte solutions get saturated ((e)), the electrostatic repulsion is very weak and particles attract each other.

Two materials may adhere by forming a compound at the joint like ionic bonding, covalent bonding, metallic bonding or hydrogen bonding. But the attractions from the ionic and covalent bonds are only effective in a short range less than one nanometer. Adhesion between two polymeric materials can be explained by diffusion theory, which states that molecules of one polymer chain diffuse into the other and form a mechanical tethering at the interface. This can be extended to sintering where atoms diffuse from one particle to the other and all the particles coagulate after metal or ceramic powders are pressed together and heated.
1.1.3 Adhesion effects

Adhesion is advantageous when being used as tools or becoming the working mechanism for some structures like gecko foot and cell adhesion to form tissues. Adhesion of capsules to cells is a crucial step for raising the efficacy of drug delivery [15]. The capsules coated with functional molecules interact with and target specific cells, tissues and organs. By changing the surface composition, the adhesion of capsules can be controlled for drug delivery applications. Also the bacterial adhesion are present in water treatment [16, 17]. By increasing adhesion, bacteria can stick together and easily deposit on a porous medium during water purification. The aforementioned gecko adhesion is attributed to the van der Waals forces between surfaces and
the spatula of gecko foot. Taking advantage of the fibrillar structures, specific materials are fabricated to simulate the gecko locomotion with binding-on and lifting-off from various surfaces [18]. Rogers et al [19] recently developed an epidermal electronic “smart skin” (Figure 1.3) to monitor electrical signals from the heart, brain, and muscles by simply attaching the flexible electronic device to the skin without any mechanical fixtures or adhesive tapes. The van der Waals forces are sufficient to maintain conformal contact between the device and the skin, withstanding normal body movements over long periods without cracking or delamination.

Adhesion also brings disadvantages. This is especially true in nanotechnology where adhesion is dominant and limits both the fabrication yield and operation lifetime of many MEMS and nano devices [20, 21]. A typical RF switch is shown in Figure 1.4. The electrostatic force pulls the top thin film bridge to contact with the grounded pad when the electrical voltage is applied [22] to the bridge. The circuit is turned on and outputs signal “1”. When the voltage is removed, the electrostatic force is lost and the thin film at bridge returns to its original position. The circuit is cut off and “0” is output. When the gap between the bridge and the grounded pad shown in Figure 1.4(b) is too narrow, adhesion is significant that makes the bridge stick to the grounded pad even in the absence of applied voltage. The RF switch then fails. For other nano structures, working environment such as temperature and RH (relative humidity) may alter the adhesion properties that causes collapse of the structures [23]. Similarly, adhesion can also be detrimental for biomaterials and their applications/implementations. Contact lenses are widely used by millions of people each year. If adhesion between the cornea and the hydrogel surface of the lens is strong, trauma can be caused to the epithelial layer of the cornea when the lens is taken off. This leads to epithelial thinning, which can lead to serious infections and corneal pathologies.
The aforementioned examples show the necessity of the study of adhesion. Whether it is optimizing a strong adhesive force for bacterial removal to make portable water, or minimizing the adhesion in RF switches, a thorough understanding of the mechanisms of adhesion will benefit society at large.

Figure 1.3 The epidermal electronics attach to the skin [19]

Figure 1.4 Typical MEMS R-F switch [22]. (a) “ON” stage and (b) “OFF” stage
1.2 Review of solid adhesion

1.2.1 Hertz contact theory

The classical Hertz contact theory [24] was firstly proposed by Hertz in 1881 and it accounts for contact between two spheres but neglecting friction and adhesion. Radius of the contact circle $a_H$ was related to the external compressive load $P$, the radius of the spheres $R_1$ and $R_2$, and elastic properties of the contacting materials:

$$a_H = \left(\frac{PR}{K}\right)^{1/3} \tag{1.1}$$

where $\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2}$, $\frac{1}{K} = \frac{3}{4} \left(\frac{1-v_1^2}{E_1} + \frac{1-v_2^2}{E_2}\right)$, $v$ and $E$ are the Poisson ratio and Young’s modulus of each material respectively.

The elastic displacement of the two spheres or distance of approach is

$$\delta_H = \frac{a_H^2}{2R} \tag{1.2}$$

The Hertz theory to predict the deformed profile of two spheres in contact is shown in Figure 1.5 where the arrows indicate the applied compressive load $P$. Relations between the applied load, contact radius and the penetration depth are given in Figure 1.6. In the absence of adhesion, Hertz contact theory has shown great success to accurately describe the contact between elastic bodies.
Figure 1.5 Comparison of different adhesion models. Normal load $P$ is applied to compress two spheres.
1.2.2 JKR theory

Bradley [25] also studied the force needed to separate two spheres named pull-off force, which is proportional to the radius of the spheres and the work of adhesion. The theory is applicable to the case of rigid sphere in contact with zero contact radius. But in reality, most of the objects in contact are deformable. At micrometer or nanometer scale, adhesion arising from
attractive surface forces is not negligible and the Hertz contact theory is no longer valid. The first successful theory of adhesive contact came in 1971 which was developed by Johnson, Kendall and Roberts, now known as JKR theory [26]. The paper published in the proceeding of Royal Society is to this day one of the most highly cited papers in the history of science. The theory shows that the contact region between two frictionless spheres would be larger than what the Hertz theory predicts. When the spheres are brought into contact under a normal force, a flat circular contact region forms and infinite tensile stress occurs at the contact edge, which causes a larger contact area than Hertz theory (Figure 1.5). The JKR theory assumes that the adhesion only exists at the contact edge and an infinite tensile stress is caused in the contact circle. A “pseudo-parabolic” neck is formed at the contact circle because of the sharp discontinuity of stress. The contact radius has the following expression

$$a_{JKR}^3 = \frac{PR}{K} \left[ 1 + \frac{3\pi \gamma R}{P} + \left[ 2\left( \frac{3\pi \gamma R}{P} \right) + \left( \frac{3\pi \gamma R}{P} \right)^2 \right]^{1/2} \right]$$

(1.3)

where $\gamma$ is the interfacial adhesion energy. The term between the curly brackets is the correction to the Hertz’s theory. The relation of contact radius as a function of applied load for JKR model is given in Figure 1.6(a). Even when the external load is reduced to zero, a measurable contact area exists (point A). In order to decrease the contact radius a tensile load is required to separate two spheres. In a load-controlled measurement, two spheres separate with none zero contact radius at point C. The phenomenon is known as pull-off and the contact radius and required force are

$$a_0 = \left( \frac{3\pi \gamma R^2}{2K} \right)^{1/3}$$

(1.4)

$$P_0 = -\frac{3}{2} \frac{\pi \gamma R}{P}$$

(1.5)
For displacement control, the contact radius can be reduced along curve CD. Pull-off occurs at point D. Other relations between applied load, penetration depth and contact radius are also given in Figure 1.6. Great success has been achieved by applying JKR theory to the contact mechanics of rubber or gelatine sphere on a glass flat [26]. By measuring the applied force and contact radius at pull-off, the adhesion energy can be obtained.

### 1.2.3 DMT theory

Derjaguin et al [27] incorporated long-range intersurface forces into solid-solid adhesion interfaces and led to the Derjaguin-Muller-Toporov (DMT) model in 1975. This model assumes an attractive force being applied in the annular region just outside the contact zone, contrasting JKR model which assumes adhesion only at the contact edge. The contact radius predicted by DMT theory is given,

$$a_{DMT} = \left( \frac{PR}{K} \left( 1 + \frac{2\pi \gamma R}{P} \right) \right)^{1/3}$$

(1.6)

The relation of contact radius as a function of applied load for DMT model is shown in Figure 1.6(a). Similar to JKR model, contact radius is nonzero even the applied load is removed (point M). In order to reduce the contact radius to zero, a tension is needed (point N),

$$P_{DMT} = -2\pi \gamma R$$

(1.7)

This pull-off force is significantly different from the result of JKR theory. As the contact profile of the adhering spheres in DMT model is taken to be identical to Hertz theory, the relations of penetration depth as a function of contact radius of two theories coincide. The normal stress at
the contact edge is zero rather than infinite in JKR theory. The contact circle assumes a cusp like geometry as contrasted to a “pseudo-parabolic” shape from JKR theory.

1.2.4 Dugdale-Barenblatt-Maugis model

The stress distribution, pull-off force and contact shape predicted from JKR and DMT are inconsistent. These two models were originally believed to be conflicting. Tabor noted the existence of a neck at the contact edge in the JKR model and obtained the height of the neck [28],

\[ h^* = \left( \frac{R \gamma^2}{E^2} \right)^{1/3} \]  

The ratio of the neck height to the equilibrium distance between atoms, named \( z_0 \), was defined by Tabor as the dimensionless parameter,

\[ \mu = \left( \frac{R \gamma^2}{E^2 z_0^3} \right)^{1/3} \]  

This Tabor parameter finally resolves the inconsistence between the JKR and DMT. The JKR model should be used for soft solids with large radius and high energy of adhesion where \( \mu >> 1 \), while DMT theory is good for hard solid material with a small radius and low adhesion energy where \( \mu << 1 \). Maugis [29] later adopted the Dugdule-Barenblatt cohesive zone approximation to model finite range and magnitude of intersurface forces, and therefore derived the transition from JKR to DMT limits shown in Figure 1.7. The modified parameter \( \lambda \) is 1.16 \( \mu \).

The Lennard-Jones potential is used as an approximate model to describe the interaction between atoms or molecules and shown as the solid curve in Figure 1.8. It contains the Pauli repulsion at short ranges due to overlapping electron orbitals and van der Waals attraction at long
ranges. The pressure due to these two forces is defined as disjoining pressure and is shown as the vertical axis in Figure 1.8. The horizontal axis is the intersurface separation. Though the Lennard-Jones potential is good to describe the interfacial interaction, the mathematical function is too complex to solve real problems. In order to simplify the calculation, forces in the Dugdale model are assumed to be uniform instead of Lennard-Jones potential and to act in annular region outside the contact area shown in Figure 1.8. The product of attractive force magnitude and range equals the adhesion energy which is the area under the Lennard-Jones potential curve. When the intersurface force is long range and force magnitude is small, DMT limit is valid. JKR model is best suited for short range intersurface force with infinite magnitude. This Heaviside function assumption is modified by other forms where the enclosed area is a triangular or trapezoid [30]. Independent of the mathematical forms, the area under the curve is fixed to be the same as the area under the Lennard-Jones potential curve, which represents the work needed to create a new unit surface.

Figure 1.7 Relation between contact radius and applied load for various $\lambda$. [29]
1.2.5 Adhesion map for solids contact

A map [31] for the contact mechanics of elastic spheres was constructed by Johnson and Greenwood based on the Tabor parameter and is shown in Figure 1.9. The vertical axis is the ratio of the applied load to the product of work of adhesion and the radius of the sphere. The horizontal axis is the modified parameter. $\delta_1$ is the approach displacement due to elastic deformation and $\delta_0$ is the distance due to adhesion. When the applied load is large enough to make the adhesion force to be negligible, Hertz theory is valid shown as the top part in the map. If normalized load is not large and adhesion should be taken into account, the selection of the adhesion model is dependent on the modified parameter or the Tabor parameter. For stiff materials at sufficiently light loads, the elastic deformation is quite smaller than the range of the adhesion force. The spheres can be considered as rigid ones and their behaviors can be described by Bradley theory.
cannot be neglected, DMT model is applicable. JKR model is valid for larger Tabor parameter and shown as the right part of the map. The intermediate region is described by Maugis theory. This map attributes the application regimes of different adhesion models depending on the material properties and is also called ‘adhesion map’.

![Adhesion map for the contact of elastic spheres](image)

Figure 1.9 Adhesion map for the contact of elastic spheres [31]

1.2.6 Other adhesion models

The above discussed adhesion models were originally used for the contact properties between two spheres or spheres with flat surface. Recently, the adhesion problems for other geometries are studied as well. Johnson and Greenwood implemented an approximate JKR theory for elliptical contacts [32]. The transition from JKR behavior for cylindrical contacts with parallel axis governed by Tabor parameter was also discussed [33]. Jin and Hui [34] developed a novel numerical method to solve asymmetric adhesive contact problems and discussed the
adhesive contact between a sphere and a cylinder and two identical cylinders placed at a skew angle was also considered.

Thin shell structures like cells, polymerized vesicles and carbon nanotubes are typical geometries. They conform to the substrate geometry by deforming in plate bending, membrane stretching, or mixed bending-stretching mode that causes stress in the center contact to be zero. Compression increases rapidly from center contact to a sharp spike at the contact edge contrasted to the parabolic distribution of solid objects from Hertz theory due to the geometrical incompatibility. Such structures are also susceptible to buckling, snap phenomenon and wrinkling which cannot be captured by the aforementioned solid adhesion theories. These specific properties have drawn high interests from researchers.

Tamura [35] studied the adhesion induced buckling of spherical shells onto a rigid substrate by means of numerical minimization of the sum of the elastic and adhesion energies. The collapse of single-walled carbon nanotubes under the influence of self-van der Waals interactions has been investigated by Tang et al [36]. Springman and Bassani [37, 38] discussed the mechano-chemical coupling in the adhesion of thin-shell structures and also analyzed the snaps transitions in adhesion of nonlinear spherical caps adhered to a rigid substrate. Carmel and Wan [39] constructed an adhesion model for two dissimilar cylindrical shells with parallel axes and considered a range of stiffness and radius. The adhesion of an elastic spherical shell and cylindrical shell onto a rigid plate were discussed by Shi and Wan [40, 41]. The JKR pull-off force for the spherical shell was found to be dependent on the elastic modulus and thickness of the shell and the pull-off radius for cylindrical shell was zero, which were distinctly from the classical JKR theory for solid objects.
Most of the adhesion models assume the contact surface to be clean and smooth. But in reality, this assumption cannot be satisfied because of surface roughness and contaminants. Lots of work has been done to understand the influence of surface roughness on the adhesion of elastic solids. Ziberman and Persson [42] presented analytical results for adhesion between elastic bodies with rough surfaces. Guduru analyzed the mechanics of detachment of a rigid solid from an elastic wavy surface and performed experimental verification [43, 44]. The JKR-DMT transition solution for adhesive rough surface contact was derived by Morrow et al [45]. Adhesion between elastic bodies with random asperities was discussed by Persson [46].

1.3 Review of thin film adhesion

Notwithstanding the many colossal applications and rich physical insights of these celebrated adhesion models, they are inadequate to account for thin film adhesion. For instance, most cells are thin-walled capsules with an ultra thin lipid bilayer membrane with thickness down to 10 nm. Interactions between cells are achieved by thin film adhesion. The stiction of RF switch is also governed by thin membrane behavior. Rather than inducing a compression within the contact area, flexible thin film conforms to the substrate geometry and undergoes bending or stretching deformation. The strain field and the resulting interfacial adhesion-delamination mechanics are expected to be distinctly different from the classical Hertz contact and aforementioned solid adhesion models. A number of methods for measuring thin film adhesion are documented in the literature as follows.
1.3.1 Peel test

Peel test is commonly used to measure adhesion of thin films and coatings. A strip is pulled by a force $F$ at some angle $\theta$ as shown in Figure 1.10. The width, thickness and Young’s modulus of the strip are $b$, $h$, and $E$ respectively. The energy release rate which describes the energy dissipated during fracture per unit of newly created surface was given by Kendall [47],

$$G = \frac{F}{b} (1 - \cos \theta) + \frac{F^2}{2b^2 Eh}$$

(1.10)

For inextensible thin film, the second term on the right side of above equation can be neglected. The state of the crack is dependent on the relation between the energy release rate $G$ and interfacial adhesion energy $\gamma$. (i) $G > \gamma$, the strip delaminates from the substrate. (ii) $G < \gamma$, the strip adheres to the substrate. (iii) $G = \gamma$, system stays at equilibrium and the crack is stable.

The peel test is quite likely the method of choice when measuring the adhesion of flexible thin film because of its simple and straightforward geometry and analysis. But for strong adhesion, a considerable amount of peeling energy goes into plastic yielding of the peeled strip in bending rather than going into crack tip processes. The above equation for energy release rate becomes invalid. Other disadvantages of this method include (a) the crack front is not straight and (b) the difficulty in initiating a peel strip for coatings with strong adhesion.
1.3.2 Blister test

Blister test, introduced by Dannenberg [49] and Williams [50], is a widely used method to measure the work of adhesion between thin film and solid substrate. In the standard blister test (Figure 1.11(a)), hydrostatic or air pressure applied via a bore in the substrate drives an axisymmetric delamination along the membrane-substrate interface. A simple energy balance entails a catastrophic propagation once the delamination initiates, which is consistent with many experimental evidences over the years [51]. Dillard et al modified the classical pressurized blister test and introduced the first constrained blister test (Figure 1.11(b)) [52-54]. A rigid plate is placed above the membrane such that the blister height is limited and thus stabilizes the delamination process. Dillard et al further modified the constrained blister by clamping a freestanding membrane at the periphery [55]. Upon an external pressure, the membrane bulges and makes adhesion contact with the fixed plate above. By simultaneously measuring the applied pressure and contact radius, the adhesion energy and the magnitude and range of the disjoining pressure can be decided. Xu and Liechti [56] recently conducted the experiment with smooth and structured acrylate layers on a PET carrier film contacting a glass substrate. The interfacial
adhesion energy was deduced by measuring the contact radius, applied pressure and profile of the deformed thin transparent films using a homemade moiré deflectometry. Island blister (Figure 1.11(c)) is also used to characterize thin film adhesion, where a small pillar is attached in the center of a detached annulus [57, 58]. The delaminated region is shown as the gray part in the top view of island blister test in Figure 1.11(c). The interface crack is propagated by pressurizing the annular blister and the radius of the inner circle is reduced. One problem with the island blister test is that it tends to be unstable. The energy release rate is very large as the debonding front is reduced to a small length, and a low applied pressure may cause the full delamination of the inner island. To overcome this difficulty, Dillard and Bao [59] conceived the peninsular blister test (Figure 1.11(d)) where delamination occurs along a narrow “peninsular” which extends into the blister region. This version of blister test maintains high driving force for a steady delamination. Williams [48] studied the energy release rates for both peeling and different blister tests.
Figure 1.11 Blister models. (a) Standard pressurized blister. (b) Constrained blister. (c) Island blister. (d) Peninsular blister. The left part is the side view from the cross section of dash line and right part is the top view. The adhered regions and delaminated regions are shown in different colors.
1.3.3 Punch test

Another alternative testing method is to replace the uniform pressure by a mechanical load to drive a delamination (Figure 1.12) known as punch test [60, 61]. A cylindrical punch makes contact with a clamped membrane, before tension is applied to drive the delamination and thus diminishing the contact radius. Interfacial adhesion can be characterized by the mechanical response. This configuration is used to study the adhesion between thin membranes and substrates and also the stiction and adhesion in biological, biomedical and MEMS structures. Wan derived the adhesion-delamination mechanics of 1-D rectangular and 2-D axisymmetric membranes in the presence of zero-range intersurface forces (JKR limit) and mixed plate-bending and membrane-stretching deformation [62-64]. Duan built the solid mechanics model for the thin film in a capacitive MEMS-RF switch and numerically analyzed the associated pull-in (initially contact with non-zero radius) phenomenon for both a 1-D rectangular bridge and a 2-D axisymmetric film [65]. The ratio of film-pad gap to film thickness was found to play a critical role in the electromechanical behavior of film based RF switch. The effect of the residual
stress to the pull-in behavior of the thin film actuated by an electrostatic potential was discussed as well [66].

However, most of the blister models and punch tests are based on the JKR assumption. These models work well for characterization of macro scale thin films because the intersurface force range is neglected compared to the dimension of the material. While for micro or nano scale, the intersurface force may have the same magnitude as material dimension, the effect of adhesion should be considered. This can be verified by taking graphene as an example in the next several chapters. Sally [67] investigated the DMT limit and JKR limit of a constrained blister from thin membrane to rigid plate with Dugdale model. Wan established the model for a circular membrane clamped at the periphery [68] and relaxed the JKR-DMT constraint by allowing finite magnitude and range of intersurface forces. DMT limit, JKR limit and the transition were discussed. Following this method, different adhesion models in the long range intersurface force will be discussed in Chapter 2.

1.4 Graphene and its adhesion property

Recently, as a promising nano material, graphene has drawn high interests from both academic research and industrial applications. It is the firstly found real two-dimensional material which is a monolayer of carbon atoms packed into a hexagonal lattice [69, 70]. The sheet has ultrahigh mechanical strength, conductivity with high electron mobility and optical transparency [71-74]. These exceptional properties make it a promising material for flexible or transparent electronics, micro/nano-electromechanical systems (M/NEMS), bio-sensors etc [75-79]. However, the nanometer thickness of graphene makes adhesion property to be significant.
The ability of graphene to integrate or to adhere to electronic substrates is crucial for the implementation and reliability in electronics systems such as transparent electronics and display panels. The world’s thinnest balloon (Figure 1.13) created by a monolayer graphene membrane shows that graphene is impermeable to even nimble helium atoms [80]. Adhesion between the graphene and the silicon substrate prevents the balloon to be blown up. Usually, flat graphene sticks well to a flexible substrate by van der Waals interaction. But delamination or even fracture may be expected when the structure is under high levels of strain [81]. In order to overcome this problem, researchers buckle graphene into 3D periodical structures. The pre-buckled thin sheet on elastomeric substrate can undergo large deformation indicating the potential use as flexible electronics. Interlayer adhesion also imposes influence on the fracture behaviors of the macroscopic graphene oxide papers [82].

Figure 1.13 The world’s thinnest balloon [80]

Because of the significant adhesion property of graphene, the conventional adhesion problems in M/NEMS, such as the stiction in RF-switch and micro cantilevers [22, 83], and collapse of a comb structure in micromachined accelerometer [23] can also happen to graphene based devices. In order to hold promise for future application in NEMS, it is necessary to
characterize the adhesion behavior of graphene. For the first time, Zong [84] reported a method to directly measure graphene adhesion on silicon substrate by intercalation of nanoparticles (Figure 1.14). Adhesion energy of the typical graphene-silicon interface is measured to be $151\pm28 \text{ mJ/m}^2$. This result is consistent with Bunch’s estimated value $100 \text{ mJ/m}^2$ [80]. Wang [85] measured the adhesion energy of graphene with liquid, also graphene oxide with liquid and found that the graphene oxide was hydrophilic, while graphene was hydrophobic. Lu [86] studied the nanomechanics of a graphene sheet adhered to a substrate with cavity sidewalls. Line loads were applied to the sheet that resulted in peeling from cavity sidewalls followed by either sliding along or decohesion from the top surface of the substrate. The nanoscale peeling of graphene sheet was numerically studied by molecular mechanics simulation [87]. Buehler [88] investigated the self-folding of mono- and multilayer graphene sheets due to its self adhesion and obtained the critical self-folded length. The van der Waals interaction energy between a monolayer graphene and substrate was numerically calculated and the graphene morphology on substrate surface was discussed as well [89, 90]. Scharfenberg [91] examined the mechanical and adhesion properties of graphene by placing it on a microscale-corrugated elastic substrate. The graphene adhered to the substrate surface and substantially deformed it shown in Figure 1.15. In the voluminous relevant literature, most studies are theoretical and simulation work with rarely any direct experimental data. The only existing experiment results are about graphene and silicon substrates. For other widely used materials in M/NEMS, like silicon nitride, gold, or even mica, the adhesion properties with graphene are unknown. Recently, scientists obtained atomically flat graphene on mica substrates [92] and also visualized the structures of water molecules using a sheet of graphene on mica substrate [93]. The graphene-mica interface is claimed to have much higher adhesion energy than graphene-silicon interface, but no direct experiment is implemented.
to verify this result. Rudenko investigated the adhesion and electronic properties of graphene on a muscovite mica surface using the density functional theory with van der Waals interactions and discussed the role of surface morphology. One objective of this thesis is to investigate the adhesion property of graphene and the associated morphology of graphene on undulated substrate. More details will be given in Chapter 4 and 5.

Figure 1.14 Direct measurement of graphene adhesion using nano-particles [84]
1.5 Research objectives

This thesis mainly includes two parts: (i) theoretical study of thin film in the presence of long range intersurface force, (ii) investigation of the adhesion property of graphene and its associated morphology on electronic substrates. As mentioned before, the adhesion models for solid objects are not valid for thin film. The adhesion-delamination mechanics of thin film should be derived from first principles and a new Tabor parameter governing adhesion transition from DMT-limit to JKR-limit is needed. This parameter would be applied for several thin film delamination geometries. Based on this new parameter, an adhesion map for thin film similar to that for solid objects adhesion [31] will be constructed. On the experimental front, adhesion property between graphene and gold will be discussed and the morphology of graphene on
undulated substrates will be experimentally examined. Molecular mechanics simulation will be conducted to study the adhesion behavior of graphene and graphene interfaces.

1.6 Organization of the thesis

This thesis is organized in six chapters.

Chapter 1 is an introduction to adhesion and discusses the history of theory development from bulk solid adhesion to thin film adhesion. Graphene and its mechanical and adhesion properties are introduced.

Chapter 2 discusses the adhesion mechanics of thin film in the long range intersurface force. A new Tabor parameter for the transition from DMT-limit to JKR-limit of thin film is found and verified by different adhesion models including punch test, standard pressurized blister model and constrained blister model. A new adhesion map for thin film is constructed which describes the transition from DMT-limit to JKR-limit of thin film adhesion and also transition from bending to stretching.

Chapter 3 discusses the loading-unloading hysteresis of a rigid punch adhered to a clamped membrane. Both rectangular and circular membrane are considered. Similarity between the punch test and classical indentation is also discussed.

Chapter 4 explores the adhesion between two graphene layers using molecular mechanics simulation. Basic theory of molecular mechanics simulation is introduced followed by three models to determine the elastic modulus and effective thickness of graphene. Interfacial adhesion energy between two graphene layers is also estimated. Delamination of two adhering graphene layers is discussed and compared to the continuum model. Crystallographic misorientation of the adhering graphene layers is also accounted for.
Chapter 5 introduces the experiment to measure adhesion of graphene with electronic substrates, as well as morphology of graphene on undulated substrates. Fabrication procedures of the electronic substrate with patterned gold nano pillars and preparation of graphene from chemical vapor deposition (CVD) method are given. After the transfer process, the morphology of graphene on these pillars is obtained by scanning electron microscopy (SEM) and atomic force microscopy (AFM). A theoretical model is built to analyze the experiment data and the adhesion energy of graphene-gold interface is obtained. The effects to change the morphology of graphene on undulated substrates are discussed.

Chapter 6 summarizes the significant contributions and conclusions of this study and proposes the future work.
Chapter 2 Thin film adhesion in the long range intersurface force

This chapter focuses on the adhesion-delamination mechanics of thin film in the presence of long range intersurface force. A new Tabor parameter governing thin film adhesion transition from DMT-limit to JKR-limit is derived and then applied to a range of adhesion models. An adhesion map to discuss theoretical behavior of membrane under bending-stretching is then built based on the obtained new Tabor parameter.

2.1 New Tabor parameter

Wan recently showed how the combination of magnitude and force range of the disjoining pressure or intersurface forces played a crucial role in determining the mechanical response of a membrane upon delamination [68]. To quantify the transition from JKR to DMT limits for thin films, a new Tabor parameter is constructed.

Figure 2.1(a) shows the schematic of a circular membrane clamped at the periphery. A cylindrical punch with a planar surface makes adhesion contact with the diaphragm, before a tension is applied to the punch to delaminate the membrane. In order to make the model to be universal, variables are normalized and their dimensionless equivalences are listed in Table 2.1. Bold symbols represent the physically measureable quantities. Figure 2.1(b) shows a schematic of half the membrane profile, \( w(r) \), from the center to the clamped edge, \( 0 \leq r \leq 1 \). Horizontal dimensions are scaled by the membrane radius, \( a \), while vertical dimensions by the membrane thickness, \( h \). The long-range intersurface force or disjoining pressure, \( p \), acting across the membrane-substrate gap gives rise to a cohesive zone immediately behind the delamination front.
$(r = c)$. The cohesive edge $(r = b)$ divides the freestanding membrane into an inner cohesive zone where $p$ acts $(c \leq r \leq b)$ and a traction free outer region $(b \leq r \leq 1)$.

Figure 2.1 (a) Schematic of a clamped circular membrane adhered to a rigid substrate. (b) Schematic of half the membrane profile drawn in normalized coordinates.
Table 2.1 Normalized coordinates and variables.

<table>
<thead>
<tr>
<th>Physical parameters (Bold)</th>
<th>Normalized parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometrical parameters</td>
<td></td>
</tr>
<tr>
<td>( r ) = horizontal distance</td>
<td>( r = \frac{r}{a} ),</td>
</tr>
<tr>
<td>( w_0 ) = vertical displacement of punch or blister height</td>
<td>( w = \frac{w}{h}, \quad w_0 = \frac{w_0}{h} )</td>
</tr>
<tr>
<td>( a ) = half membrane width in 1D model or membrane radius in 2D model (or hole radius in standard pressurized blister test)</td>
<td>( c = \frac{c}{a}, \quad b = \frac{b}{a} )</td>
</tr>
<tr>
<td>( c ) = half contact width in 1D model or radius of contact circle in 2D model</td>
<td></td>
</tr>
<tr>
<td>( b ) = half cohesive edge in 1D model or radius of cohesive edge in 2D model</td>
<td></td>
</tr>
<tr>
<td>( h ) = membrane thickness</td>
<td></td>
</tr>
<tr>
<td>Material parameters</td>
<td></td>
</tr>
<tr>
<td>( v ) = Poisson’s ratio</td>
<td>( s = \sigma^{1/2} \left( \frac{12(1-v)a^2}{Eh^2} \right)^{1/2} )</td>
</tr>
<tr>
<td>( E ) = elastic modulus</td>
<td>( \gamma = \gamma \left( \frac{12(1-v)a^4}{Eh^5} \right) )</td>
</tr>
<tr>
<td>( \sigma ) = tensile membrane stress</td>
<td>( p = p \left( \frac{12(1-v)a^4}{Eh^4} \right) )</td>
</tr>
<tr>
<td>( \gamma ) = interfacial adhesion energy</td>
<td>( y = \frac{y}{h} )</td>
</tr>
<tr>
<td>( p ) = disjoining pressure</td>
<td></td>
</tr>
<tr>
<td>( y ) = surface force range</td>
<td></td>
</tr>
<tr>
<td>Mechanical loading</td>
<td></td>
</tr>
<tr>
<td>( F ) = applied external force</td>
<td>( F = F \left( \frac{12(1-v)a^2}{\pi Eh^4} \right) )</td>
</tr>
<tr>
<td>( f ) = applied pressure</td>
<td>( f = f \left( \frac{12(1-v)a^4}{Eh^4} \right) )</td>
</tr>
<tr>
<td>( U ) = energy terms</td>
<td>( U = U \left( \frac{12(1-v)a^3}{Eh^5} \right) )</td>
</tr>
</tbody>
</table>
The form of exact disjoining pressure is mathematically involved [94], though the net effect is here taken to be attractive in the present context. A finite magnitude, \( p \), and a finite range, \( y \), according to the Dugdale-Barenblatt-Maugis model [95, 96], are assumed such that

\[
\Phi(w) = \begin{cases} 
  p & \text{within the cohesive zone, } c < x \leq b \text{ and } 0 < (w_0 - w) \leq y \\
  0 & \text{without the cohesive zone, } b < x \leq 1 \text{ and } y < (w_0 - w) \leq w_0 
\end{cases}
\]

(2.1)

The JKR-limit corresponds to \( y \to 0, p \to \infty \) and \( b \to c \), and the DMT limit \( y \to \infty, p \to 0 \) and \( b \to 1 \). The interfacial adhesion energy, \( \gamma = p y \), is a material parameter.

No membrane wrinkling is allowed and residual stresses are not considered. For demonstration purposes, a classical energy balance method is adopted. The disjoining pressure considered here acts perpendicular to the adhering surfaces. Should mixed opening-shearing be considered, the lateral component of \( p \) has to be considered. This mode mixity will lead to a modified membrane profile and force-displacement relationship, which is beyond the scope of this thesis. The flexural rigidity of a membrane is given by \( \kappa = \frac{E h^3}{12(1 - v^2)} \). In the presence of an external load, the thin film is deformed by mixed bending (\( \kappa \cdot \nabla^4 w \)) and stretching (\( -\sigma h \cdot \nabla^2 w \) with \( \sigma \) the tensile membrane stress), and the thin film profile \( w(r) \) is governed by,

\[
\kappa \cdot \nabla^4 w - \sigma h \cdot \nabla^2 w = p , \quad \text{within the cohesive zone} \quad (2.2)
\]

\[
\kappa \cdot \nabla^4 w - \sigma h \cdot \nabla^2 w = F \cdot \delta(r) , \quad \text{without the cohesive zone} \quad (2.3)
\]

where \( \nabla^2 \) is the Laplacian operator and \( \delta(r) \) is the Dirac’s delta function denoting the applied load. The above two equations have been recast using the dimensionless variables shown in Table 2.1 by Wan in his circular punch model [68]. Equations (2.4) and (2.5) show the dimensionless expression,

\[
\nabla^4 w - s^2 \cdot \nabla^2 w = p , \quad \text{within the cohesive zone} \quad (2.4)
\]
\[ \nabla^4 w - s^2 \nabla^2 w = F \cdot \delta(r), \quad \text{without the cohesive zone} \quad (2.5) \]

However, the normalized adhesion energy \( \gamma \) was assumed to be 1 which prevented the conclusion to be universal in Wan’s work. Following this normalized method, it is found that the dimensionless force \( F \) is proportional to \( \gamma^{3/4} \) and \( w \) is proportional to \( \gamma^{1/4} \) for a pure stretching membrane. This reminds us to obtain a universal JKR-DMT transition parameter or new Tabor parameter, \( \psi_{\text{stretching}} \), for a thin flexible membrane possessing zero flexural rigidity and deforming under pure stretching by doing the following simplification,

\[
\psi_{\text{stretching}} = \frac{p}{\gamma^{3/4}} = \left[ \frac{6(1-v)a^4}{\gamma^3 Eh} \right]^{1/4} p
\]

The membrane behavior transits from JKR to DMT as \( \psi \) spans a range of values specific to different blister geometries, which will be discussed in the next few sections. Note that a similar parameter, \( \lambda = (p^4a^4/Eh\gamma^3)^{1/3} \), was recently introduced by Xu and Liechti [56] following our work. This comes from a different normalized method and thus \( \lambda = \psi^{4/3}/(6(1-v))^{1/3} \).

For a thick and stiff membrane under pure bending with negligible stretching, \( F \propto \gamma^{1/2} \) and \( w \propto \gamma^{1/2} \) and this introduces the universal JKR-DMT transition parameter, \( \psi_{\text{bending}} \), for a thick plate with neglecting membrane stress,

\[
\psi_{\text{bending}} = \frac{p}{\gamma^{1/2}} = \left[ \frac{6(1-v)a^4}{\gamma Eh^3} \right]^{1/2} p
\]

Though both \( \psi_{\text{stretching}} \) and \( \psi_{\text{bending}} \) are dimensionless, their distinct dependencies on the membrane geometry and materials parameters are notable.

However, the true deformation of a thin film must be mixed bending and stretching, not just these two limits. Lots of studies have focused on the deformation of a thin film transition from a rigid plate at small deformation to a flexible membrane at large deformation [97-100].
This has been applied to investigate the nonlinear bending and stretching by indentation of a clamped graphene [101]. To be valid for the thin film mixed bending and stretching, the new Tabor parameter can be extended to the following form:

$$\psi_{SB} = \left(\frac{y}{a}\right)^{-1} \left(\frac{\gamma}{Eh}\right)^{m} \left(\frac{a}{h}\right)^{n}$$

(2.8)

where, $y/a$ is the force range, $\gamma/ (Eh)$ represents interfacial adhesion energy and $a/h$ is the dimension ratio. For a thin film, when the deformation is close to its thickness, pure bending is dominant and equation (2.8) can be simplified to equation (2.7) by applying $m = \frac{1}{2}$ and $n = 1$. When the deformation is large compared to film thickness, pure stretching limit is valid and the index $m$ and $n$ decrease to $\frac{1}{4}$ and 0, respectively. Equation (2.8) is simplified to equation (2.6).

This new parameter reminisces the famous Tabor parameter for the adhesion of bulk solids, $\mu = (16 \frac{R}{9} \gamma^2 K^2 y^3)^{1/3}$, or, $\mu = \frac{p(16 R / 9 K^2 \gamma)^{1/3}}{2E / 3(1 - v^2)}$. It is interesting to find that these two parameters are not isolated, but correlated in some form. The new Tabor parameter can be rearranged to the form like equation (1.9) by taking $m = 2/3$ when the radius of the sphere $a$ is assumed to be the same as thickness $h$. From this point, we can say that a universal parameter to govern the adhesion from flexible membrane to bulk solid is found. We will show how the new dimensionless parameter $\psi$ is used to gauge the JKR-DMT transition for adhesion-delamination of thin membrane from a rigid substrate in the next several parts and also demonstrate how $\psi$ manifests in different blister geometries, which can be extended to other inward or outward bound delamination configurations.
2.2 Punch test model

2.2.1 Rectangular film under pure stretching

We take the rectangular punch test model as an example to verify the obtained new Tabor parameter. Figure 2.2(a) shows a rectangular membrane of unit width being clamped at the opposite ends and adhered to the planar surface of a flat punch with the same length and width. Upon an external tensile load applied to the punch, delamination occurs reducing the contact area. Figure 2.2(b) gives the model drawn in normalized coordinates. All variables and their dimensionless equivalences are defined and listed in Table 2.1. A few basic assumptions are taken to construct the new adhesion model: (i) the membrane is deformed by membrane-stretching only with negligible plate-bending (i.e. zero flexural rigidity), (ii) the debonding angle, $\theta$, is small with $dw/dx = \tan \theta \approx \sin \theta \approx 0$, (iii) any residual stress and sliding in the contact region are ignored [102]. Mechanical equilibrium requires $F = 2p(b - c)$. Upon loading, small punch displacement with $w_0 \leq y$ requires the cohesive zone to extend to the clamped edge ($x = 1$), alluding to a pseudo DMT-limit. Large displacement with $w_0 > y$ causes the cohesive edge to retract from the edge and give rise to a fully developed cohesive zone entirely confined to the freestanding region.

The external load applied to the punch is balanced by the disjoining pressure, resulting in a deformed membrane profile governed by

$$
\left\{
\begin{array}{ll}
-\sigma h \nabla^2 w = p & \text{for } c < x \leq b \\
-\sigma h \nabla^2 w = (F/2) \delta(x) & \text{for } b < x \leq a
\end{array}
\right.
$$

(2.9)

where $\nabla^2 = d^2/dx^2$ is the Laplacian operator and $\delta(x)$ is the Dirac’s delta function denoting the applied load at the centerline ($x = 0$).
Figure 2.2 (a) Schematic of a clamped rectangular membrane adhered to a planar punch surface. (b) Drawing in normalized coordinates and variables.

Equation (2.9) can be rewritten as

$$
\begin{align*}
- s^2 \frac{d^2 w}{dx^2} &= p x & \text{for } c < x \leq b \\
- s^2 \frac{d^2 w}{dx^2} &= p (b - c) & \text{for } b < x \leq 1
\end{align*}
$$

(2.10)

which can be solved exactly to yield

$$
w = \begin{cases} 
\frac{p}{2s^2} (-x^2 + 2cx + 2b - b^2 - 2c) & \text{for } c < x \leq b \\
\frac{p(b-c)}{s^2} (-x+1) & \text{for } b < x \leq 1
\end{cases}
$$

(2.11)
Figure 2.3 shows typical profiles for $c = 0.1$ and a range of $p$. Note the “cusp”-like geometry in the cohesive zone leading to the contact edge in reminiscence of the Barenblatt’s crack [95, 96, 103], and the linear profile in the traction-free region alluding to the Griffith’s parabolic geometry [104]. In the limit of $p \to \infty$ and $b \to c$, the cusp vanishes and the freestanding region is linear throughout.

![Figure 2.3 Membrane profile for fixed half contact length $c = 0.1$ and a range of disjoining pressure.](image)

The punch displacement is given by

$$w_0 = w(x = c) = -\frac{p}{2s^2}(b + c - 2)(b - c)$$

(2.12)
and the surface force range

\[ y = w_0 - w(x = b) \]  \hspace{1cm} (2.13)

Total energy of the membrane-substrate system is given by \( U_T = U_E - U_S \), with \( U_E \) the elastic energy due to membrane stretching and \( U_S \) the surface energy to create new surfaces. For delamination to occur, \( (\partial U_T / \partial c)_{w_0=\text{constant}} = 0 \). Since the mechanical response of a thin flexible membrane is always cubic with \( F \propto w_0^3 \), \( U_E = \int F \, dw_0 = \frac{1}{4} F \, w_0 \). Alternatively, the energy density of \( s^4/24 \) leads to \( U_E = \text{energy density} \times \text{area}. \) The average membrane stress is given by

\[
s^2 = \begin{cases} 
\frac{12}{b-c} \int_c^b \frac{1}{2} \left( \frac{dw}{dx} \right)^2 \, dx & \text{for } c < x \leq b \\
\frac{12}{1-b} \int_b^1 \frac{1}{2} \left( \frac{dw}{dx} \right)^2 \, dx & \text{for } b < x \leq 1
\end{cases}
\]  \hspace{1cm} (2.14)

Substituting \( w \) in equations (2.11) into (2.14),

\[
s = \begin{cases} 
2^{1/6} (b-c)^{1/3} p^{1/3} & \text{for } c < x \leq b \\
6^{1/6} (b-c)^{1/3} p^{1/3} & \text{for } b < x \leq 1
\end{cases}
\]  \hspace{1cm} (2.15)

The elastic energy is therefore given by

\[
U_E = \frac{s^4}{24} \cdot \frac{2(b-c)}{24} \cdot \left( \frac{1}{2} \right) \left( \frac{dw}{dx} \right)^2 \, dx + \frac{s^4}{24} \cdot \frac{2(1-b)}{24} \cdot \left( \frac{1}{2} \right) \left( \frac{dw}{dx} \right)^2 \, dx
\] \hspace{1cm} (2.16)

Substituting \( s \) in equations (2.13) and (2.15) into (2.16),

\[
U_E = \frac{16}{3(b-c)^2} y^4 + \frac{3}{4(1-b)^3} (w_0 - y)^4
\] \hspace{1cm} (2.17)

The surface energy per unit area has a maximum in the contact zone with \( U_S = \gamma (2c) \), decreases in the cohesive zone, and reaches zero at the cohesive edge. Therefore,
\[ U_s = 2c\gamma + 2 \int_c^b p \left[ y - (w_0 - w) \right] dx \quad (2.18) \]

Substituting equation (2.11), (2.12) and (2.13) into (2.18),

\[ U_s = 2c\gamma - (b - c) \left\{ \left( \frac{2}{3} \frac{b - c}{2 - b - c} \right) pw_0 - 2\gamma \right\} \quad (2.19) \]

In the JKR-limit, \( y \to 0, p \to \infty \) and \( b \to c \). The disjoining pressure turns into a Dirac’s delta function at the contact edge, the cohesive zone width \( b - c \) reduces to zero, and the traction free freestanding membrane becomes linear, and is given by

\[ w = w_0 \left( \frac{1 - x}{1 - c} \right) \quad \text{with} \quad w_0 = \frac{F}{2s^2} (1 - c) \quad (2.20) \]

The mechanical response without delamination is found to be

\[ F = \frac{12w_0^3}{(1 - c)^3} \quad (2.21) \]

which is cubic for fixed \( c \). The energy terms reduce to

\[ U_E = \frac{3w_0^4}{(1 - c)^3} \quad \text{and} \quad U_s = 2c\gamma \quad (2.22) \]

An energy balance yields the delamination trajectory,

\[ w_0 = \frac{2^{1/4}}{3^{1/2}} (1 - c)^{1/4} \gamma^{1/4} \quad \text{and} \quad F = 4 \left( \frac{2^{3/4}}{3^{1/2}} \right)^3 \gamma^{3/4} \quad (2.23) \]

Equations (2.20) to (2.23) are consistent with earlier results [105]. Figure 2.4 shows \( F(w_0) \) in the JKR-limit. As \( F \) increases from null, the contact area remains intact until \( F \) reaches a maximum at \( F_{\max} = (4 \times 2^{3/4} / 3^{1/2}) \gamma^{3/4} \approx 3.884 \gamma^{3/4} \) (N.B. \( F_{\max} = 4 \gamma^{3/4} \) in Figure 2.4 for reasons discussed later), which is consistent with reference report [105]. In a displacement control configuration,
A further increase in \( w_0 \) leads to a steady delamination along \( JJ' \) at constant \( F_{max} \) under neutral equilibrium. At \( J' \), the contact area reduces to a central line contact \((c = 0)\). An incremental increase in \( w_0 \) requires the membrane to snap from the substrate or pinch-off at

\[
w_0^* = \left( \frac{2^{1/4}}{3^{1/2}} \right) \gamma^{1/4} \approx 0.6866 \gamma^{1/4}.
\]

Since the membrane-punch gap now exceeds the disjoining pressure range \((w_0 > \gamma)\) herein, the membrane no longer senses the presence of the substrate and thus returns to its non-deformed plane.

![Figure 2.4 Mechanical response for a range of disjoining pressure.](image)
Figure 2.5 Energy as function of contact length for punch displacement $w_0 = 0.5 \gamma^{1/4}$ and a range of disjoining pressure
Figure 2.6 Total energy of the membrane-punch system for disjoining pressure
In the neo-DMT-limit, \( y \to \infty, p \to 0 \) and \( b \to 1 \). Here we consider a pseudo-DMT-limit (abbreviated as DMT-limit hereafter) where \( b = 1 \), but \( p \) does not necessarily vanish and \( y \geq w_0 \). The cohesive zone is underdeveloped, and the disjoining pressure is present in the entire non-contact freestanding region. The “cusp”-like membrane profile is found from equation (2.11) to be

\[
w = w_0 \left( -x^2 + 2cx - 2c + 1 \right) \frac{1}{c^2 - 2c + 1} \quad \text{with} \quad w_0 = \frac{p}{2s^2} (c^2 - 2c + 1) \quad (2.24)
\]

The constitutive relation without delamination is therefore

\[
F = \frac{32 w_0^3}{(1-c)^3} \quad (2.25)
\]

The energy terms become

\[
U_E = \frac{16 w_0^4}{3 (1-c)^3} \quad \text{and} \quad U_S = 2 Y - \frac{2}{3} p w_0 (1-c) \quad (2.26)
\]

Energy balance requires

\[
w_0 = \left( \frac{p}{16} \right)^{1/3} (1-c)^{4/3} \quad \text{and} \quad F = 4p^{3/4} w_0^{3/4} \quad (2.27)
\]

Figure 2.4 shows \( F(w_0) \) for \( \psi = 0.1 \). At \( O \) (\( F = 0, w_0 = 0 \)), the membrane is in full contact with the punch. As delamination proceeds along path OA, \( F \) monotonically increases while the contact area shrinks. At A, the contact area reduces to a line with \( c = 0 \). Further increase in \( w_0 \) causes the membrane to pinch-off. Regardless of the surface force range, the initial loading (\( w_0 = 0 \) and \( y > w_0 \)) always begins with the DMT-limit. The pinch-off locus hereafter denoted by the asterisk can be obtained by putting \( c \to 0 \) into equation (2.25), yielding \( F^* = 32 (w_0^*)^3 \). The condition \( w_0^* \leq y \) implies that the punch displacement falls short of the surface force range when
the membrane completely separates from the punch. In order words, the membrane can still sense the presence of the punch and remains deformation until \( w_0 > y \). The special case of \( w_0^* = y \) denoted by the dagger superscript requires \( b = 1 \) and \( p^\dagger = 16 (y^\dagger)^3 \), which is consistent with our earlier result [106]. Now \( \gamma = p^\dagger y^\dagger \), \( p = p^\dagger = 16^{1/4} \gamma^{3/4} = 2 \gamma^{3/4} \), which is the maximum possible disjoining pressure for DMT-limit to remain valid, and \( y^\dagger = 0.5 \gamma^{1/4} \). The two limits according to JKR and DMT present distinctly different delamination processes.

For disjoining pressure with intermediate range and magnitude, a Mathematica code is developed for fixed \( w_0 \) shown in Appendix 1. The cohesive edge is first determined by numerically solving equation (2.13), followed by solving for \( U_E \), \( U_S \) and \( U_T \) as functions of \( c \). Figure 2.5(a) to 2.5(c) show the energy terms for \( w_0 = 0.5 \gamma^{1/4} \) and a range of \( p \). At large \( \psi (> 100) \), all energy terms approach the JKR-limit. In Figure 2.5(c), the local minimum indicates a stable equilibrium. Figure 2.6(a) to 2.6(c) show \( U_T(c) \) for fixed \( p \) and a range of \( w_0 \). In Figure 2.6(a), \( p = 0.5 \gamma^{3/4} \) and DMT-limit applies throughout. As the punch moves from \( w_0 = 0 \) to \( 0.1 \gamma^{1/4} \), the contact area decreases until pinch-off at \( w_0^* \). Delamination proceeds along the dashed curve connecting the \( U_T \) minima from left to right. In Figure 2.6(b), \( p = 5 \gamma^{3/4} \) and \( y = 0.2 \gamma^{1/4} \). DMT-limit is valid for \( w_0 \leq 0.2 \gamma^{1/4} \). Further punch displacement leads to DMT-JKR transition and the cohesive zone becomes fully developed. Figure 2.6(c) shows the JKR-limit.
Figure 2.7 Mechanical response for a range of disjoining pressure.

The full mechanical response, $F(w_0)$, for a range of $\psi$ is shown in Figure 2.4. For $\psi \leq \psi^{\dagger}$, the DMT-limit is expected. All such curves ($\psi = 0.1, 1$ and $2$) terminate at the locus OABC with $F^* = 16 (w_0^*)^3$. For $\psi > \psi^{\dagger}$, all curves begin with the DMT-limit prior to DMT-JKR transition at $w_0 = \gamma$. For instance, when $\psi = 4$, DMT is valid until $w_0 = \gamma / p = 0.25 \gamma^{1/4}$ at $R$. In a load-controlled measurement, pull-off occurs at $R$ since further increase in load is no longer confined to this energy balance curve. In a displacement-controlled measurement, further increase in $w_0$ is possible beyond $R$. Along $RR'$, the contact area reduces while external load remains constant at $F = 4 \gamma^{3/4}$. The energy balance allows one to obtain the last loading point at $R'$, where $c = 0$ and the
membrane pinches off the substrate. In the JKR-limit, the loading curve rises sharply in $F$ till $F = 4 \gamma^{3/4}$ at $J$. Further increase in $w_0$ reduces contact area while $F$ remains at $4 \gamma^{3/4}$ till pinch-off at $J'$. The same DMT-JKR transition is predicted for $\psi = 10$ along path OPP'. Useful expressions for $F(c)$ and $w_0(c)$ are shown in Figure 2.7 and Figure 2.8 respectively. In Figure 2.7, delamination proceeds from bottom right ($c = 1$ and $F = 0$) to the left ($c = 0$). For $\psi > \psi^*$, external load keeps constant at $F_{\text{max}}$ with decreasing contact area. The curves terminate at $c = 0$. In Figure 2.8, the DMT-limit is sufficient for $w_0 \leq y$. For $w_0 > y$, DMT-JKR transition occurs and the curve becomes linear till pinch-off at $c = 0$. The dashed line annotated “DMT-JKR” is the locus of DMT-JKR transition and is found to be $w_0 = (1 - c)/2$. Figure 2.9 shows the varying cohesive edge as a function of half contact length. For $\psi \leq \psi^*$, DMT-limit is valid and the cohesive zone extends to the membrane edge ($b = 1$). For $\psi > \psi^*$, the trajectory deviates from the DMT-limit at $F_{\text{max}}$ and $b$ decreases till pinch-off.
Figure 2.8 Punch displacement as a function of half contact length for a range of disjoining pressure.

The above calculation leads to a slightly larger maximum force $F_{\text{max}} = 4 \gamma^{3/4}$ compared to the classical JKR-limit of $F_{\text{max}} = 3.884 \gamma^{3/4}$ in Wan’s work [105] (c.f. Figure 2.4). The 3% inconsistency lies in the average membrane stress approximation within and without cohesive zone (c.f. Equations (2.14) and (2.17)) in computing the membrane profile and ultimately the energy balance. A proper method is to allow membrane stress to vary as a function of distance from the contact edge. However, discontinuity and non-differentiability will become inevitable at the cohesive edge, let alone an analytical solution. An exact numerical solution is beyond the scope of this paper. Nevertheless, the small discrepancy does not change the trend of DMT-JKR
transition when disjoining pressure approaches JKR-limit. The JKR-limit is therefore stated to be \( F = 4 \gamma^{3/4} \) instead of \( 3.884 \gamma^{3/4} \) in Figure 2.4.

![Figure 2.9 Cohesive edge as a function of half contact length for a range of disjoining pressure.](image)

It is worthwhile to contrast the 1-D model with a 2-D axisymmetric membrane. Wan earlier derived a model for a circular membrane clamped at the periphery with a radius \( a_c \) and adhered to a circular punch of the same radius, in reminiscent of the current rectangular geometry [68]. To make a meaningful comparison, we choose to equate the normalized applied load. In 1-D, the membrane is here taken to be a square with the same width and length, and the
normalized applied load is redefined to be \( F = \frac{F}{\sqrt{\frac{2}{1} \pi \frac{1}{\text{hE}} a^2}} = \frac{6 \left(1 - \nu\right) a_c^2}{\pi E h^4} \),

implying comparable characteristic length scale, \( a_c = (2\pi)^{1/2} a \). Considering a membrane-substrate interface with a specific interfacial disjoining pressure \( p \), the normalized quantities are given by \( p_{1D} = p \frac{12 \left(1 - \nu\right) a^2}{E h^4} \) and \( p_{2D} = p \frac{6 \left(1 - \nu\right) a_c^4}{E h^4} = 2\pi^2 p_{1D} \approx 20 p_{1D} \). As an illustration, Figure 2.10 compares the 1-D and 2-D mechanical responses. In the DMT-limit \( (p_{1D} = 0.05 \gamma^{3/4} \text{ and } p_{2D} = 1 \gamma^{3/4}) \), delamination in both 1-D (path OA) and 2-D (path OB) is accompanied by a monotonic increasing applied load till “pinch-off”. The DMT-JKR transition \( (p_{1D} = 5 \gamma^{3/4} \text{ and } p_{2D} = 100 \gamma^{3/4}) \) shows contrasting 1-D (path OPP') and 2-D (path OQQ') behavior. The circular membrane reaches a maximum prior to the transition and decreases monotonically till “pull-off” occurs at a non-zero radius. It is obvious that a gradual 1-D “pinch-off” causes less damage than an unstable 2-D pull-off. An ideal elliptical membrane delamination will follow an intermediate path bounded by the 1-D and 2-D limits.

The new model has significant impacts on the design of a number of cell-tissue adhesion, micro-devices, and micro-/nano-structures. For instance, it is showed that the stability of a micro-truss structure depends on combination of the bridge span, separation, and materials properties of the trusses, as well as the adhesion energy [107]. The finite magnitude and range of intersurface forces add a new dimension to the stability consideration and require new design guidelines.
Figure 2.10 Comparison of mechanical response, \( F(w_0) \), between 1-D model (solid) and the 2-D axisymmetric membrane.
2.2.2 Rectangular film under pure bending

A rectangular film under pure bending is also discussed. The model is the same as Figure 2.2. The governing equations (2.2) and (2.3) can be simplified into the following dimensionless forms with membrane stretching term neglected.

\[
\begin{align*}
\frac{d^4 w}{dx^4} &= p \quad \text{for } c < x \leq b \\
\frac{d^4 w}{dx^4} &= 0 \quad \text{for } b < x \leq 1
\end{align*}
\]  

(2.28)

These equations can be exactly solved and the deformed profile of the film can be obtained:

\[
w = \begin{cases} 
\frac{p}{24c} (4c(c-b)x^3 - 2(2c^3 - 3b^2c + b^3)x^2 + c(c^4 - 2b^3c + b^4)) & \text{for } c < x \leq b \\
\frac{p}{24c} (c-x)^2(c^3 - 2b^3 + 2c^2x - cx^2) & \text{for } b < x \leq 1
\end{cases}
\]  

(2.29)

Total energy of the film-substrate system is given by $U_T = U_E - U_S$, with $U_E$ the elastic energy due to film bending and $U_S$ the surface energy to create new surfaces. For delamination to occur, 

\[
(\partial U_T / \partial c)_{w_0=\text{constant}} = 0.
\]

\[
U_E = \begin{cases} 
2 \int_c^b \frac{1}{2} \left( \frac{d^2 w}{dx^2} \right)^2 dx \quad & \text{for } c < x \leq b \\
2 \int_b^1 \frac{1}{2} \left( \frac{d^2 w}{dx^2} \right)^2 dx \quad & \text{for } b < x \leq 1
\end{cases}
\]  

(2.30)

Substituting $w$ in equations (2.29) into (2.30), the elastic energy is therefore obtained. The surface energy per unit area decreases in the cohesive zone, and reaches zero at the cohesive edge. The equation for surface energy is the same as equation (2.18).

The JKR limit, DMT limit and DMT-JKR transition are discussed as well and the applied force as a function of punch displacement is shown in Figure 2.11. Mathematica programs for
the calculations are given in Appendix 2. It clearly shows that the mechanical property of a thin film under pure bending has significant difference from the membrane under pure stretching. When the parameter $\psi$ is smaller than $4.89898$, DMT limit is valid and the applied force increases as the punch moves far away until the contact is fully lost. Regardless of the surface force range, the initial loading ($w_0 = 0$) always begins with the DMT-limit. The condition $w_0 \leq y$ implies that the maximum central deflection falls short of the surface force range and the whole film is in cohesive zone. The special case of $w_0 = y$ is denoted by the maximum central deflection for DMT-limit to remain valid and this corresponds to the peak points of the force versus displacement curves in Figure 2.11.

For the mediate value of $\psi$, the disjoining pressure has finite range and magnitude and DMT-JKR transition is expected. For $w_0 \leq y$, the whole film is under the intersurface force range and the DMT-limit is valid. The applied force reaches the maximum at $w_0 = y$ shown as the peak points of the curves in Figure 2.11 and dramatically decreases after the displacement of the punch goes beyond the range of the intersurface force until the contact is totally lost.

When $\psi$ is greater than 200, JKR limit is approaching shown as the dash curve in Figure 2.11. The constant force for pure stretching membrane cannot be seen here. The applied external load decreases as the displacement of the punch increases to make the delamination propagate. Another difference with the pure stretching membrane is that the maximum normalized punch displacement here is about 0.3 which is much smaller than the pure stretching result of 0.6 from Figure 2.4. This phenomenon is reasonable as the membrane under pure stretching behaves more flexible and has the ability to undergo large deformation.
Figure 2.11 Mechanical response of a clamped rectangular membrane under pure bending.

2.2.3 Circular film under pure stretching

Figure 2.1(a) shows the schematic of a circular membrane with radius, $a$, clamped at the periphery. Figure 2.1(b) gives the model drawn in normalized coordinates. Measuring simultaneously the applied load, $F$, punch displacement, $w_0$, the contact radius, $c$, and the membrane profile allows one to deduce the magnitude and range of the disjoining pressure. Recently, Wan deduced the adhesion-delamination mechanics of this model and also discussed the DMT-JKR transition [68]. While that work was derived based on an assumption, albeit
arbitrary, adhesion energy, $\gamma = 1$. Though valid, the new parameter $\psi$ takes into account of the variation in $\gamma$. The calculations are similar to Wan’s work and not shown here.

Figure 2.12 shows the mechanical behavior of an initially stress-free membrane. Throughout the loading process, the contact circle continues to shrink (not shown). For $\psi < 1.86121$, the cohesive zone spans the entire freestanding membrane with $b = a$. Delamination proceeds in a stable manner under either fixed load ($F = \text{constant}$) or fixed grips ($w_0 = \text{constant}$), and the membrane ultimately pinches off from the substrate with $c = 0$ at the maximum external load on the dashed curve OD, resembling the DMT-limit. For $1.86121 < \psi < 10$, the cohesive zone becomes a shrinking annulus as delamination proceeds ($c < b < a$). After reaching a maximum load, $F_{\text{max}}$, the applied load decreases to maintain equilibrium until the final pinch-off on BC. For $\psi \geq 10$, the contact radius is non-zero ($c \neq 0$) at the final pull-off, resembling the JKR-limit. The full JKR solution becomes apparent in the limit of $\psi \rightarrow \infty$. The dashed curve OADCF traces the loci of pinch-off and pull-off.
Figure 2.12 Mechanical response of a clamped circular membrane under pure stretching.

Figure 2.13 Mechanical response of a clamped circular membrane under pure bending.
2.2.4 Circular film under pure bending

As a comparison with the pure stretching membrane, the clamped circular film under pure bending is discussed. The model is the same as Figure 2.1. The governing equation is

\[
\begin{align*}
\nabla^4 w &= p & \text{for } c < r \leq b \\
\nabla^4 w &= 0 & \text{for } b < r \leq 1
\end{align*}
\] (2.31)

Using the normalized variables in Table 2.1, above equation can be simplified as,

\[
\begin{align*}
\left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr}\right)\left(\frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr}\right) &= 2p & \text{for } c < r \leq b \\
\left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr}\right)\left(\frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr}\right) &= 0 & \text{for } b < r \leq 1
\end{align*}
\] (2.32)

The energy density of a deformed circular plate is given by \( \int \frac{1}{2} \left(\frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr}\right)^2 r dr \), which is different from the expression for a rectangular plate. Elastic energy \( U_E = \text{energy density} \times \text{area} \). Then we have:

\[
U_E = \begin{cases}
2 \int_c^b \frac{1}{2} \left(\frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr}\right)^2 r dr & \text{for } c < r \leq b \\
2 \int_b^1 \frac{1}{2} \left(\frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr}\right)^2 r dr & \text{for } b < r \leq 1
\end{cases}
\] (2.33)

The surface energy per unit area decreases in the cohesive zone, and reaches zero at the cohesive edge. Therefore,

\[
U_S = \gamma c^2 + \int_c^b p \cdot (y - (w_0 - w)) 2r dr
\] (2.34)

Total energy of the film-substrate system is given by \( U_T = U_E - U_S \) and delamination occurs when \( \frac{\partial U_T}{\partial c} \bigg|_{w_0 = \text{constant}} = 0 \). The mechanical response can be obtained by solving above
equations and Mathematica programs are given in Appendix 3. Figure 2.13 shows the delamination process for a stiff membrane under pure bending. Transition from DMT to JKR occurs at $\psi = 4\sqrt{2} \approx 5.657$, where the force curve terminates at B. For $\psi < 5.657$, the DMT-limit prevails and the delamination terminates at pinch-off point on the dashed curve. A larger $\psi$ raises $F_{\text{max}}$ which indicates the onset of cohesive zone shrinkage. In the limit of $\psi \to \infty$, pull-off dominates in the JKR-limit.

2.3 Pressurized blister model

2.3.1 Rectangular pressurized blister under pure stretching

Figure 2.14(a) shows a blister delamination of half width, $c$, and height, $w_0$, driven by a uniform pressure, $f$, via a bore of half width, $a$, in the substrate. The cohesive zone is shown as $b < x < c$. The half width of the hole is $a$, all the horizontal variables are normalized by $a$. The external pressure applied through the hole is balanced by the disjoining pressure, resulting a deformed membrane profile governed by the dimensionless equations

$$
\begin{cases}
-s^2 \frac{d^2 w}{dx^2} = f - p & \text{for } b < x \leq c \\
-s^2 \frac{d^2 w}{dx^2} = f & \text{for } 0 < x \leq b
\end{cases}
$$

Equation (2.35) is solved exactly to yield,

$$
w = \begin{cases}
\frac{1}{2s^2} (c-x)((c+x)(f-p)+2bp) & \text{for } b < x \leq c \\
\frac{1}{2s^2} ((c^2-x^2)f-(c-b)^2p) & \text{for } 0 < x \leq b
\end{cases}
$$

The average membrane stress is given by
The elastic energy is therefore given by

\[
U_E = \begin{cases} 
\frac{12}{c-b} \int_b^c \frac{1}{2} \left( \frac{dw}{dx} \right)^2 \, dx & \text{for } b < x \leq c \\
\frac{12}{b} \int_0^b \frac{1}{2} \left( \frac{dw}{dx} \right)^2 \, dx & \text{for } 0 < x \leq b
\end{cases}
\]  \tag{2.37}

The surface energy per unit area is similar to equation (2.18) for the rectangular punch model under pure stretching,

\[
U_S = -2c\gamma + 2 \int_b^c p \left( y - w \right) \, dx
\]  \tag{2.39}

Total energy of the film-substrate system is given by \( U_T = U_E - U_S \) and delamination occurs when \( \frac{\partial U_T}{\partial c} \bigg|_{w_0=\text{constant}} = 0 \). Mathematical programs for the solution are given in Appendix 4.

For a range of disjoining pressure, Figure 2.15 shows the mechanical responses of a pressurized rectangular membrane under pure stretching. All curves are independent of \( \gamma \). Initial pressurization leads to a small rise in \( w_0 \) without delamination until the blister grows beyond the venting hole and the applied pressure is a simple cubic function of central displacement. Further increase in \( f \) expands \( c \). For \( w_0 < y \), the entire freestanding membrane remains under the influence of the disjoining pressure that counterbalances the applied pressure. The relation \( f(w_0) \) is a monotonic increasing function and the delamination process is stable. A maximum pressure, \( f_{\text{max}} \), is reached when the blister height finally catches up with the surface force range, \( w_0 = y \). Further increase in \( f \) until \( w_0 > y \) renders the cohesive zone residing to an annulus around the contact edge \( (b < c) \) such that the cohesive zone width \( (b - c) \) continues to diminish. Hereafter \( f(w_0) \)
becomes monotonic decreasing, in that, pressure increase leads to an ebbing blister height despite an expanding delamination radius. At \( f_{\text{max}} \), the delamination grows spontaneously and catastrophically till it reaches the physical edge of the sample substrate. One possible way to stabilize the blister is to allow a fixed mass of working gas in the blister void while the delamination is driven by reducing the external pressure. The internal pressure drops while the working gas expands.

The long range disjoining pressure manifests itself as follows. For small \( \psi \), the blister height is relatively small because the entire blister lies within the cohesive zone \( (b = c) \), and \( p_{\text{max}} \) is also small. A large \( \psi \) approaches the JKR-limit shown as the dash curve in Figure 2.15. Here \( \psi \) is not well defined since the half width of bore, \( a \), is the only fixed dimension other than the membrane thickness. The \( a \)-dependency of \( \psi \) becomes negligible as the blister expands outwards beyond the hole \( (c >> a) \). Nonetheless, increase of \( \psi \) from 10 to 100 in Figure 2.15 demonstrates the fact that a large \( \psi \) approaches the JKR-limit.
Figure 2.14 (a) Schematic of a standard pressurized test. (b) Model drawn in normalized coordinates.
Figure 2.15 Mechanical response of a pressurized rectangular blister under pure stretching.

Figure 2.16 Mechanical response of a pressurized rectangular blister under pure bending.
2.3.2 Rectangular pressurized blister under pure bending

A rectangular film under pure bending is pressurized to deform to the profile shown in Figure 2.14(a). The dimensionless governing equations are

\[
\begin{aligned}
\frac{d^4 w}{dx^4} &= f - p & \text{for } b < x \leq c \\
\frac{d^4 w}{dx^4} &= f & \text{for } 0 < x \leq b
\end{aligned}
\]  

(2.40)

The elastic energy of the film can be obtained by putting the solved deformed profile from equation (2.40) into the following,

\[
U_E = \begin{cases}
2 \int_b^c \frac{C}{b} \left( \frac{d^2 w}{dx^2} \right)^2 \, dx & \text{for } b < x \leq c \\
2 \int_0^b \frac{1}{2} \left( \frac{d^2 w}{dx^2} \right)^2 \, dx & \text{for } 0 < x \leq b
\end{cases}
\]  

(2.41)

Equation (2.39) can also be used to calculate the surface energy and total energy of the film-substrate system is given by \(U_T = U_E - U_S\). For delamination to occur, \(\frac{\partial U_T}{\partial c}|_{c=0} = \text{constant} = 0\). The calculations are implemented by Mathematica programs given in Appendix 5.

Figure 2.16 shows the applied pressure as a function of central displacement for a pressurized thin film under pure bending. The thin film has very small deformation in the beginning and no delamination occurs. The applied pressure is proportional to the central displacement. The cohesive zone is the same as the half width of the hole. After the peak point, the cohesive zone propagates and the applied pressure decreases with the increasing central displacement. It is similar to the previous pure stretching case, JKR limit will be reached when \(\nu\) goes to a larger value.
2.3.3 Circular pressurized blister under pure stretching

Figure 2.17(a) shows a circular blister delamination of radius, $c$, and height, $w_0$, driven by a uniform pressure, $f$, via a bore of radius, $a$, in the substrate. The cohesive zone is shown as $b < r < c$. All the horizontal variables are normalized by hole radius $a$. The external pressure applied through the hole is balanced by the disjoining pressure, resulting in a deformed membrane profile governed by the dimensionless equations

$$
\begin{align*}
-s^2 \left( \frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right) &= 2(f - p) \quad \text{for } b < r < c \\
-s^2 \left( \frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right) &= 2f \quad \text{for } 0 < r \leq b
\end{align*}
$$

Equation (2.42) is solved exactly to yield,

$$
w = \begin{cases} 
\frac{p}{2s^2} b^2 \left( \log \left( \frac{c^2}{r^2} \right) - 1 + \frac{r^2}{c^2} \right) & \text{for } b < r \leq c \\
\frac{p}{2s^2} \left( b^2 \log \left( \frac{c^2}{b^2} \right) - \left(1 - \frac{b^2}{c^2}\right) r^2 \right) & \text{for } 0 < r \leq b
\end{cases}
$$

The average membrane stress is given by

$$
s^2 = \begin{cases} 
\frac{6}{c^2 - b^2} \int_b^c \left( \frac{\partial w}{\partial r} \right)^2 2rdr & \text{for } b < r \leq c \\
\frac{6}{b^2} \int_0^b \left( \frac{\partial w}{\partial r} \right)^2 2rdr & \text{for } 0 < r \leq b
\end{cases}
$$

The elastic energy is therefore given by

$$
U_E = \frac{s^4}{24} (c^2 - b^2) + \frac{s^4}{24} b^2 \quad \text{for } b < r \leq c \quad \text{for } 0 < r \leq b
$$

The surface energy per unit area is given
Total energy of the film-substrate system is given by \( U_T = U_E - U_S \). For delamination to occur, \((\partial U_T / \partial c)_{w_0=\text{constant}} = 0\). The mechanical response can be obtained by solving above equations and the Mathematical programs are given in Appendix 6. Figure 2.18 shows the applied pressure as a function of central displacement of the membrane. In the beginning period shown as the curve AB, the membrane bulges up with very small deformation and no delamination happens. The applied pressure is a simple cubic function of central displacement. Further increase of the pressure will cause the delamination to propagate while the cohesive zone range keeps the same as the radius of the hole before reaching the peak points in the curves of pressure as a function of the central displacement. The relation \( f(w_0) \) is a monotonic increasing function and the delamination process is stable, which is quite unexpected according to the classical unstable pressurized blister [51]. After that, the cohesive zone will be larger than the radius of the hole and increase with central displacement after the maximum points. In order to keep the balance and make steady delamination, the applied pressure should be decreased while the central displacement of the film is still increased. In real experiments, this can only be achieved by volume control method, not force control. Similar experiment has been done by Shirani and Liechti [108] to study the adhesion between polymer films with aluminum substrates. The dash curve in Figure 2.18 shows the JKR-limit. When \( \psi \) increases to larger value, it approaches the JKR limit.
Figure 2.17 (a) Schematic of a standard pressurized test. (b) Model drawn in normalized coordinates.
Figure 2.18 Mechanical response of a standard pressurized blister under pure stretching.

Figure 2.19 Mechanical response of a standard pressurized blister under pure bending.
2.3.4 Circular pressurized blister under pure bending

The profile of a deformed circular film under pure bending is governed by

\[
\begin{align*}
\left\{ \begin{array}{l}
\left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) \left( \frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right) = 2(f - p) & \text{for } b < r \leq c \\
\left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) \left( \frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right) = 2f & \text{for } 0 < r \leq b \\
\end{array} \right.
\end{align*}
\] (2.47)

The above equation can be solved and the central displacement of the film is given by

\[
w_0 = w(r = 0) = \frac{P}{32} b^2 (3c^2 - 3b^2 - 2b^2 \log\left(\frac{c^2}{b^2}\right))
\] (2.48)

and the surface force range

\[
y = w(r = b) = \frac{3P}{32} b^2 (c^2 - \frac{b^4}{c^2} - 2b^2 \log\left(\frac{c^2}{b^2}\right))
\] (2.49)

The energy density of a deformed plate is given by \( \int \frac{1}{2} \left( \frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right)^2 r \, dr \) and \( U_E = \text{energy density} \times \text{area} \). Then we have:

\[
U_E = \left\{ \begin{array}{l}
2 \int_b^c \frac{1}{b} \left( \frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right)^2 r \, dr & \text{for } 0 < r \leq b \\
2 \int_b^c \frac{1}{b} \left( \frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right)^2 r \, dr & \text{for } b < r \leq c \\
\end{array} \right.
\] (2.50)

Substituting \( w \) in equation (2.47) into (2.50), the elastic energy is therefore found. The surface energy per unit area decreases in the cohesive zone, and reaches zero at the cohesive edge. Therefore,

\[
U_S = -b^2 y + \int_b^c P \cdot (y - w) 2r \, dr
\] (2.51)
Surface energy is found by substituting equations (2.47) and (2.49) into (2.51),

\[ U_s = -b^2 \gamma + 2 \left( b^2 + \frac{2b^6 - 6b^4 c^2 + 3b^2 c^4 + c^6}{3c^2 (3b^2 - 3c^2 + 2b^2 \log(c^2/b^2))} \right) r_p w_0 \]  \hspace{1cm} (2.52)

Total energy of the film-substrate system is given by \( U_T = U_E - U_S \) and \((\partial U_T / \partial c)_{w_0=\text{constant}} = 0\) when delamination occurs. Mathematica programs for the calculations are given in Appendix 7. Figure 2.19 shows the applied pressure as a function of central displacement of the film under pure bending. No delamination occurs in the initial part when the membrane bulges up with very small deformation. The whole membrane stays in the intersurface force range. The relation \( f(w_0) \) is a simple linear function. Further increase of the pressure will cause the delamination to propagate while the cohesive zone radius \( b \) keeps the same as the radius of the hole \( a \) before reaching the peak points. After that, the cohesive zone radius goes beyond the radius of the hole as delamination keeps propagation. In order to keep balance and make steady delamination, the applied pressure should be decreased while the central displacement of the film is still increased. The dash curve in Figure 2.19 shows the JKR-limit. When \( \psi \) increases to larger values, it approaches the JKR limit.

2.4 Constrained blister model

2.4.1 Circular constrained blister under pure stretching

In the classical constrained blister test (Figure 2.20(a)), the top plate limits the blister height, \( w_0 \), to a fixed constant. Increase in \( f \) presses the membrane against the top plate into an adhesion contact. Reduction in \( f \) therefore delaminates the membrane and shrinks the contact.
circle. The theoretical adhesion-delamination mechanics in the JKR and DMT limits and the associated JKR-DMT transition have been extensively investigated by Dillard et al. for both linear and nonlinear elastic plate and membrane under bending or stretching [109]. Experimental investigations and associated theoretical models are recently reported in literature. Xu and Liechti built a Moiré interferometer to map the profile of polyethylene terephthalate (PET) films deformed in a constrained blister configuration, with and without the adhesion at the contact interface [56, 110, 111]. Flory et al. used the constrained blister test to measure interactions between a soft polymer membrane on a rigid substrate and constructed a theoretical model based on the JKR limit and large deformation instead of small strain in linear elasticity [112]. Hui et al. constructed a detailed model based on JKR limit and large deformation [113]. Here we will study the JKR limit, DMT limit and DMT-JKR transition for the constrained blister model shown in Figure 2.20. The dimensionless governing equations are

\[
\begin{align*}
-s^2 \left( \frac{d^2 w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right) &= 2(f + p) \quad \text{for } c < r \leq b \\
-s^2 \left( \frac{d^2 w}{dr^2} + \frac{1}{r} \frac{dw}{dr} \right) &= 2f \quad \text{for } b < r \leq 1
\end{align*}
\]

(2.53)

The profile of the deformed membrane can be obtained,

\[
w = \begin{cases} 
\frac{1}{2s^2} (f(1-r^2 + c^2 \log(r^2)) - p(b^2 - c^2)\log(r^2)) & \text{for } b < r \leq 1 \\
\frac{1}{2s^2} (f(1-r^2) + p(b^2 - r^2 - b^2 \log(b^2)) + c^2 (f + p)\log(r^2)) & \text{for } c < r \leq b
\end{cases}
\]

(2.54)
The average membrane stress is given by

\[
    s^2 = \begin{cases} 
        \frac{6}{b^2 - c^2} \int_c^b \frac{1}{2} \left( \frac{\partial w}{\partial r} \right)^2 2rdr & \text{for } c < r \leq b \\
        \frac{6}{1-b^2} \int_b^1 \frac{1}{2} \left( \frac{\partial w}{\partial r} \right)^2 2rdr & \text{for } b < r \leq 1
    \end{cases}
\]  

(2.55)

Substituting \( w \) from equation (2.54) to (2.55), the average membrane stress is found,
The intersurface force range $y$ and the height of the blister $w_0$ can be obtained from equation (2.54) and (2.56) and the delamination behavior can be solved by a force balancing method which has been used by Plaut et al [55, 114]. Appendix 8 gives the Mathematica programs for the calculations. Figure 2.21 shows the contact radius as a function of applied pressure for a constrained circular membrane under pure stretching. Both the normalized adhesion energy $\gamma$ and blister height $w_0$ equal 0.8. Raising $f$ from null leads to blister bulging but does not immediately incur adhesion contact because of the weak disjoining pressure. Interfacial contact occurs once $f$ exceeds critical thresholds, $f_{\text{min}}$, which are shown as the intersection points of curves with horizontal axis. For $\psi \leq 3$, the adhesion contact starts with one point contact ($c = 0$) and so is delamination upon unloading, in reminiscent of the DMT-limit. Increase in $\psi$ in this range reduces $f_{\text{min}} / \gamma^{3/4}$ until it reaches 1.23. For $\psi > 3$, the function $c(f)$ shows an infinite slope at $f_{\text{min}}$ with $(dc / df) \to \infty$ and $c(f_{\text{min}}) > 0$, indicating a pull-in where the membrane jumps into adhesion contact at $f_{\text{min}}$. Upon unloading, pull-off is expected at $f_{\text{min}}$ where the membrane spontaneously snaps from the plate, resembling the JKR-limit with $\psi \to \infty$. The JKR-DMT transition is apparent.

\[
\begin{align*}
  s &= \begin{cases} 
    \frac{3}{2} f ((1 + b^2 - 4c^2) f + 4(b^2 - c^2) p) - \frac{6(b^2 p - c^2 (f + p))^2 \log(b)}{1 - b^2}^{1/6} & \text{for } b < r \leq 1 \\
    \frac{3}{2} \frac{(f + p)^2}{(b^2 - c^2)} (b^4 - 4b^2 c^2 + 3c^4 + 2c^4 \log(\frac{b^2}{c^2}))^{1/6} & \text{for } c < r \leq b
  \end{cases}
\end{align*}
\]
Figure 2.21 Mechanical response of a constrained circular blister under pure stretching.

Figure 2.22 Mechanical response of a constrained circular blister under pure bending.
2.4.2 Circular constrained blister under pure bending

The schematic model for a constrained blister under pure bending is the same as Figure 2.20. The governing equations are

\[
\begin{align*}
\left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr}\right)\left(\frac{d^2 w}{dr^2} + \frac{1}{r} \frac{dw}{dr}\right) &= 2(f - p) \quad \text{for } c < r \leq b \\
\left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr}\right)\left(\frac{d^2 w}{dr^2} + \frac{1}{r} \frac{dw}{dr}\right) &= 2f \quad \text{for } b < r \leq 1
\end{align*}
\]

(2.57)

The deformed profile of the blister can be solved from above equation and the mechanical response can also be obtained using same force balancing method. Mathematica programs for the calculations are shown in Appendix 9. It should be mentioned that the normalized adhesion energy \(\gamma\) and blister height \(w_0\) take value 0.22 and 0.055 respectively which is not the same as above pure stretching model. The reason is that the film under pure bending is hard to get a large deformation as pure stretching membrane. The previous rectangular punch model under pure bending has been found to have a smaller pinch-off displacement than the model under pure stretching. Figure 2.22 shows the contact radius as a function of applied pressure. For \(\psi \leq 2\), delamination process resembles the DMT-limit with a point contact \((c = 0)\) at the beginning of loading and end of unloading. For \(2 < \psi \leq 2000\), decrease in \(f\) leads to delamination until pressure equilibrates on both sides of the membrane with \(f = 0\), then the contact circle is arrested with a non-zero radius \((c > 0)\). For \(\psi > 2000\), the JKR like pull-off is expected.
2.4.3 Rectangular constrained blister under pure stretching

The rectangular constrained blister is discussed as well. Figure 2.23(a) shows the schematic of a constrained blister test. The thin film is rectangular shape and only deformation from membrane stretching is considered here. The dimensionless governing equations are

\[
\begin{cases}
-s^2 \frac{d^2 w}{dx^2} = f + p & \text{for } c < x \leq b \\
-s^2 \frac{d^2 w}{dx^2} = f & \text{for } b < x \leq 1
\end{cases}
\]  

(2.58)

The membrane profile is then found as follows,

\[
w = \begin{cases}
\frac{1}{2s^2} ((1-x)(f(1+x-2c)+2p(b-c))) & \text{for } b < x \leq 1 \\
\frac{1}{2s^2}((1-x)(f(1+x)-2cf-2cp) + p(2b-b^2-x^2)) & \text{for } c < x \leq b
\end{cases}
\]  

(2.59)

The intersurface force range \( y \) and the height of the blister \( w_0 \) can be obtained from equation (2.59) and the delamination behavior will be solved by the force balancing method (Appendix 10). Figure 2.24 shows the half contact width as a function of applied pressure for a rectangular constrained blister under pure stretching. In order to make comparison, the normalized adhesion energy \( \gamma \) and blister height \( w_0 \) take the same value 0.8 as the circular model. For \( \psi < 4 \), initial small external pressure leads the membrane to bulge up without delamination and the model is simplified to a standard pressurized blister. Interfacial contact occurs once \( f \) exceeds a critical thresholds, \( f_{\text{min}} \), which are shown as the intersection points of curves with horizontal axis in Figure 2.24. The membrane first touches with the substrate in a line shape not a point contact for the circular model. Delamination happens during the unloading period, in reminiscent of the DMT-limit. Increase in \( \psi \) in this range reduces \( f_{\text{min}} / \gamma^{3/4} \) until it reaches 0 when \( \psi = 4 \) which provides the critical disjoining pressure that is strong enough to pull up the
membrane and make a line contact with substrate even no external pressure is applied for this configuration of $\gamma$ and $w_0$. For $\psi > 4$, the membrane makes none zero contact with the substrate even no external pressure is applied. This is different from the circular model where pull-off is expected before the pressure is reduced to zero. The result shows that the 1-D model has less damage to the contact than 2-D model which has an unstable pull-off and this is consistent with the previous comparison between 1-D punch model and 2-D punch model. If the adhesion energy here is weaker or the blister height is larger enough, the membrane may lose the contact before the pressure reduces to zero which is similar to the result shown in Figure 2.21. The dash line is the JKR-limit with $\psi \to \infty$ and JKR-DMT transition is apparent.

Figure 2.23 Schematic of a constrained blister test. (b) Model drawn in normalized coordinates.
Figure 2.24 Mechanical response of a constrained rectangular blister under pure stretching.

Figure 2.25 Mechanical response of a constrained rectangular blister under pure bending.
2.4.4 Rectangular constrained blister under pure bending

The dimensionless governing equations for a rectangular constrained blister under pure bending are

\[
\begin{align*}
\frac{d^4w}{dx^4} &= f + p \quad \text{for } c < x \leq b \\
\frac{d^4w}{dx^4} &= f \quad \text{for } b < x \leq 1
\end{align*}
\] (2.60)

The deformed profile of the membrane can be solved from equation (2.60) and the mechanical response of the blister is obtained using the force balancing method. Mathematica programs for the calculations are shown in Appendix 11. The normalized adhesion energy $\gamma$ and blister height $w_0$ take value 0.22 and 0.055 respectively which are the same as previous constrained circular blister under pure bending. Figure 2.25 shows the half contact width as a function of the applied pressure. The result is very similar to the pure stretching model shown in Figure 2.24. Initial small external pressure bulges up the film without contact with the substrate until reaching the threshold $f_{min}$ shown as the intersection points of the curves with the horizontal axis. For $\psi < 4$, the thin film will snap from the substrate upon unloading before the applied pressure is reduced to zero. While for $\psi > 4$, the film still contacts with the substrate even no pressure is applied. The dash curve shows the JKR limit and DMT-JKR transition is apparent.

2.4.5 Discussion

It should be mentioned that thin film in our above constrained blister model is clamped at the periphery and contacts with the top rigid substrate. It is possible that the constraint of the film can be released and delamination occurs at the interface with bottom substrate as well. When the applied external pressure is large enough, the thin film bulges up and contacts with the substrate
while delamination happens at the bottom. J. G. Williams [48] investigated the energy release rate of this model and concluded that the energy release rate at the bottom was much higher than that at the top. While, back to our model with long range intersurface force, more variables will come in and the calculation will be very complex if delamination is allowed at the bottom. Recently, Hui et al. [113] discussed the similar constrained blister model under large deformation and figured out the relations among pull-off pressure, pull-off radius and the work of adhesion. This reminds us to review our above models again by playing with these parameters. Actually, the punch test model, pressurized blister and constrained blister can be correlated by changing these parameters. In Figure 2.20, the initial small pressure bulges up the membrane without contact and the constrained blister is simplified to pressurized blister. After the contact, the change of the pressure brings the mechanical response for the constrained blister shown in Figure 2.21. However, if the pressure keeps constant after the membrane contacts with the substrate, the increase of the blister height can shrink the contact area and pull-off occurs at some critical height. This looks like the punch test model shown in Figure 2.1. The relations among the pressure, the adhesion energy and the height of the blister need to be found and it is worthy to compare our results with Hui’s conclusion.

The constrained blister model used here is same as Figure 2.20 and only membrane stretching is considered. The governing equation is still equation (2.53) and the membrane profile is given in equation (2.54). The average membrane stress is thus obtained using equation (2.55). In order to simplify the calculation, only JKR limit is discussed and cohesive zone radius $b$ equals zero. In section 2.4.1, a force balancing method is used to get the relation between the contact radius and the applied pressure shown in Figure 2.21. Here, the energy balance method is used which has been used before for the punch test model and pressurized blister model. The
energy density of \( s^4/24 \) leads to elastic energy \( U_E = \text{energy density} \times \text{area} \). Surface energy here \( U_S = \gamma c^2 \). Total energy of the film-substrate system is given by \( U_T = U_E - U_S \) and delamination occurs when \( \left( \frac{\partial U_T}{\partial c} \right)_{w_0=\text{constant}} = 0 \). The mechanical response can then be found by solving this equation. The effects of blister height \( w_0 \) and adhesion energy \( \gamma \) to the pull-off properties of the blister will be discussed.

For the fixed adhesion energy between membrane and the substrate, the change of the external pressure will cause the membrane to bulge up to contact with substrate or to snap from the substrate at pull-off upon unloading. Here, the external pressure is defined to be positive when the membrane is bulged up to contact with substrate. The negative pressure drives the membrane to delaminate from the substrate. Figure 2.21 shows the contact radius as a function of applied pressure for a constrained blister with given blister height. However, these mechanical properties especially the pull-off points will change for different blister height. The contact radius should be smaller for a larger blister height with same external pressure. In another words, for a given external pressure, the increase of the blister height will cause the contact radius to shrink and fully delaminate from the substrate at some critical separation. Figure 2.26 shows the contact radius as a function of blister height for different external pressure when the adhesion energy \( \gamma = 1 \). All curves begin with contact radius \( c = 1 \). Locus of “pull-off” is shown as ABCDEGHI. Here the pull-off contact radius decreases when the applied external pressure increases. Figure 2.27 shows the pull-off contact radius as a function of blister height for different adhesion energies. Figure 2.28 shows the pull-off contact radius as a function of external pressure for different adhesion energies. All curves converge to one point with contact radius of 0.1945 when the external pressure is zero. It is not difficult to understand this conclusion. When there is no external pressure applied to the membrane, the constrained blister
model is exactly a punch test model where the pull-off radius is 0.1945 according to the results in section 2.1.3. The figure also shows that stronger adhesion gives a larger contact radius for the same external pressure. Figure 2.29 plots the blister height or plate separation at pull-off as a function of external pressure. Larger external pressure allows the blister to have higher clearance to pull-off and stronger adhesion also gives a larger blister height at pull-off.

Figure 2.26 Contact radius as a function of plate separation. Adhesion energy $\gamma = 1$. Points A, B, C, D, E, G, H and I represent the pull-off points for different external pressure.
Figure 2.27 Pull-off contact radius as a function of plate separation for fixed adhesion energy. The corresponding pull-off pressure is shown in Figure 2.26.

Figure 2.28 Pull-off contact radius as a function of pull-off external pressure for fixed adhesion energy.
In the above discussion, adhesion energy is fixed and the blister height is variable which simplifies the constrained blister to a punch test model. Let us consider the situation when the blister height is fixed while the adhesion energy varies. Figure 2.30 shows the contact radius as a function of external pressure when the blister height \( w_0 = 1 \). If there is no adhesion between the membrane and substrate, point contact occurs once the external pressure exceeds the critical value shown as the intersection point of red curve with the horizontal axis. As the adhesion energy increases from zero to larger value, pull-in occurs at the critical external pressure. The red dash curve shows the pull-off points for different adhesion energies during unloading. It clearly shows that the existence of adhesion always gives none zero contact when the membrane snaps from the substrate and a smaller external pressure is needed at pull-off for stronger adhesion, but a larger pull-off radius is obtained. For the critical adhesion energy \( \gamma = 9.993 \), the required
external pressure is zero at pull-off. Larger than that adhesion energy, negative pressure is needed to drive the membrane snap from the substrate. Figure 2.31 shows the pull-off contact radius as a function of external pressure for different blister heights. All the curves intersect one point where the pull-off radius is 0.1945 when the applied pressure is zero shown as the dash line. This has been illustrated in the previous and consistent with the result of punch test model. The intersect points of the curves with the horizontal axis represent the point contact at the critical external pressure without adhesion. The higher blister, the larger pressure is required to bulge up the membrane to contact with the substrate. Figure 2.32 and Figure 2.33 show the pressure and contact radius at pull-off as function of adhesion energy respectively.

Figure 2.30 Contact radius as a function of external pressure. Blister height \( w_0 = 1 \).
Figure 2.31 Pull-off contact radius as a function of pull-off pressure for fixed plate separation

Figure 2.32 Pull-off pressure as a function of adhesion energy for fixed plate separation
Experiments can be implemented to verify the results shown in Figure 2.30 to Figure 2.33 for the fixed plate separation model. The thin film can be bulged up to contact the constrained top plate. During the unloading, the decrease of the applied pressure will shrink the contact radius and cause pull-off. The experiment data of applied pressure and contact radius for loading and unloading can be recorded. By fitting the experiment data with the theoretical curves shown in Figure 2.30, the interfacial adhesion energy of thin film can be obtained. This has been carried out by Xu to measure interfacial adhesion energy of a laminate of polyethylene terephthalate (PET) film with aluminum substrate [56]. The film was bulged up to contact with the top substrate. Contact radius was measured by a homemade moiré interferometry during the loading and unloading process. The interfacial adhesion energy of the film with substrate was deduced by fitting the data with the theoretical curve of contact radius with applied pressure.
In order to make comparison between our result and Hui’s work [113], our above result based on the normalized variables listed in Table 2.1 was recalculated according to Hui’s method using the following different dimensionless variables,

\[ w_0 = \frac{w_0}{a}, \quad p = \frac{p a}{E h}, \quad \gamma = \frac{\gamma}{E h} \]  

(2.61)

Figure 2.34 and Figure 2.35 show the pull-off pressure and contact area as function of normalized work of adhesion respectively. Our result (Figure 2.34(a) and Figure 2.35(a)) is different from Hui’s model (Figure 2.34(b) and Figure 2.35(b)). The reason is that our model has an assumption that the deformation is small and the average stress can be expressed in equation (2.55). For large deformation, this expression for average membrane stress is no longer valid. The deformation in Figure 2.34 and Figure 2.35 is very close to the radius of the membrane indicating a large deformation. In this condition, Hui’s neo-Hookean membrane model for large deformation is more reasonable.

Figure 2.34 Pull-off pressure as a function of work of adhesion. (a) our model; (b) Hui’s result [113]
Figure 2.35 Pull-off contact area as a function of work of adhesion. (a) our model; (b) Hui’s result [113]

2.5 New adhesion map for thin film

Previously, we deduced a new Tabor parameter to govern the adhesion transition from DMT-limit to JKR-limit for thin films. Based on this parameter, a new adhesion map for thin films has been constructed shown in Figure 2.36, similar to the adhesion map given by Johnson and Greenwood presenting the JKR-DMT transition of solids adhesion governed by the Tabor’s parameter. The vertical axis is the normalized displacement which is the ratio of the out of plane deformation $w_0$ to the membrane thickness $h$. The horizontal axis is the new Tabor parameter $\psi$. When the film deformation is smaller than its thickness, bending deformation is dominant shown as the bottom blue region in Figure 2.36. When the deformation is large compared to the film thickness, stretching is dominant shown as the top pink region. In the middle, it is the mixed bending and stretching region. The continuous change of the color indicates that there is no obvious boundary for pure bending and stretching. As a rough estimate, membrane is subjected
to mixed bending-stretching deformation when the maximum displacement lies between 1 to 5 times the membrane thickness. For application, it is widely accepted that when the deformation of thin film is ten times greater than the membrane thickness, pure bending effect can be neglected and only stretching is taken into account. The horizontal axis shows how this new Tabor parameter \( \psi \) governs the transition from DMT limit to JKR limit. The solid curve with inverse function shape represents the intersurface force range. Small Tabor parameter means the intersurface force is long range and whole film is still under the influence of adhesion even the contact is lost. When the film deformation is beyond the force range, some parts of the film become freestanding while others are still in force range and Maugis-Dugdale (M-D) model is approached. This is illustrated in the previous DMT-JKR transition of the rectangular punch model. When the Tabor parameter \( \psi \) is larger enough (greater than 100), the value of the solid curve goes close to zero and this means the force range is very small and JKR-limit is approached. DMT-limit is always valid for the initial loading when the membrane deformation is small and the displacement does not go beyond the force range and the whole film stays in the cohesive zone, which is different from the classical solid adhesion map (Figure 1.9). It also should be admitted that this new adhesion map for thin films cannot exactly quantify the application regimes of different adhesion models. Here, it only roughly points out the transition tendency from DMT-limit to JKR-limit according to the value of the new Tabor parameter.
Figure 2.36 A new adhesion map for thin film.
Chapter 3 Hysteresis of loading and unloading a rigid punch to a clamped membrane

In previous chapter, we discussed the adhesion-delamination mechanics of a clamped rectangular or circular membrane with a rigid punch [68, 115]. Initially it is full contact and then the contact region shrinks until pull-off occurs. This is like the unloading process when an AFM tip or indenter leaves the sample. Loading and unloading hysteresis can be found in a typical AFM indentation test because of adhesion [116, 117]. Here, we will continue to study the loading process where the rigid punch is coming to contact with the membrane. Hysteresis of loading and unloading for thin films will be discussed.

3.1 Rectangular film

The rectangular model is the same as shown in Figure 2.2. But no contact occurs until the punch moves to some specific position. Figure 3.1 shows the loading and unloading process of a punch to a membrane when the disjoining pressure $p$ picks up value $1 \gamma^{3/4}$ which represents the DMT-limit case. We redraw the delamination result denoted by curve OC in Figure 3.1(a). In the unloading process at point O, the punch fully contacts with the membrane. Along curve OC, the punch moves away and the contact region decreases and shrinks to a line at point C where pinch-off occurs. However, the membrane is still deformable at that point though the contact is lost. The long range intersurface force makes the membrane still stay in the cohesive zone. Mechanical equilibrium requires $F = 2 \gamma^{3/4}$. So from C to B, the applied force keeps a constant. Once the punch moves beyond the force range denoted by point B here, the applied force
decreases as mechanical equilibrium requires $F = 2pb$. Following the curve BD, the applied force decreases until the whole membrane is fully out of the force range and returns to its planar shape at point D. It should be noted that the applied force does not decrease to zero at point D, but loses its deformation abruptly instead.

For the loading case, when the punch is far from the membrane, no adhesion can be felt and the membrane still keeps its planar shape. The applied force is zero shown as the gray arrow toward point A in Figure 3.1(a). Once the punch goes into the force range, the membrane will deform instantaneously and the applied force jumps to the constant value. But no contact exists at point B though the membrane deforms. When the punch moves closer to the membrane, the applied force will keep the constant value following curve BC until the punch makes a line contact with membrane at point C named pinch-in. Moving the punch much closer to the membrane, the applied force will go through the same path as the unloading process until full contact occurs at point O. Comparing the loading path and the unloading one, we can see that there is a jump to deform event in loading process. The reason is the assumption of the Dugdale-Barenblatt-Maugis model which assumes that a constant disjoining pressure exists in some region. This makes the disjoining pressure not continuous, while the exact disjoining pressure should decrease to zero continuously.
Figure 3.1 Mechanical characterization of loading and unloading a rigid punch to a clamped rectangular membrane
For a fixed adhesion energy, when the disjoining pressure is large, the force range becomes smaller and the denoted force range of point B should move left. The constant force region CB gets shorter and shorter until comes to the limit case where point B coincides with C. This limit case has the maximum disjoining pressure $p$ for DMT-limit shown in Figure 3.1(b). The initial unloading result follows curve OB which has been reported before. When the contact of the membrane with punch shrinks to a line, the punch reaches the intersurface force range at point B in the mean time. A little further movement will make some part of the membrane out of the force range and the applied force decreases. Along curve BD, the deformation of the membrane decreases until it returns to its original planar shape at point D. For the loading part, the applied force is zero initially because the membrane is out of the force range until the punch comes to point A, where pinch-in occurs. The punch reaches the force range and the membrane jumps to make a line contact with punch at point A. The next loading path is the same as the unloading result following curve BO until the punch makes a full contact with membrane at point O.

We set the disjoining pressure $p$ to be $4 \gamma^{3/4}$ to see the JKR-limit as Figure 3.1(c) shows. The initial unloading path was discussed in the rectangular punch model in Chapter 2 and redrawn here. Just as said above, when the disjoining pressure $p$ gets larger value, the force range will shrink much shorter. When the punch comes to the force range denoted by point B, the membrane still has a none zero contact. After this point B, some part of the membrane goes out of the force range and the contact shrinks. The applied force keeps a constant value until the contact decreases to a line. After point C, the membrane remains deformable but contact has lost. At point D, the whole membrane returns to its planar shape. When the punch is loading to the membrane, the initial applied force is always zero. Once the punch comes to the force range at
point A, the membrane jumps to make a none zero contact which is called “pull-in”. The coming loading path is the same as unloading case following curve OB.

It should be noted that both DMT-limit and JKR-limit have a constant force period. But they are different, not only for the force magnitude, also for the physical meaning. The constant force period in DMT-limit is showed in dash curve where the contact has lost while the membrane is still deformable. The whole membrane is under the influence of the intersurface force and the deformation of the membrane does not change. But in JKR-limit, the membrane reduces contact with the punch at the constant force period until pinch-off occurs. This constant force period has been discussed and verified in experiments [99].

3.2 Circular film

Figure 3.2(a) shows the loading and unloading result for a clamped circular membrane when the disjoining pressure $p$ picks up value $1 \gamma^{3/4}$. For the initial unloading state, the force-displacement relation follows curve OB reported by Wan [68]. At point B, the contact of the membrane to the punch decreases to a point and totally loses after that. Because of the long range force, the whole membrane still feels the adhesion and the deformation keeps constant along BC. Once the punch goes beyond the force range denoted by point C, some parts of the membrane get free standing and the applied force decreases until the whole membrane returns to planar shape at point D. When the rigid punch is loading onto the membrane from far away, the initial state is always force free because the whole membrane is out of the force range and no adhesion can be felt shown as the gray line pointing to A. A jump event occurs at point A as the membrane feels the adhesion. Along curve CB, the punch moves closer to the membrane and the force keeps a
constant, but no contact exists until point contact occurs at B. Following BO the punch is loading closer to the membrane until makes a full contact at point O.

Figure 3.2(b) shows the loading and unloading result when the disjoining pressure obtains the maximum value for the DMT-limit, \( p = 1.861 \gamma^{3/4} \). The initial unloading result is given by Wan and redrawn here shown as curve OB. At point B, the contact decreases to a point and the punch comes to the intersurface force range. Moving the punch further causes the contact totally lost, but the membrane remains deformable. The applied force decreases until the whole membrane returns to planar shape at point D. The loading case is similar to above DMT-limit. Only difference is that no constant force period exists in this case. The reason is that when the loading punch comes to the force range the membrane deforms to make a point contact with the punch. Further loading process will increase the contact radius following the same path as unloading case.

For JKR-limit, we take the disjoining pressure \( p \) to be \( 5 \gamma^{3/4} \). The initial unloading path follows curve OB in Figure 3.2(c). At point B, the punch moves to the force range with a none zero contact. After point B, some parts of the membrane get out of the force range and become free standing. The applied force decreases along curve BC. Pull-off occurs at point C with a none zero contact lost instantaneously. Along curve CD, the deformation of the membrane decreases until returns to planar shape at point D. When the punch is loading close to the membrane, the applied force is zero until it moves to the force range. At point A, the membrane jumps to contact with the punch and pull-in happens. The next loading path follows the same curve with unloading case.
Figure 3.2 Mechanical characterization of loading and unloading a rigid punch to a clamped circular membrane
3.3 Discussion

It is found that hysteresis exists between loading and unloading process for both rectangular and circular membrane. The membrane has deformation only after the punch moves into the intersurface force range in loading process. While in unloading case, the membrane still keeps deformation even contact is lost and the punch moves beyond the force range. The deformable shape of the membrane makes some parts of it stay in the force range. This behavior is not predicted by the classic contact mechanics for solids.

An important application of the above analysis is to determine the adhesion energy ($\gamma$), intersurface force magnitude ($p$) and range ($\gamma$) according to measurable quantities: applied load ($F$), substrate displacement ($w_0$), contact area ($c$), and membrane deformed profile $w(r)$, which cannot be obtained by classical Hertz model or JKR model of solid adhesion. Another significant application is to supply the prediction of pull-in voltage or critical depth of the MEMS/NEMS device. Graphene, the two dimensional material has been introduced in Chapter 1, is considered as an ideal material in nanotechnology because of its significant mechanical, electrical and optical properties and many graphene-based devices have been fabricated [72, 75, 76]. Kong’s group made a graphene electromechanical switch and conducted the electrical measurements [118]. A pull-in contact occurs as the voltage increases to some critical value. The electrostatic force here can be treated as the disjoining pressure mathematically and this has been discussed by Wan before [65]. The mechanical model obtained here can help to extract the minimum separation to avoid the adhesion problem when designing this kind of nano-switch. On the other hand, in order to make contact to produce signal in a circuit, this model can help to predict the minimum working voltage that needed to be applied to the circuit [22]. This is useful to improve the performance and durability of nano devices.
Since atomic force microscopy (AFM) was invented around 25 years ago, many kinds of measurements have been done and AFM is therefore recognized as a very useful tool in nanotechnology [119]. One of the most important applications is the adhesion measurement and typical loading and unloading curve is well known. Here, we will make a theoretical prediction when the AFM tip is loading and unloading a membrane under the influence of long range intersurface force. It should be pointed out that our named AFM tip is not the typical one with a sharp V shape or sphere end, but a cylindrical punch with a flat end in contact with the same size membrane. In former case, the ratio of tip radius to the dimension of sample is small and a point load can be assumed. However, our prediction here is coming from the previous punch test model, and the tip radius cannot be ignored. Rein et al, recently compared the difference of two kinds of AFM probes when imaging the free-standing biomimetic polymer membrane [120]. The normal tetrahedrally shaped tip and the flat ended nanoneedle tip show different behaviors during loading and unloading.

Figure 3.3 shows our theoretical prediction of an AFM tip with an ideal infinite stiffness to indent a membrane under the influence of intersurface force. It can be realized in the intersurface force microscope (IFM) constructed by Kenneth M. Liechti and his group [121, 122]. The loading curve is shown as green arrow and the unloading curve is in blue. When the AFM tip is loading to the membrane initially, the membrane has no deformation. Once the tip comes to the force range, the membrane jumps up to contact with the tip. The next loading step goes along the gray curve and the membrane returns to original planar shape at point O. The further loading will compress the membrane shown as the inset figure. The main purpose of this study is the loading and unloading hysteresis, the details of membrane compression are beyond the scope of this paper. When the AFM tip is unloaded from the deformable membrane, the initial result is the
It is needed to figure out the limit of our results discussed above. Our model is simply based on the pure stretching assumption and no bending effect of the membrane is taken into account. However, for a real sample, it is always mixed bending and stretching deformation. Just as Wan’s experiment [123], the deformation of the rubber membrane is small compared to its thickness and bending moment contributes most to the deformation. The loading and unloading
behavior is slightly different from our result above. But this does not deny the application of our model. When the deformation is large, stretching deformation is dominant and bending effect can be ignored.

Figure 3.3 Theoretical prediction of an AFM tip to indent a membrane under the influence of intersurface force. The green arrow is the loading path and the blue arrow shows the unloading path. The pink area is the hysteresis of the loading and unloading result because of the adhesion. The inset shows the schematic of compression and tension of the membrane by AFM indentation.

In previous two models and the AFM prediction, the punch has the same dimension as the membrane and makes a full contact initially. The dimensionless pull-off radius is 0.194545 for the circular membrane [68]. However, in AFM measurement the tip radius is always much smaller than that of the sample. The previous conclusion is not valid any more. Here, we will
discuss the case when the punch is smaller than the membrane size. For simplification only JKR limit is considered. Figure 3.4 shows a typical tip-membrane adhesion model.

The profile of the deformed membrane is given by Wan [68]:

$$w = \frac{F}{2s^2} \log\left[\frac{1}{r^2}\right]$$  \hspace{1cm} (3.1)

Elastic energy and the surface energy can be obtained:

$$U_E = \frac{6}{(1-c^2)\log\left[\frac{1}{c^2}\right]^2} w_0^4; \hspace{1cm} U_S = \gamma c^2$$  \hspace{1cm} (3.2)

$$U_T = U_E - U_S$$, energy release rate has expression:

$$\partial_c U_T = -2c\gamma + \frac{24}{c(1-c^2)\log\left[\frac{1}{c^2}\right]^3} w_0^4 + \frac{12c}{(1-c^2)^2\log\left[\frac{1}{c^2}\right]^2} w_0^4$$  \hspace{1cm} (3.3)

From the Griffith’ criteria, we know that when \(\partial_c U_T > 0\), the crack will propagate; \(\partial_c U_T < 0\) the crack will heal and only get equilibrium at \(\partial_c U_T = 0\). For a initially full contact model, contact
radius will decrease as the punch moves far away. Pull-off occurs at \( c = 0.194545 \). In our model, the punch radius \( R \) is smaller than membrane radius \( a \) and the following cases will be discussed:

1. \( R/a > 0.194545 \), we find that no delamination happens initially and the contact radius keeps \( R \) as \( \partial_c U_T \) is always negative. The initial punch movement is accommodated by stretching the annular membrane without interfacial delamination. The applied force is a simple cubic function of punch displacement. At some point where \( \partial_c U_T = 0 \), delamination occurs and it follows the same path as obtained in circular membrane model where punch has the same size as membrane until pull-off occurs at \( c = 0.194545 \). Figure 3.5(a) shows the relation between the contact radius and punch displacement when the dimensionless tip radius is 0.5.

2. \( R/a < 0.194545 \). Initially, no delamination occurs and the force follows the cubic function of displacement until reaching a critical point where \( \partial_c U_T = 0 \) and pull-off occurs simultaneously. In a typical AFM measurement, the tip radius is much smaller than the sample dimension and this is why no delamination is observed before pull-off occurs. Figure 3.5(b) shows the result when the dimensionless tip radius is 0.1. The critical displacement of the tip and the applied force have the expressions:

\[
\begin{align*}
    w_0^* &= \left( \frac{R^2 (1 - R^2)^2 \log \left[ \frac{1}{R^2} \right]^3}{6(2 - 2R^2 + c^2 \log \left[ \frac{1}{R^2} \right])} \right)^{1/4} \\
    F^* &= \frac{24}{(1 - R^2) \log \left[ \frac{1}{R^2} \right]^2} w_0^3
\end{align*}
\]

(3.4)

For fixed adhesion energy between tip and the membrane, the pull-off force and displacement have the relations with tip radius shown in Figure 3.6 (a) and (b) respectively.
Figure 3.5 Contact radius versus punch displacement: (a) Tip radius $R = 0.5a$  (b) Tip radius $R = 0.1a$

Figure 3.6 (a) Pull-off force versus tip radius;  (b) Pull-off displacement versus tip radius
Chapter 4 Molecular mechanics simulation of graphene-graphene adhesion

As it is difficult to directly measure the adhesion of graphene and graphene interfaces, molecular mechanics simulation is performed here instead. Young’s modulus and effective thickness of monolayer graphene will be determined and the adhesion energy between two graphene layers will be extracted. Using these parameters, adhesion properties of rectangular and circular graphene models will be discussed and compared to the continuum model. The effect of misorientation between two graphene layers to their adhesion properties will be investigated as well.

4.1 Molecular mechanics simulation method

Molecular mechanics simulation is performed with the HyperChem program employing MM+ force field which describes a molecule as a collection of atoms that interact with each other by simple analytical functions [124]. The system total energy is a sum of bond stretching, bond-angle binding, improper dihedral, and van der Waals terms.

\[ E_{Total} = E_{Stretching} + E_{Bending} + E_{Dihedral} + E_{Van\,der\,Waals} + E_{Electrostatic} + \ldots \]

\[ E_{Stretching} = \sum K_r (r - r_0)^2; \]

\[ E_{Bending} = \sum K_\theta (\theta - \theta_0)^2; \]

\[ E_{Dihedral} = \sum \frac{V_n}{2} (1 + \cos(n\,\phi - \phi_0)); \]
\[ E_{\text{van der Waals}} = \sum \left( \frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^6} \right); \]

\[ E_{\text{Electrostatic}} = \sum \frac{q_i q_j}{\varepsilon R_{ij}} \]

where, \( k_r, k_\theta \) and \( V_n \) are bond stretching, angle bending and torsional constants respectively. \( r_0, \theta_0, \Phi_0 \) are equilibrium constants. \( n \) is the periodicity of the Fourier term. \( A_{ij} \) and \( B_{ij} \) are van der Waals parameters. \( q_i, q_j \) and \( R_{ij} \) are point charges and the distance between them respectively. \( \varepsilon \) is the effective dielectric constant. The geometry optimization will help the system to find the minimum energy potential and reach the equilibrium state. It should be pointed out that molecular mechanics does not treat electrons explicitly, thermal motions and temperature-dependent contributions. Molecular mechanics calculations cannot describe bond formation, bond breaking, or system in which electronic delocalization or molecular orbital interactions play a major role in determining geometry or properties. Thus the fracture and buckle behavior or the temperature effects are beyond the scope of this work and molecular dynamics simulation (MD) is needed [125, 126].

### 4.2 Young’ modulus and effective thickness of graphene

In order to quantify the mechanical properties of graphene, atomic force microscopy (AFM) was used to indent the monolayer graphene suspended over a cavity on the silicon substrate and the elastic modulus was found around 1 TPa by assuming the effective thickness of graphene to be 0.34 nm [127]. This result is a little different from the result 0.5 TPa obtained by Frank [128]. Other simulation results show the variation of the elastic modulus from 6.88 TPa to
1 TPa while the effective thickness changes from 0.052 nm to 0.34 nm [101, 129]. Huang [130] pointed out that the thickness and Young’s modulus of graphene or carbon nanotube depend on the types of loading and the chirality when the tube radius is smaller than 1 nm. Here, three different configurations including plane stretching, point load indentation and clamped central region indentation are built to extract the Young’s modulus and effective thickness of graphene.

First, a square shape graphene sheet with 80 nm width was built using software HyperChem shown in Figure 4.1. The left edge of the sheet was fixed and the right side can be moved to different positions. In order to simulate the stretching of the graphene sheet, the carbon atoms at the right edge was shifted along the x direction by small incremental steps, and the entire graphene sheet was allowed to relax using the conjugate-gradient method [124]. After the system finds the equilibrium position by energy minimization the total potential change of the system was obtained by comparing with the initial stage. The data points in Figure 4.2 show the total potential change with the displacement of the right edge. In the mean time, a continuum thin film with thickness $h$ and Young’s modulus $E$ is under plane stretching, the elastic energy can be calculated using the following equation,

$$
U_E = \int \frac{F^2}{2EA} dx = \frac{F^2}{2EA} L_x \frac{L_y}{2} \frac{Eh}{w_0^2}
$$

(4.1)

where $w_0$ is the displacement of the moving edge, $L_x$ and $L_y$ is the length of film in $x$ and $y$ direction respectively. Our model used here is square shape and thus $L_x = L_y$. By fitting the simulation data points with continuum model, the product of $E$ and $h$ is found around 340 J/m$^2$. This is consistent with the widely used value of 1 TPa for Young’s modulus of graphene and 0.34 nm for the effective thickness. However, when the effective thickness gets different values, Young’s modulus also varies. That’s why there are different pairs of $E$ and $h$ for graphene from
plenty of simulation results. In order to decide the values for $E$ and $h$ in our current simulation, more deformed configurations of graphene are needed.

Figure 4.1 Schematic of a plane stretching graphene sheet with left edge fixed and right edge can be moved

![Figure 4.1 Schematic of a plane stretching graphene sheet with left edge fixed and right edge can be moved](image)

Figure 4.2 Total potential change as a function of displacement. The data points are from the molecular mechanics simulation and the solid curve is from the continuum model.

![Figure 4.2 Total potential change as a function of displacement](image)
Here, a circular graphene sheet with radius of 35.1 Å was built shown in Figure 4.3(a). The periphery of the sheet was clamped and the central carbon atom was pulled up along the vertical direction by small incremental steps and the entire sheet was allowed to relax. The equilibrium state of the system was found by energy minimization and the total potential change with the displacement of the central atom was obtained as the data points shown in Figure 4.4. Considering the graphene sheet with radius \( a \) subjected to a central point load \( F \) shown in Figure 4.3(b), the central displacement \( w_0 \) has already been solved by Wan [131]:

\[
w_0 = \frac{F a^2}{2 \pi D h \beta^2} \left\{ \frac{(1 - \beta K_1(\beta))(1 - I_0(\beta))}{\beta I_1(\beta)} - \log\left(\frac{2}{\beta}\right) + \lambda + K_0(\beta) \right\} \tag{4.2}
\]

where the dimensionless membrane stress is defined as \( \beta = \sqrt{\frac{N a^2}{D}} \) and \( N \) is the tensile membrane stress. The function \( I_i(x) \) and \( K_i(x) \) are the \( i \)th order of the first and second modified Bessel functions, respectively and \( \lambda = 0.577216 \) is the Euler-Mascheroni constant. The applied load \( F \) has also been shown in equation (37) in reference [131] which is not given here because of the complex expression. The elastic energy of the thin film was calculated by \( U_E = \int F \, dw_0 \). The theoretical relation between elastic energy and the central displacement was found and shown as the solid curves in Figure 4.4. Keeping the product of \( E \) and \( h \) to be the constant 340 J/m\(^2\) obtained above, several pairs of \( E \) and \( h \) were selected which gave different theoretical curves in Figure 4.4. Only when \( E \) and \( h \) take 2.5 TPa and 0.14 nm respectively, the theoretical curve fits much better with the molecular mechanics simulation data points. However, the initial part of the theoretical curve with slope 2 where the bending deformation is dominant varies far from the simulation data points. It should be pointed out that deformation at this initial stage is even much smaller than the carbon-carbon bond length which is 0.14 nm and this small deformation cannot be exactly accounted from the simulation which gives error compared to the theoretical curve.
When the deformation is close to the stretching dominant region, the carbon bonds around the central carbon atom elongate very large. That’s why the largest central displacement stops at around 1 nm where the largest elongated carbon bond length is close to 0.177 nm which is the critical length before the carbon bond breaks [132]. In order to avoid the singularity problem of central point load and also verify the values of $E$ and $h$ obtained here, another out of plane deformation model is discussed in the next part.

![Continuum Model](image)

Figure 4.3 (a) A graphene sheet with the central atom pulled up and the periphery is clamped. The radius of the sheet is 35.1 Å. (b) Theoretical model of a clamped thin film with point load applied in the center.
Figure 4.4 Potential change as a function of central displacement. The data points are the simulation result and the solid curves with different color represent different pairs of Young’s modulus and thickness of graphene.

Figure 4.5(a) shows a circular graphene sheet fixed at the periphery and three different central areas were clamped. The radius of the sheet is 35.1 Å which is the same as the above point load model. In the above model, only the central carbon atom was pulled up, here the clamped region with radius $c$ was pulled up instead and the entire sheet was left to relax to reach the equilibrium state and the total potential change with the central displacement was thus obtained. The molecular mechanics simulation results for three different clamped radiiuses are
shown in Figure 4.6. The corresponding continuum model is also discussed by Wan in [131] and the central displacement of the sheet \( w_0 \) is given:

\[
w_0 = \frac{F a^2}{2\pi D h \beta^2} \left\{ C_1 \left[ I_0 \left( \beta \frac{c}{a} \right) - I_0 (\beta) \right] - C_2 \left[ K_0 \left( \beta \frac{c}{a} \right) - K_0 (\beta) \right] - \frac{1}{\beta} \log \left( \frac{c}{a} \right) \right\}
\]

where, constants \( C_1 \) and \( C_2 \) are given:

\[
C_1 = \frac{1}{\beta^2} \left\{ \frac{K_1 \left( \beta \frac{c}{a} \right) - K_1 (\beta) \frac{a}{c}}{I_1 (\beta) K_1 \left( \beta \frac{c}{a} \right) - I_1 (\beta) \frac{c}{a} K_1 (\beta)} \right\}
\]

\[
C_2 = \frac{1}{\beta^2} \left\{ \frac{I_1 \left( \beta \frac{c}{a} \right) - I_1 (\beta) \frac{a}{c}}{K_1 (\beta) I_1 \left( \beta \frac{c}{a} \right) - K_1 (\beta) \frac{c}{a} I_1 (\beta)} \right\}
\]

The applied load \( F \) has been shown in equation (31) in reference [131] which is not given here because of the complex expression. The elastic energy of the thin film was calculated by \( U_E = \int F \, dw_0 \). Applying \( E \) and \( h \) to be 2.5 TPa and 0.14 nm respectively, the theoretical curves for three different clamped areas are shown as solid curves in Figure 4.6 and fit well with the simulation data points except the initial stage where the displacement is smaller than the carbon-carbon bond length and the error here can be ignored. The Young’s modulus and effective thickness of graphene sheet obtained here are consistent with the previous two configurations.
Figure 4.5 (a) Graphene sheet with different clamped regions in the center. The radius of the sheet is 35.1 Å. (b) Theoretical model of a clamped punch model.
Figure 4.6 Potential change as a function of central displacement. The data points are the simulation result and the solid curves with different color represent different clamped radius in the center.
4.3 Adhesion energy of two graphene layers

Two graphene layers were built with HyperChem and shown as the inserted top figure in Figure 4.7. The radius of the sheet is 41 Å. All atoms of the graphene sheets were fixed in plane and no out of plane deformation was allowed. For each different separation between two graphene sheets, the system was allowed to relax to find the total potential density which is shown as the black curve in the inserted bottom figure in Figure 4.7. Derivation of the surface potential density gives the intersurface pressure shown with solid curve in Figure 4.7. The intersurface pressure reaches a maximum at distance 4.2 Å and decreases to negligible value when the separation is larger than 1.3 nm. This means that no adhesion can be felt when the separation goes beyond the interaction force range 1.3 nm. The area under the intersurface pressure curve in Figure 4.7 shown as gray part represents the adhesion energy of two graphene sheets which gives the number around 500 mJ/m² and this is consistent with previous experimental and theoretical values of the graphene-graphene interaction energy 30 meV/Å² or 481 mJ/m² [133-135].

The interaction potential between a flat monolayer and a flat substrate surface was given by Huang [90] in an analytical form:

\[
U_{vdw}(z) = -\Gamma_0 \left[ \frac{3}{2} \left( \frac{h^0}{z} \right)^3 - \frac{1}{2} \left( \frac{h^0}{z} \right)^9 \right]
\]

where \( U_{vdw} \) is the monolayer-surface interaction energy per unit area, \( z \) is the distance between the monolayer and the substrate surface, \( h^0 \) is the equilibrium separation, and \( \Gamma_0 \) is the interfacial adhesion energy per unit area. This equation can also be applied to calculate the adhesion energy of two graphene sheets. Actually, the adhesion energy per unit area equals to the total interaction energy at the equilibrium state according to equation (4.6). Our above simulation result indicates
that the total interaction potential energy density at equilibrium is 450 mJ/m² corresponding to the minimum point of surface potential density curve in Figure 4.7. This is also consistent with above result. Figure 4.7 also shows that the equilibrium separation between two graphene sheets is around 3.44 Å, where the interaction force is zero. There is a little difference with the commonly used layer-to-layer spacing in bulk graphite 3.42 Å. The size effect of the sheet to the result is taken into account as well. A smaller model of radius 14.5 Å was built and the results are shown as the gray curves. The results are almost the same as the larger radius model. And we can say that the result of graphene with radius of 41 Å is representative and the adhesion energy between two graphene layers is around 500 mJ/m².
Figure 4.7 Intersurface pressure as a function of separation between two graphene sheets. The black data points are from larger model with radius of 41 Å and the gray data points are from the smaller model with radius of 14.5 Å. The top inserted figure shows two graphene sheets with radius of 41 Å. The bottom inserted figure shows the surface potential as a function of graphene-graphene separation. The black points are from the larger model and the gray ones are from the smaller model.

4.4 Adhesion mechanics between graphene-substrate

In this part, we will discuss the adhesive behavior and mechanical properties of two graphene sheets with different configurations including rectangular shape and circular shape. The adhesion-delamination mechanics from the molecular mechanics simulation will be compared with the previous punch test model. Figure 4.8(a) shows two circular graphene sheets built in HyperChem. The single layer carbon sheet has radius of 40 Å and 2065 atoms. The top circular graphene film was clamped at the periphery and deformed to contact with the bottom graphene
film, which was fixed as a rigid substrate. Here, it should be pointed out that the contact defined here is not the same as classical meaning. The two graphene layers cannot truly touch because of the repulsion force when they come closer. The equilibrium separation between two graphene layers is 3.44 Å according to the previous result. We consider this smallest separation to be in contact. Initially, the two graphene layers are full contact. Then a displacement, here denoted by \( w_0 \), was set for the rigid bottom layer to move away from the top layer. The system automatically found a new equilibrium state and output the change of the total energy of the system, \( \Delta U_t \). Figure 4.9 shows that the minimum separation changes when the bottom layer moves away. It is clearly seen that the separation keeps constant 3.44 Å initially and increases to large value abruptly at last. This means that the contact radius shrinks and two graphene layers snap-off and contact is totally lost finally. The relation of applied external load \( F \) and the displacement \( w_0 \) is shown in Figure 4.10 with a series of dots.

In order to compare the result of molecular mechanics simulation with continuum model, theoretical adhesion model of graphene is built here. The top deformed graphene layer is treated as a thin film and the bottom graphene layer is considered as a rigid substrate. This is the typical punch test model for charactering thin film adhesion. Figure 4.8(b) shows the schematic of the model. \( a \) is the radius of the film, \( c \) is the contact radius, \( w_0 \) is the punch displacement and \( h \) is thickness of the film. The film has flexible rigidity \( D = \frac{E h^3}{12(1-\nu^2)} \) with an elastic modulus, \( E \), and Poisson’s ratio, \( \nu \). The bottom graphene layer is fixed at the periphery. The external load \( F \) is applied to the punch to delaminate the contact interface. The dimensionless membrane stress is defined as \( \beta = \frac{\sqrt{N a^2}}{D} \), where \( N \) is the tensile membrane stress. Wan [98] solved the punch displacement:
\[ w_0 = \frac{F \alpha^2}{2 \pi DH \beta^2} \{ C_1 \beta \left[ I_0 \left( \frac{\beta c}{a} \right) - I_0 (\beta) \right] - C_2 \beta \left[ K_0 \left( \frac{\beta c}{a} \right) - K_0 (\beta) \right] - \log \left( \frac{C}{a} \right) \} \quad (4.7) \]

where, constants \( C_1 \) and \( C_2 \) have the same forms as shown in equation (4.4) and (4.5). But \( c \) represents the contact radius here instead of the clamped radius in the previous. The applied force has the relation with punch displacement: \( F \propto w_0^n \), \( 1 \leq n \leq 3 \). \( n=1 \) refers to the pure bending limit and \( n=3 \) is for a pure stretching membrane. In order to find the relationship between \( F \) and \( w_0 \) at the equilibrium state, energy balance is needed. The potential energy of the external load, \( U_P = -Fw_0 \), the elastic energy stored in the film, \( U_E = \int F \, dw_0 \), and surface energy, \( U_S = - (\pi c^2) \gamma \), are defined respectively. Where, \( \gamma \) is the adhesion energy of the graphene-substrate interface which is 500 mJ/m\(^2\) according to previous results. At equilibrium, it can be defined as:

\[ \gamma = - \frac{\partial}{\partial (\pi c^2)} (U_P + U_E) \bigg|_{F} = \frac{\partial U_E}{\partial (\pi c^2)} \bigg|_{w_0} \quad (4.8) \]

The relation between external load \( F \) and displacement \( w_0 \) was found by solving equations (4.7) and (4.8) and shown as the gray curve in Figure 4.10. It clearly shows that this theoretical JKR model does not fit well with the simulation data points. The reason for this mismatch is not difficult to understand. Adhesion is only considered at the contact edge and the surface energy is simplified to the product of adhesion energy with the contact area in above theoretical calculation named JKR model. But Figure 4.7 shows that the real intersurface pressure is not short range compared to the graphene thickness. The force range 1.3 nm is larger than the maximum punch displacement and this means that the deformed graphene sheets can still feel the adhesion from the substrate even before the contact is lost. The full surface force potential should be considered rather than the Dugdale model. Another reason may be due to the zero membrane stress assumption in our theoretical model. The membrane is assumed to stick to the rigid
substrate and no sliding is allowed during the delamination. However, simulation shows that two graphene layers do not stick together but keep an equilibrium separation in the center region and stretching is allowed. Also the detail lattice of graphene are not considered here, especially when separation of the interacting surfaces are down to lattice spacing. Here graphene can no longer be treated as continuum membrane in macroscopic sense.

Figure 4.8 (a) Side view of the graphene graphene adhesion model in molecular mechanics simulation. The top deformable graphene layer is clamped at the periphery. The bottom layer is fixed as a rigid substrate. The radius of the graphene membrane is 40 Å. (b) Continuum model of a clamped circular film adhered to a rigid substrate.

Figure 4.8 (a) Side view of the graphene graphene adhesion model in molecular mechanics simulation. The top deformable graphene layer is clamped at the periphery. The bottom layer is fixed as a rigid substrate. The radius of the graphene membrane is 40 Å. (b) Continuum model of a clamped circular film adhered to a rigid substrate.
Figure 4.9 Central separation between two graphene sheets as a function of displacement. The inserted figure shows the deformed profile of the two sheets.
Figure 4.10 Applied force as a function of punch displacement. The results of JKR model DMT model are shown as the solid lines. The data points with different shapes are for different clamped regions.
As JKR model is not valid for the adhesion of two graphene sheets, we are trying to build a long range intersurface model named DMT model to compare with the simulation data points. The adhesion energy between two graphene sheets is a constant which equals the product of intersurface force range and the force magnitude. According to our previous theoretical model for the membrane under the long range intersurface force [68], we can change the force range and get different configurations. It should be mentioned that in our theoretical model, only membrane stretching is considered and the bending effect is ignored. Here, the graphene has thickness of 0.14 nm and bending is only dominant in the initial deformation. The larger deformation can be assumed to stretching dominant. The black curve in Figure 4.10 is the DMT limit where the disjoining pressure is assumed in the range of 1.3 nm according to the result of Figure 4.7. This makes the whole graphene sheet under a constant disjoining pressure. But again the result does not fit well with the simulation data points. In nano scale, the dimension and deformation of the material has the same magnitude as the intersurface force range, the typical short range model and long range model named JKR limit and DMT limit respectively cannot survive any more.

The two graphene layers in the above simulation have the same size and the bottom layer is restrained as a rigid substrate. The periphery of the top layer is fixed as the boundary condition. However, how many carbon atoms should be restrained at the edge and would this affect the results too much? In order to figure out these questions, boundary conditions with different size of restrained areas are considered. The diamond shape data points are the result of a larger clamped radius which gives the free membrane radius of 35.1 Å. The triangular shape data points are the result of free membrane radius of 36.5 Å. The circular shape data points represent the case only the atoms at the edge are fixed and this gives the free membrane radius of 38 Å. It
clearly shows that boundary conditions have significant effects to the final results from Figure 4.10. It is not hard to understand the differences of these three cases. Even though the carbon atoms were fixed by the coordinate at the edge, they did not disappear and still had interactions with the bottom layer. This extra contribution has significant effects at the small separation where intersurface force is strong between carbon atoms. But as the clamped radius is small enough, the edge effect can be ignored and the circular data points can be considered more accurate.

Theoretically speaking, the adhesion-delamination mechanics of rectangular model is quite different from the circular model according to our previous results [98, 99]. Pull-off occurs in the circular contact while line contact exists for rectangular model. Here, a rectangular graphene adhered to a rectangular rigid punch with same size was built and shown in Figure 4.11(a). Our model here is a square shape with width of 85 Å. The top graphene layer was clamped at two opposite edges and two other edges were kept free. The bottom graphene layer was fixed as a rigid punch. Just as the circular model, the total potential change of the system can be obtained by giving different displacements of the bottom layer. The rectangular contact area shrinks until the two layers totally delaminate. Figure 4.12 shows the central separation between two graphene sheets. It keeps the equilibrium separation of 3.44 Å initially and increases abruptly at some position where the two graphene sheets delaminate completely. Data points in Figure 4.13 show the relationship between the applied force and the displacement. Different boundary conditions are discussed as well. The diamond data points are the result of two arrays of carbon rings fixed at the armchair edges and the freestanding width is 80 Å. The circular data points show the result when the carbon atoms at the edge are fixed and this gives the freestanding width to be 84 Å. While in these two cases, the bottom graphene sheet treated as a
rigid substrate has the same size of 85 Å. Figure 4.13 clearly shows that a bump is formed at small separation. When the size of the clamped region is small enough, the bump should disappear and the curve gets smooth. The reason that causes this edge effect is the same as the above circular model. The clamped atoms can still interact with other atoms even their coordinates are fixed. The star shape data points are the result when the carbon atoms at the zig-zag edges are fixed while the armchair edges are free. There is no much difference between the armchair fixed and zig-zag fixed boundary conditions.

Figure 4.11 (a) Side view of the graphene graphene adhesion model in molecular mechanics simulation. The top deformable graphene layer is clamped at the periphery. The bottom layer is fixed as a rigid substrate. The width of the graphene membrane is 85 Å. (b) Continuum model of a clamped rectangular film adhered to a rigid substrate.
Figure 4.12 Central separation between two graphene sheets as a function of displacement. The inserted figure shows the deformed profile of the two sheets.
Figure 4.13 Applied force as a function of punch displacement. The gray curve is the JKR model result and the black curve is the DMT model result. The data points with different shapes are for different clamped regions.
We also try to compare the result from molecular mechanics simulation with the continuum model. According to Wan’s previous model, the central displacement of the punch can be calculated:

\[
 w_0 = \frac{F a^3}{2 D h \beta^3} \left\{ \frac{[\cosh(\beta \frac{C}{a}) - 1]^2}{\sinh(\beta \frac{C}{a})} - \sinh(\beta \frac{C}{a}) + \beta \frac{C}{a} \right\}
\]  

(4.9)

The potential energy of the external load, \( U_P = - F w_0 \), the elastic energy stored in the film, \( U_E = \int F dw_0 \), and surface energy, \( U_S = - 2a \gamma \), are defined respectively. At equilibrium, the adhesion energy can be defined as:

\[
 \gamma = - \frac{\partial}{\partial (2a)} (U_P + U_E) \bigg|_F = \frac{\partial U_E}{\partial (2a)} \bigg|_{w_0}
\]

(4.10)

The relation between external load \( F \) and displacement \( w_0 \) can be found by solving equations (4.9) and (4.10) and shown as the gray curve in Figure 4.13. It is not surprising to see that this theoretical JKR model does not fit well with the molecular simulation data points. The reason for this mismatch is the same as the circular model. The solid curve is the DMT limit where the intersurface force range is assumed to be 1.3 nm according to the result in Figure 4.7. The whole graphene sheet is under the intersurface force even before the contact is lost. This DMT model cannot fit well with the simulation data points just as the circular model. The assumption of zero membrane stress in the contact region can also contribute to the mismatch of the theoretical model with the simulation data points.
4.5 Adhesion mechanics between two graphene layers

In the previous part, one layer graphene was clamped at the boundary and another was fixed as a rigid substrate. The molecular simulation result was compared with the punch test model. Here, two graphene layers were clamped at the boundaries shown in Figure 4.14. The circular graphene has radius of 40 Å and 2065 carbon atoms, which is the same as the previous circular graphene-substrate model. The top layer was clamped at the periphery and deformed to contact with the bottom film. The two graphene layers could not truly contact because of the repulsion force but stayed at the equilibrium separation which is 3.44 Å according to the previous result. Once a displacement, here denoted by \( w_0 \), was set for the top layer to move away from the bottom layer, the system automatically found a new equilibrium state and output the change of the total energy of the system, \( \Delta U_T \). The derivation of the energy change then gave the external force. The relation of applied external load \( F \) and the central displacement \( w_0 \) is shown as the circular shape data points in Figure 4.15. The rectangular model shown in Figure 4.14(b) is a square shape with width of 85 Å. The triangular shape data points in Figure 4.15 give the mechanical response of rectangular graphene-graphene model. In order to make comparison with the previous graphene-substrate model, the previous simulation results of circular and rectangular model are replotted and shown as gray data points in Figure 4.15.

The relation between applied force and central displacement of graphene-graphene model is similar to graphene-substrate model but the magnitude is different. For two films model shown in Figure 4.14(c), the pull-off displacement is larger than graphene-substrate model because two films are more compliant. But it is not two times of the graphene-substrate model. This is due to the variation of the intersurface force which depends on the separation between two films and the
exact relation is shown in Figure 4.7. Once the separation goes beyond the critical value, the attraction force between two films decreases as separation increases.

Figure 4.14 (a) Side view of the circular graphene-graphene adhesion model built in HyperChem. Two deformable graphene layers are clamped at the periphery. The radius of the graphene membrane is 40 Å. (b) Side view of the rectangular graphene-graphene adhesion model. The width of the graphene is 85 Å. (c) The theoretical model of two films adhesion.
Figure 4.15 The applied force as a function of central displacement. The circular data points are the simulation result of rectangular graphene-graphene model and the triangular shape is for circular graphene-graphene model.
4.6 Misorientation effect to the adhesion property of graphene

The adhesion properties of two graphene layers including rectangular shape and circular shape discussed above are from the identical model. However, some graphene used in experiments are twisted to nonzero angles and a series of moiré pattern are formed. This kind of misoriented graphene behaves different electronic properties [136-138]. Here, we study the effect of misorientation to adhesion properties of two graphene layers. Figure 4.16 shows moiré patterns when two graphene layers are twisted with different angles. The hexagonal lattice resumes zero orientation every 60 degree. 30 degree misorientation has the smallest interference patterns. We redo the adhesion energy measurement of two graphene layers as before by changing the inter separation. The only difference is that two graphene layers are identical in previous, but twisted to be different angles here. The relations between the total potential change and separation of two graphene layers are shown in Figure 4.17(a) for different angles. Also the intersurface forces are obtained as well. It is found that the results are almost the same as previous identical case. The adhesion energy keeps 500 mJ/m² and does not depend on the twisted angles. In order to check the effect of the misorientation to the adhesion mechanics of two graphene layers, the two thin films in Figure 4.8(a) are misoriented with different angles and the simulation is implemented again. Figure 4.17(b) shows the results of different twisted angles. It proves again that misorientation of two graphene layers does not have effect to the adhesion properties. Actually, this conclusion is not difficult to understand. The above simulation models always have the relative movement perpendicular to the graphene plane. As the adhesion property is related to the projection of the work of interaction force in the perpendicular direction, the result is the same no matter which angle two circular graphene sheets with same size are misoriented. When the two graphene sheets slide from each other, we find the
misorientation only has minor effects at very small displacements and can be neglected at most time.

Figure 4.16 Different moiré patterns are formed when two graphene sheets are twisted various angles.
Figure 4.17 (a) The intersurface force as a function of separation when two graphene sheets are twisted different angles. (b) The applied force as a function of punch displacement in the circular graphene adhesion model for different twisted angles.
Chapter 5 Graphene on electronic substrates

5.1 Introduction

Ultrahigh mechanical strength, conductivity with high electron mobility and optical transparency of graphene make it to be an attractive material for flexible or transparent electronics, micro/nano electromechanical system (M/NEMS) etc [75-79]. There are, however, technical difficulties in graphene preparation and deposition that restrain its wide applications. Rudimentary mechanical exfoliation method using scotch tape peels fragmented graphene flakes off highly oriented pyrolytic graphite (HOPG) surface in a random fashion. The obtained sheets are typically multilayer with micrometer size and do not allow deposition over a precisely defined location on the electronic substrate. The uncontrollability and low efficiency of this method limit its application. Chemical vapor deposition (CVD) of organic vapor on transition metals such as nickel [71], ruthenium [139], and copper [140] is promising to create monolayer graphene of several inches, which can be transferred to other electronic substrates. The key for a successful transfer is to keep the thin film flat and have a clean and smooth substrate to avoid cracking graphene. In reality, substrate surface may have contaminates or structures on it which will affect the morphology of graphene. It is found that the electronic properties of graphene are closely related to its morphology and controlling the graphene morphology over large areas is essential in future graphene-based devices [141, 142]. Recently, a lot of theoretical calculations have been done showing that the morphology is determined by graphene-substrate adhesion, number of multi-layered graphene and substrate stiffness [89, 90, 143-145]. Generally, multi-layers render higher bending rigidity to the film attributing distinct mechanical behavior drastically different from monolayer. Bunch [146] recently pointed out that the higher adhesion
of monolayer graphene than multilayer was possibly due to the smaller bending rigidity which makes the monolayer graphene flexible to conform to the substrate contours. The influence of the substrate stiffness to the morphology of graphene was studied by Scharfenberg et al [91] by placing an exfoliated graphene onto a compliant polydimethysiloxane (PDMS) substrate with sinusoidal shape trench patterns.

Virtually all existing models assume the substrate to be in sinusoidal geometry such that deformation in x-y plane is limited. In order to obtain more representative morphology on substrates with micro-structures, we designed an array of gold pillars on silicon substrate as shown in Figure 5.1. The transferred graphene films from CVD attached strongly to substrates via natural intersurface attraction (e.g., van der Waals). These significant adhesion forces can tightly hold the sheet suspended over a cavity of micron dimensions even under the indentation of atomic force microscopy tip [127] or by hydrostatic pressure [80]. The morphology of graphene on substrate regulated by the adhesion property is sketched in Figure 5.2. When the adhesion is strong the blisters stay isolated. Weak adhesion causes coalescence of blisters.

However, direct measurement of graphene adhesion is rather difficult. The traditional methods for macroscopic films introduced in Chapter 2 are unsuitable in dealing with the samples of extremely small dimension. For example, the typical peel test or punch test becomes highly challenging in setting up experiment configurations and precise determination of the interfacial cracking for ultra-thin films. Recently, the intercalation of nanoparticles method is successful to measure adhesion of graphene with silicon [84]. However, nano particles randomly placed on a silicon substrate easily aggregate and are hard to locate. On the other hand, it is quite difficult to get large area single layer graphene by mechanical exfoliation method using scotch
tape. This causes a low efficiency to trap a nano particle by monolayer graphene to form a blister.

Here, an array of gold nano-pillars of desirable dimension is fabricated on a silicon substrate. Graphene prepared by CVD is transferred to the nano-patterned substrate. Intersurface attraction pulls the graphene into intimate contact with the substrate, leaving blisters being wedged open by the pillars and adhesion contact conforming to the substrate. Interfacial adhesion strength can be measured as a function of the radius of isolated blisters and pillar height. In addition, the change of the geometrical parameters of the pillars such as height or separation can also regulate the graphene morphology, e.g., adjacent blisters may stay isolated or coalesce.
5.2 Experiment

5.2.1 Sample preparation

Gold nano pillars were fabricated by our collaborator (Mr Cihan Yilmaz) from Center for High-rate Nanomanufacturing (CHN) in Northeastern University using a directed nanoparticle assembly process [147] shown in Figure 5.3.

1. 100 nm thick gold layer was sputtered on a silicon substrate of square shape with width and thickness 12 mm and 380 μm respectively.

2. 150 nm thick poly-methyl-methacrylate (PMMA) was spin coated on the gold/silicon substrate forming a sandwich shape with thin gold layer in the middle.

3. Arrays of nano vias were produced by conventional electron-beam lithography in the PMMA coating.
4. An AC electric field was applied between the patterned substrate and a counter electrode submerged in a gold nanoparticle suspension. Nanoparticles precisely assembled into the nanoscale vias.

5. The assembled nanoparticles were fused by passing a DC current, resulting in nanopillar formation in the vias.

6. PMMA was dissolved by acetone.

The desired nano pillar dimensions were obtained by controlling the dimensions of the holes as well as the experimental parameters such as the amplitude and the frequency of the applied voltage. The room-temperature and non-vacuum based nanorod fabrication process was carried out in an aqueous environment. Figure 5.4 shows our fabricated gold pillars with height $w_0 = 60 \pm 10 \text{ nm}$, radius $R = 25 \text{ nm}$ and inter-pillar separation $H = 500 \text{ nm}$. 

Figure 5.3 Procedures for nano pillar fabrication
Figure 5.4 Fabricated gold pillar patterns with height $w_0 = 60\pm10$ nm, radius $R = 25$ nm and inter-pillar separation $H = 500$ nm. The bottom figure shows the zoom in region.

Macroscopic sheets of graphene were grown directly on 25 $\mu$m thick copper foils (Alfa Aesar) using CVD [140] by our collaborator (Dr Xiaohong An) from Laboratory for Graphene Research in Northeastern University. The experiment set up and operation parameters such as time and pressure are shown in Figure 5.5. Copper foils (1.5 cm by 1.5 cm) were preheated in a
chamber at $T = 900-1000^\circ C$ in the presence of a flowing mixture of hydrogen and argon, which annealed the copper surface and removed surface adsorbates / impurities and oxides. Methane then fed into the furnace disintegrated into atomic carbon atoms that were in turn absorbed onto the metal surface. Upon cooling to room temperature, formation of the hybridized C=C $sp^2$ bonds produced large, continuous (though polycrystalline) graphene hexagonal lattice covering the metal surface.

Figure 5.5 Procedures for CVD grown graphene [140]. The top figures illustrates the experiment set up. The bottom one shows the operation parameters.
The weakly bonded graphene sheet was then transferred to the nano-patterned substrate using method [148] shown in Figure 5.6. The following steps give more details of this transfer process.

1. As graphene grew on both sides of the copper foil, one side of the sample was carefully scraped by super fine sand paper. The thin film was then moderately compressed between two sterilized microscope glass slides to keep the sheet flat to avoid cracking graphene.

2. 500 nm Poly (methyl methacrylate) (PMMA) was spun onto the graphene surface using spinner coating machine in Kostas center in Northeastern University (Laurell Spinner, Laurell Technology Inc., North Wales, PA) at 4000 RPM for 60 seconds. The sample was kept for a while to make the PMMA dry.

3. The sample was then carefully placed onto the surface of Ferric Chloride solution with the PMMA layer facing up. The thin film floated on the surface. The sample was kept in the solution overnight and the copper was etched away leaving the PMMA-graphene membrane floating on the solution.

4. The membrane was scooped from the etchant solution with a sterilized microscope glass slide and immersed in deionized (DI) water, with the PMMA side facing up. The membrane was thoroughly rinsed with fresh DI water repeatedly for 6 times.

5. The membrane was scooped from the DI water using the patterned substrate with the pillar array, leaving graphene contacting the pillars. The scoop operation in step 4 and 5 is very delicate and meticulous because buoyancy increases the difficulty to keep graphene flat to contact with the substrate. Samples with wrinkles will be discarded.

6. The sample was left to dry overnight.
7. The chip was immersed into acetone for overnight to remove PMMA.

8. The chip was rinsed with Isopropyl alcohol (IPA) and DI water repeatedly.

After drying, the sample was now ready for examination using scanning electron microscope (SEM, Surpa 25, Carl Zeiss SMT Inc., Peabody, MA) and atomic force microscopy (AFM, Agilent 5500, Agilent Technologies Inc., Palo Alto, CA).

![Diagram of graphene transfer process]

Figure 5.6 Transfer process of CVD grown graphene

5.2.2 Blister formation

Raman spectroscopy (HORIBA Jobin Yvon, France) verified the graphene to be monolayer with G-band around 1589 cm\(^{-1}\) and 2D-band at 2680 cm\(^{-1}\) shown in Figure 5.7. An array of graphene blisters with an inter-pillar separation \(H = 0.5 \mu m\) are shown in Figure 5.8-Figure 5.10. The high-angle viewed SEM images were taken with 30 degree tilting holder for the
The gold coating on the silicon substrate was characterized to have a grain size of ~ 50 nm with an inter-grain trough of ~1.5 nm in depth measured by AFM. Blisters did not conform to the ideal circular geometry but irregular shape with lateral corrugation.

Figure 5.7 Raman Spectra of graphene on gold. The position of G-band is around 1589 cm$^{-1}$ and 2D-band position is 2680 cm$^{-1}$. The intensity of 2D-band is more than two times of the G-band and this verifies the graphene to be single layer.

Figure 5.8(a) is the SEM image taken from an angle of 60° to the horizon. Three graphene blisters in the middle in good shape will be used later to deduce the adhesion energy between graphene and gold substrate. Figure 5.8(b) is the top view of the same region under
SEM and the nano connections among blisters can be seen. Figure 5.8(c) is the SEM image after the AFM scanning. By comparing with the initial image in Figure 5.8(a), it is obvious that the pillars A, B, and C were removed by the AFM tip and the blister D was destroyed. The AFM image is shown in Figure 5.8(d). Shadow effects are obvious at the edges of blisters or pillars. The AFM tip (Model: Contact-A from Veeco Instruments Inc., USA) used in our experiment has a triangular pyramid shape. The scanning was from the top to bottom in Figure 5.8(d). Once the tip climbed over pillars, the edge surfaces of pillars in the bottom could not be touched and the shadow was formed [149]. Same effects were seen in the AFM images in Figure 5.9 and Figure 5.10. Sharper tip and slower scan speed can help to reduce this shadow effect.

Figure 5.9(a) shows the blisters in another region. Well formed circular blisters are seen from the left side of Figure 5.9(a) and top view image of Figure 5.9(b). Coalescence of the blisters occurred and the graphene was suspended between two pillars without contacting the substrate. The pillars for this configuration are not single rods but a fusion of gold particles which were caused during the fabrication process. The height and radius of those irregular pillars are larger than the regular ones and thus gives a larger blister radius which may cause the blisters to interact with one another. Figure 5.9(c) is the SEM image taken from an angle of 60° to the horizon after AFM scanning. The pillars L, M and N were destroyed by the AFM tip during the scanning. The AFM image of the same region is shown in Figure 5.9(d).

Another pillar array was fabricated with inter-pillar separation 0.5 μm and pillar height around 100 nm shown in Figure 5.10. Some pillars are irregular because of the random distribution of gold particles during the fabrication process. Coalescence of blisters occurred and the graphene was suspended between two pillars without contacting the substrate. Those irregular shape blisters are larger than the well formed pillars. Also taller pillars increase the
blister radius and causes the blisters to interact with one another. Some irregular pillars collapsed during the graphene transfer procedures. Figure 5.10(b) shows the top view under SEM and Figure 5.10(c) is the SEM image taken from an angle of 60° to the horizon after AFM scanning. The pillars Q was destroyed by the AFM tip during the scanning. The AFM image of the same region is shown in Figure 5.10(d).

Figure 5.8 SEM and AFM image of the graphene on gold pillars with 0.5 μm separation. (a) High-angle viewed SEM image, scale bar is 100 nm. (b) Top view of the same region in SEM. (c) High-angle viewed SEM image of the same region after the AFM scanning. Pillars A, B, and C were removed by the AFM tip. The blister D was destroyed by AFM tip. (d) AFM image of the same region.
Figure 5.9 SEM and AFM image of the graphene on gold pillars with 0.5 μm separation in a different region. (a) High-angle viewed SEM image, scale bar is 100 nm. The radial corrugations of blisters are clear to see. (b) Top view of the same region in SEM. (c) High-angle viewed SEM image of the same region after the AFM scanning. Pillars L, M and N were destroyed by AFM tip during scanning. (d) AFM image of the same region.
Figure 5.10 SEM and AFM image of the graphene on gold pillars with 0.5 μm separation in a different pattern region. (a) High-angle viewed SEM image, scale bar is 100 nm. The radial corrugations of blisters are clear to see. (b) Top view of the same region in SEM. (c) High-angle viewed SEM image of the same region after the AFM scanning. Pillar Q was destroyed by AFM tip during scanning. (d) AFM image of the same region.
5.3 Model and Analysis

According to Zhang et al [145], the morphology of graphene are determined by graphene-substrate adhesion, number of graphene layers and substrate stiffness. The change of these parameters may cause the graphene fully conform to the substrate with sinusoidal surface grooves or stay flat on top of the substrate. The sharp transition between these two limits occurs at certain number of graphene layers and stiffness of substrate. Similar conclusion can be drawn from our model. If the adhesion energy between the graphene and substrate is sufficiently strong, the thin sheet can fully conform to the pillar patterns like coating while weak adhesion keeps the graphene flat and supported by pillars. However, in reality, the adhesion energy is finite and a series of blisters with some debonding regions are more likely formed and shown as Figure 5.1. We will deduce the adhesion energy of graphene-gold interface using our theoretical model. Whether these kinds of blisters will keep isolated or interact with one another is strongly associated to the geometry parameters of the pillars which are the height and separation of pillars. A dimensionless parameter will be built to predict the morphology of graphene.

Figure 5.11 shows the schematic of two isolated graphene blisters. For graphene with an elastic modulus, \( E \approx 1.0 \) TPa and thickness \( h \approx 0.34 \) nm, the tall pillar with height \( w_0 = 60 \pm 10 \) nm (\( \gg h \)) leads to membrane stretching with negligible bending. Assuming an approximate circular blister geometry, our previous model [84, 150] expresses the interfacial adhesion energy, \( \gamma \), as

\[
\gamma = \frac{E h}{32 k_{el}} \left( \frac{w_0}{a} \right)^4
\]  

(5.1)
where \( k_{el} = 1 - (2\cos\theta)^{-1} \) with \( \theta \approx 22^\circ \) the contact angle at the blister edge, and an average blister radius of \( a = 160 \pm 20 \) nm. Adhesion energy of the graphene-gold interface is found to be \( \gamma = 0.45 \pm 0.1 \) J/m\(^2\).

Figure 5.11 Schematic of two blister models. The parameters are defined as: \( w_0 \): the height of the pillar; \( a \): radius of the blister; \( H \): separation between two pillars.

Here, we have the theoretical prediction for the blisters to interact and coalesce and study the contact area change when the height of the pillars increases while the inter-pillar separation keeps a constant named \( H \). Figure 5.12(a) shows a top view of four pillars. The red spots represent the pillars and the gray region is the delaminated area. It should be pointed out that the delaminated area from the blister is a circular shape. Here we only consider the quarter section because of the symmetry. The radius of the blister is \( a \) and the separation between the pillars is \( H \) which is a fixed value. The height of the pillar \( w_0 \) can change. Equation (5.1) shows that the radius of the blister is proportional to the height of the pillar. When the pillar height is small enough, the blister size can be neglected and the whole area of graphene makes a full contact with the gold substrate. When the pillar height increases, the blisters propagate and more contact area loses. A dimensionless parameter \( \kappa \) is defined as the ratio of the delaminated area named \( A_{del} \) to the original full contact area denoted by \( A_0 \):
At the critical point where the edges of the blisters are shown as the dash curves in Figure 5.12(a), the blisters interact with one and another. The blister radius is half of the separation and the dimensionless parameter is $\kappa = \pi / 4$, the critical height of the pillar $w_0' = \frac{H}{2} \left( \frac{32 k_{el}}{E h} \right)^{1/4}$. The blisters connect together after the pillars height goes beyond this critical value and the contact edges propagate to the solid curves shown in Figure 5.12(a). The surrounded area in the center is the only contact region. After coalescence of the blisters, the dimensionless parameter can be obtained after some algebra operations,

$$\kappa = \sqrt{4 \left( \frac{a}{H} \right)^2 - 1 + \left( \frac{a}{H} \right)^2 \left( \pi - 4 \arccos \left( \frac{H}{2a} \right) \right)}$$  \hspace{1cm} (5.3)

We know that the contact region in the center must shrink when the pillar height increases further. While it cannot decrease to zero but snap off with none zero radius instead. It is not easy to find out the exact position when the snap off occurs and is beyond the scope of this paper, but we can give an estimation instead. For the limiting case, we know that the distribution of the pillars will be more like a circle not the current square shape when the pillars number increases to a large value. Then the contact region becomes close to a circular shape and the graphene sheet is likely clamped by the circular distributed pillars and delaminates with the gold surface. We have a similar model where a circular film was clamped at the periphery and delaminated from the bottom substrate [68] and pull-off occurs when the contact radius shrinks to 0.195 times of the film radius. The contact area is defined as $A_{con}$ and $A_{con}^*$ represents the critical contact area when the blisters begin to interact shown as the dash curves in Figure 5.12(a). Thus we have $A_{con} / A_{con}^* < 0.195^2$ at the snap off point and obtain the maximum height of the pillar.
The dimensionless parameter $\kappa = 0.962$ at this limit case. The graphene sheet will keep flat after fully debonding from the substrate and the dimensionless parameter holds the constant 1. Further increasing of the pillar height will not change the morphology of the graphene any more. Figure 5.12(b) plots the dimensionless parameter as a function of pillar height. The slope of curves at $w_0$ is not continuous. The reason is the energy release rate after the blisters merge together is greater than before. The sharp contact edge makes the blister easily delaminate from the substrate.
Figure 5.12 (a) Schematic of four blisters. The red spots represent four gold pillars. The gray region shows the quarter size of the delaminated region. The dash curves show the critical contact edges when the blisters begin to interact with one and another. The solid curves in the center show the contact edges after the blisters coalesce. (b) The dimensionless parameter as a function of the pillar height. The vertical axis is defined as ratio of the delaminated area to the original full contact area. $w_0$ is the height of the pillar. $w_0'$ is the critical height when the blisters begin to interact and $w_0''$ is the critical height when graphene snap off the substrate.
5.4 Discussion

Our above theoretical prediction for the morphology of graphene on pillars assumes the adhesion energy and separation of pillars to be constant and only height of pillars can change. If only separation of pillars increases with adhesion energy and height of pillars fixed, theoretically speaking, the size of blisters does not change and morphology keeps the same. The reducing of the separation of pillars may cause the blisters to coalesce. Equation (5.1) can also predict the radius of the blister if the adhesion energy is known. Two blisters will merge together when the separation $H$ decreases to a critical value $H^*=2a$. The critical aspect ratio of the pillar can be calculated in the following equation,

$$
\frac{H}{w_0} = \left(\frac{32k_{el} \gamma}{E h}ight)^{1/4} \frac{w_0}{w_0} = 2\left(\frac{E h}{32k_{el} \gamma}\right)^{1/4}
$$

(5.5)

Using the previously obtained parameters of graphene and pillars, the critical aspect ratio of the gold pillar for the blister to interact and coalesce is 5.3. In Figure 5.8, the height of the pillars is 60±10 nm and the minimum separation to avoid the coalescence of the blister is 320 nm. Ideal situation for our 0.5 μm separation pillars is that all the formed blisters have circular shape and stay isolated demonstrated as Figure 5.1. Our experiments showed that the blisters got close to trapezoidal shape and connected with some nano channels even though they did not coalesce. These nano channels have depth of 1.5 nm and are large enough to allow water molecules to move through the blisters easily. The reason why the nano channels are formed is not clear. Another reason for the irregular blisters is the extreme flexibility of monolayer graphene which readily conforms to the geometry of the gold layer on the substrate. In the previous intercalation of nanoparticles method [84], the graphene sample was multilayer (roughly 5 layers) obtained by mechanical exfoliation. The film was more rigid than our current sample and easier to form a...
circular blister. For the pillars with height of 100 nm shown in Figure 5.10, the minimum separation to avoid the coalescence of the blister is 530 nm. This critical aspect ratio is beyond the inter-pillar separation 0.5 μm and the radial corrugation of blisters is formed. If the separation $H$ decreases to very small value, the coalesced blisters may also snap off at some critical point similar to the pillar height effect.

![Figure 5.13 SEM image of graphene on pillars with separation of 1 μm. It is very difficult to form the expected blisters as previous with inter-pillar separation of 0.5 μm. Graphene was destroyed by the pillars and cracks can be seen around the pillars. The dark region is the shade after focusing on a smaller size under SEM. The edge of the graphene is clear to see.](image)

In order to check the effect of separation to the morphology of graphene on pillars, we also fabricated the pillars pattern with 1.0 μm separation while the height of pillar was around 100 nm. After the experiment we found that the pillars with 0.5 μm separation were welcomed and easy to form blister, while the pillars with 1.0 μm separation were hard to succeed. Most of them collapsed downward or formed cracks shown in Figure 5.13. One possible explanation is when the separation of pillars increases to a larger value, the number of pillars per unit area reduces and the force supported by a single pillar is much larger, which may cause the pillar to
fall down or destroy the graphene. The increases of the pillar height may also cause the pillars to
be unstable and destroyed easily.

To check the stress and strain situation in the blisters, we tried to use Raman
Spectroscopy to map out the stress of graphene on pillars. According to Wan’s model [150], the
tent shape blisters are stretched and the radial ($\beta_r$) and tangential ($\beta_t$) stress can be calculated:

$$\beta_r = \frac{Eh w_0^2}{4a^2} \log\left(\frac{a}{r}\right) + \frac{F}{2\pi w_0 \cos(\theta)}$$

(5.6)

$$\beta_t = \frac{Eh w_0^2}{4a^2} (\log\left(\frac{a}{r}\right) - 1) + \frac{F}{2\pi w_0 \cos(\theta)}$$

(5.7)

The membrane strain is:

$$\varepsilon_r = \frac{1}{Eh} (\beta_r - \nu \beta_t)$$

(5.8)

$$\varepsilon_t = \frac{1}{Eh} (\beta_t - \nu \beta_r)$$

(5.9)

The radial stress and strain decrease gradually from the center to the edge. The tangential
stress and strain reduce from the center but get negative values close to the contact edge. This
means compression is applied and wrinkles are caused, which were not observed in the
experiment. This theoretical prediction is also inconsistent with Wan’s finite element analysis
result shown in Figure 5.14 [131]. For zero initial residual stress ($\beta_0=0$), both radial and
tangential stress get singularity at the point load center and decrease gradually, but still keep
tension. The inconsistency is because of the assumptions to deduce the stress and strain in
equations (5.6)-(5.9). The profile of the blister was assumed to be linear shape which was good
for the middle region of the blister, but invalid for the center loaded region and the clamped
edge. For a single blister with radius of 160 nm and pillar height of 60 nm, the radial and
tangential stress should follow the results shown in Figure 5.14. According to Hone and Galiotis’s results [151, 152], the strain should cause the G band and 2D band to have an obvious shift, even to split the G band to two peaks named $G^+$ and $G^-$. But here, we cannot see the clear shift after our Raman Spectroscopy measurement. The reason is that our blister was too small with diameter of 320 nm and the spot size of the laser used for Raman Spectroscopy was around 1.5 μm. This very small tension area cannot make a significant contribution to the overall Raman spectra.

Figure 5.14 The radial and tangential stress of the blister as functions of radial distance [131]. $\beta_0$ is the initial residual stress.
The results obtained here are not limited to the circular pillars but can also be applied to study the morphology of graphene on substrate with different undulated surfaces. In our previous intercalation of nanoparticles method, the gold nano particles were trapped underneath the graphene and formed various blisters. The change of the diameter of the particles may also cause the blister to shrink or coalesce and the critical diameter of the particle can be obtained according to our model. The results and trends set design guidelines for graphene devices.

### 5.5 Graphene on other substrate materials

Except the above utilized gold substrate, other widely used electronic substrate materials have also been tried such as silicon dioxide and silicon nitride.

Figure 5.15(a) shows the optical image of the graphene on the silicon substrate with a silicon dioxide layer with 300 nm thickness. This special thickness gives a very good contrast which makes the graphene to be visible under optical microscope and this is the key for graphene to be experimentally found for the first time [69]. The blue region in a square shape is the transferred graphene. Figure 5.16 shows the SEM image of a nano particle trapped by the graphene on the silicon dioxide substrate. The blister is star shape here and the folding can be clearly seen which is quite different from Zong’s intercalation of nanoparticles method shown in Figure 1.14 where the blister is circular. But the result here is consistent with our previous result of graphene on gold pillars shown as Figure 5.8. The reason is the same as previous that the graphene here is single layer which is more flexible and easily to fold. Graphene in Zong’s experiment was multilayer and more rigid.

We also tried the silicon nitride substrate shown in Figure 5.15(b). However, we found it was very difficult to transfer the graphene onto the silicon nitride surface. During our transfer
process, the last step was to dissolve the Poly (methyl methacrylate) (PMMA) coated on the graphene in acetone. If graphene adheres well with the substrate, large area of graphene can be found on the substrate after the sample is dry. Here, we guess the adhesion between graphene and silicon nitride is too weak. When the sample was immersed in the acetone solution, the graphene detached from the sample surface under the effect of surface tension or other interfacial force.

Figure 5.15 Graphene transferred to silicon dioxide substrate (a) and silicon nitride substrate (b).

Figure 5.16 SEM image of copper nano particles trapped by graphene on the silicon dioxide substrate.
Chapter 6 Conclusion and future work

6.1 Significant contributions and conclusions

By reviewing the merits and shortcomings of available solid adhesion and thin film adhesion models, this thesis propose the demand for the adhesion-delamination mechanics of thin film under long range intersurface forces. A new dimensionless parameter $\psi$ was found and used to gauge the JKR-DMT transition for adhesion of thin membrane from a rigid substrate. Behavior of membrane with large $\psi$ approaches the JKR-limit, but a small $\psi$ tends to the DMT-limit. This new parameter was extended to cover the form of Tabor parameter for solid adhesion. We also demonstrated how $\psi$ manifested itself in three well known test configurations for thin films, including punch test model, pressurized blister model and constrained blister model. The adhesion-delamination mechanics of a rectangular or circular membrane to a rigid substrate was obtained by linear elasticity and thermodynamic energy balance. Pinch-off or pull-off and the associated critical force and central displacement were determined. The theoretical framework allows one to experimentally gauge the materials properties of thin membrane and interfaces and to track the delamination process. An adhesion map for thin film was constructed to show the JKR-DMT transition governed by this new Tabor parameter and also the transition from pure bending limit to pure stretching limit depending on the thin film deformation compared with its thickness.

The hysteresis of loading and unloading a rigid punch to a clamped membrane for both rectangular and circular shape were discussed. The pull-in and pull-off were found and compared with a typical AFM measurement. In our model, the membrane deforms to contact with the tip at the intersurface force range. While in a typical AFM measurement, the AFM tip contacts with
the sample with bending the tip cantilever. The effect of the punch size was discussed as well. The relation between the pull-off force or displacement and the tip radius was obtained.

We obtained the Young’s modulus and effective thickness of graphene with molecular mechanics simulation for three geometry configurations including plane stretching, point load, and clamped punch load. The adhesion energy between graphene and graphene interface was found to be 500 mJ/m² and the result is consistent with the reported value from reference. The adhesion-delamination mechanics between two graphene layers including circular and rectangular shape was discussed and compared with the continuum model. The theoretical JKR and DMT model does not match well with simulation results. The detail lattice of graphene should be considered, especially when the separation of the interacting surface are down to lattice spacing. Here graphene can no longer be treated as continuum membrane in the macroscopic sense. The full surface force potential should be considered rather than the Dugdale model. Also the assumptions in our continuum model, such as the average membrane stress, small contact angle and no sliding in contact region, cause inconsistency between simulation and continuum model. We also considered the misoriented graphene and found the misorientation did not affect the adhesion properties of two graphene layers.

By transferring the monolayer graphene grown by chemical vapor deposition onto the fabricated gold nano pillars on silicon substrate, a series of blisters were formed and the adhesion energy between graphene and gold was deduced to be 0.45 ± 0.1 J/m². The morphology of graphene on nano pillars was strongly regulated by the interfacial adhesion energy, the height and separation of pillars. The effects of these parameters to the graphene morphology were discussed. A dimensionless parameter was derived to gauge the area coverage over the substrate and the blister profile. The critical separation between pillars and the critical height of pillars
were predicted to avoid the coalescence of blisters. Graphene was also transferred onto other substrates including silicon dioxide and silicon nitride. Irregular blisters with lateral corrugation were always found on silicon dioxide substrate because of the extreme flexibility of monolayer graphene. The interfacial adhesion energy between graphene and silicon nitride was found to be weaker than graphene with silicon dioxide. The surface tension may cause graphene detach from the substrate surface during the transfer process.

6.2 Future work

There are a number of unanswered questions. First, the adhesion mechanics of thin film under mixed bending and stretching deformation is needed. Our available results are either pure stretching or pure bending when the long range intersurface force is applied, or only JKR limit is discussed when the thin film is mixed bending and stretching. No one has ever coupled the stretching and bending deformation with long range intersurface force. Actually this more accurate model is also needed to analyze our molecular mechanics simulation results for graphene. The membrane stress in our current theoretical model is averaged and the adhesion-delamination mechanics is obtained by linear elasticity. While for large deformation, the assumptions of uniform membrane stress and small contact angle in our model are not valid and this has been demonstrated by comparing our constrained blister result with Hui’s work [113]. For our punch test model, the membrane is assumed to stick to the substrate and no sliding is allowed in the contact region. Thus the membrane stress in the contact zone is not taken into account and this may cause the mismatch between the molecular mechanics simulation result and the theoretical model for the graphene work shown in Chapter 4. The future work should seek a more sophisticated model without these assumptions. In order to compare the adhesion
mechanics of graphene from molecular mechanics simulation, finite element analysis can be implemented. The long range intersurface force shown in Figure 4.7 can be defined as the interaction between two thin films.

A new Tabor parameter was found in Chapter 2 and showed the transition from a thin membrane to a rigid plate and even to a solid sphere. But in application, the value of $m$ and $n$ are unknown for a thin film under mixed bending and stretching. The variation of $m$ and $n$ between these limits are still missing. If the new adhesion model proposed above works in the future, the transition from DMT to JKR limit of a thin film mixed bending and stretching can be found and the variation of $m$ and $n$ can also be obtained. The available adhesion map for thin film should be modified.

The blisters formed by particle or nano pillars underneath the monolayer graphene shown in Chapter 5 are not ideal circular geometry but irregular shape with lateral corrugation. Though, adhesion energy between graphene and gold is obtained by assuming the blister to circular geometry, more accurate models are needed to analyze the irregular blisters like triangular and even polynomial shapes. It should be pointed out that the pillars used in our experiment is quite small with diameter of 25 nm. This dimension is almost the limit of our current fabrication technique and the pillars were not exactly the same size. Larger pillars can be made to get uniform shape which may help to form circular blisters. The reason for the lateral corrugation of blisters connected with nano channels is not clear and can be extended to the future work. Finite element analysis or molecular dynamics simulation can also be done to compare the morphology of graphene on these undulated substrates.
Table 6.1 The prediction of the blisters shape

<table>
<thead>
<tr>
<th>Set</th>
<th>Pillar height ($w_0$)</th>
<th>Inter pillar separation ($H$)</th>
<th>Aspect ratio</th>
<th>Blisters shape</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set 1</td>
<td>60 nm</td>
<td>500 nm</td>
<td>8.3</td>
<td>Isolated</td>
<td>Done</td>
</tr>
<tr>
<td>Set 2</td>
<td>100 nm</td>
<td>500 nm</td>
<td>5</td>
<td>Coalesced</td>
<td>Done</td>
</tr>
<tr>
<td>Set 3</td>
<td>100 nm</td>
<td>1000 nm</td>
<td>10</td>
<td>Isolated</td>
<td>Future work</td>
</tr>
<tr>
<td>Set 4</td>
<td>150 nm</td>
<td>1000 nm</td>
<td>6.7</td>
<td>Isolated</td>
<td>Future work</td>
</tr>
</tbody>
</table>

Our experiment results about the morphology of graphene on undulated substrates mainly come from the gold pillars with 500 nm separation and the isolated and coalesced blisters have been obtained. In order to verify the theoretical prediction of the morphology of graphene and also experimentally find the critical aspect ratio of the pillars, more configurations of pillars with different heights and separations should be fabricated to repeat the experiments shown in Table 6.1. Sets 1 and 2 have been done already and the experiments have verified the theoretical prediction. Sets 3 and 4 have larger aspect ratio than the critical value of 5.3 from equation (5.5) and the blisters are predicted to be isolated. The experimental verification can be extended to the future work. When the height of pillars is increased to form blister with larger radius, the effect of the membrane stress to the shift of the Raman Spectra of graphene on gold can be captured.
REFERENCES


133. Sabio, J., et al., *Electrostatic interactions between graphene layers and their environment.*


Appendix 1: Mathematica Program for Rectangular Punch Test Model under Pure Stretching

Without the cohesive zone \((x > b)\)

\[
\text{DSolve}\left[\left\{ -s^2 w''(x) = \frac{F}{2} \text{DiracDelta}[x], w, x \right\}\right]
\]

\[
\left\{\{w \rightarrow \text{Function}\left[\{x\}, C[1] + x C[2] - \frac{Fx \text{UnitStep}[x]}{s^2} \}\}\right\}
\]

Within the cohesive \((c < x < b)\)

\[
\text{DSolve}\left[\left\{ -s^2 w''(x) = p\right\}, w, x \right]\right]
\]

\[
\left\{\{w \rightarrow \text{Function}\left[\{x\}, -\frac{px^2}{2s^2} + C[1] + x C[2]\}\}\right\}
\]

Clear\([w, b, c, x, p, s]\):

\[
w[x_] := \frac{p(b - c)}{s^2} (1 - x) \quad \text{if} \quad 1 > x \leq b;\]

\[
w[x_] := \frac{2bp - b^2p - 2cp + 2cpx - px^2}{2s^2} \quad \text{if} \quad c \leq x < b;\]

Punch Displacement

\[
w_0 = w[x = c] = \frac{2bp - b^2p - 2cp + c^2p}{2s^2}\]

Surface force range

\[
w(x = b) = \frac{p(b - c)}{s^2} (1 - b)\]

Clear\([b, c, p, s]\)

FullSimplify\[
\frac{2bp - b^2p - 2cp + c^2p}{2s^2} - \frac{p(b - c)}{s^2} (1 - b)\]

\[
y = \frac{(b - c)^2p}{2s^2}\]
Membrane Stress within the cohesive zone

Clear\[x, \ b, \ c, \ p, \ s\]

\[
\text{wl} = \left(\frac{2 \ b \ p - b^2 \ p - 2 \ c \ p + 2 \ c \ p \ x - p \ x^2}{2 \ s^2}\right);
\]

\[
\text{dwdx} = \partial_x \ \text{wl};
\]

\[
\int \text{dwdx}^2 \ \text{dx}
\]

\[
y1[x_] := -\frac{\ p^2 \ (c - x)^3}{3 \ s^4}
\]

\[
\text{FullSimplify}\left[\frac{6 \ (y1[b] - y1[c])}{(b - c)}\right]
\]

\[
2 \ (b - c)^2 \ p^2 \ \frac{s^4}{s^4}
\]

\[
\text{Solve}\left[s^2 = \frac{2 \ (b - c)^2 \ p^2}{s^4}, \ s\right]
\]

\[
s1 = 2^{\frac{1}{6}} \ (b^2 \ p^2 - 2 \ b \ c \ p^2 + c^2 \ p^2)^{\frac{1}{3}}
\]

\[
s1' = \frac{p \ (b - c)^2}{2 \ Y}
\]

\[
F = 2 \ p \ (b - c) = \frac{32 \ p^5}{(b - c)^3}
\]

Clear\[w, \ w0, \ w1, \ w2, \ p, \ F, \ s, \ b, \ c, \ x\]

\[
D = \frac{16 \ p^3}{(b - c)^4};
\]

\[
s1 = 2^{\frac{1}{6}} \ (b^2 \ p^2 - 2 \ b \ c \ p^2 + c^2 \ p^2)^{\frac{1}{3}};
\]

\[
\text{UE1} = \text{FullSimplify}\left[2 \ \frac{(s1)^4}{24} \ (b - c)\right]
\]

\[
\frac{16}{3} \ (b - c) \ \left(\frac{y^5}{(b - c)^6}\right)^{\frac{2}{3}}
\]

\[
\text{UE1} = \frac{16}{3} \ \frac{y^4}{(b - c)^3}
\]
Membrane stress without the cohesive zone

Clear[p, b, c, s, x]

\( w_2 = \frac{p (b - c)}{s^2} (1 - x); \)

\[ \int dw_2 dx = \partial_s w_2; \]

\[ y_2[x_] := \frac{(b - c)^2 p^2 x}{s^4} \]

\[ \text{FullSimplify}\left[\frac{6 \left(y_2[1] - y_2[b]\right)}{(1 - b)}\right] \]

\[ 6 \frac{(b - c)^2 p^2}{s^4} \]

\[ \text{Solve}\left[s^2 == \frac{6 (b - c)^2 p^2}{s^4}, s\right] \]

\[ s_2 = 6^{1/6} \left(b^2 p^2 - 2 b c p^2 + c^2 p^2\right)^{1/6} \]

\[ s_2^2 = \frac{p (b - c) (1 - b)}{w_0 - y} \]

\[ \left(\frac{p (b - c) (1 - b)}{w_0 - y}\right)^3 = 6 \left(b^2 p^2 - 2 b c p^2 + c^2 p^2\right) \]

Clear[p, b, c, s_2, w_0, y]

\[ p = \frac{6 (w_0 - y)^3}{(b - c) (1 - b)^3}; \]

\[ s_2 = 6^{1/6} \left(b^2 p^2 - 2 b c p^2 + c^2 p^2\right)^{1/6}; \]

\[ \text{UE}_2 = \text{FullSimplify}\left[\frac{2 \left(s_2^2\right)^4}{24} (1 - b)\right] \]

\[ -3 (-1 + b) \left(\frac{(w_0 - y)^6}{(-1 + b)^6}\right)^{1/3} \]

\[ \text{UE}_2 = \frac{3 (w_0 - y)^4}{(1 - b)^3} \]

Elastic energy of membrane

\[ \text{UE} = \frac{16}{3} \frac{y^4}{(b - c)^3} + \frac{3 (w_0 - y)^4}{(1 - b)^3} \]
Surface Energy

Clear[w0, w1, b, c, y, p, x]

w1 = w0 \left( \frac{2 b - b^2 - 2 c + 2 c x - x^2}{2 b - b^2 - 2 c + c^2} \right);

\int p \left( y - (w0 - w1) \right) dx

p x \left( w0 x^2 + 3 c^2 (w0 - y) + 3 (-2 + b) b y + c (-3 w0 x + 6 y) \right)

3 (-2 b + b^2 - (-2 + c) c)

Clear[b, c, y, w0, p]

T[y_] := \frac{p x \left( w0 x^2 + 3 c^2 (w0 - y) + 3 (-2 + b) b y + c (-3 w0 x + 6 y) \right)}{3 (-2 b + b^2 - (-2 + c) c)};

US1 = 2 FullSimplify[T[b] - T[c]]

\frac{2}{3} (b - c) p \left( \frac{(b - c) w0}{-2 + b + c} + 3 y \right)

Energy Calculation

Clear[b, c, y, w0, y, s, p]

p = 5;

w0 = 0.5;

y = 1; y = y / p;

0 >> c.txt; 0 >> ue.txt; 0 >> us.txt; 0 >> ut.txt

cmin = 0.00001; cmax = 0.999; cinc = (cmax - cmin) / 200;

Do[S - 2^{1/6} \left( \frac{p^2 (b - c)^2 (3 - 2 b - c)}{1 - c} \right)^{1/6};

sol = FindRoot[w0 == \left( \frac{2 b - b^2 - 2 c + c^2}{2 b - b^2 - 2 c + c^2} \right)p, \{b, c + 0.01\}];

UE - N[\frac{1}{6} \left( \frac{1 - c}{2} \right)^{2/3} \left( b^2 (b - c)^2 (3 - 2 b - c) \right)^{2/3} /. sol] >>> ue.txt;

US = N[\frac{2 y c + 2 \left( \frac{(b - c)^2 p w0}{3 (-2 + b + c)} + (b - c) y \right)}{3 (-2 + b + c)} /. sol] >>> us.txt;

UT = N[UE - US] >>> ut.txt; N[\{\}] >>> c.txt; \{c, cmin, cmax, cinc\}

X = Import["C:\\Documents and Settings\\Gu.Li\\My Documents\\c.txt", "List"];

Y = Import["C:\\Documents and Settings\\Gu.Li\\My Documents\\ut.txt", "List"];

XTable = {{X[[1]], Y[[1]]}};

Do[XTable = Append[XTable, {X[[i]], Y[[i]]}], \{i, 2, Length[X]\}];

g1 = ListPlot[XTable, PlotRange -> {{0, 1}, {-2, 1}}]
Appendix 2: Mathematica Program for Rectangular Punch Test Model under Pure Bending

Governing equation

```mathematica
Clear[w1, w2, b, c, x, p, F]
DSolve[\[LeftBracket\[w1''''[x] == 0, w2''''[x] == p, w1[1] == 0, w1'[1] == 0, w1''[1] == \(\frac{F}{2}\), w1[b] == w2[b], \RightBracket], \{w1[b] == w2[b], w1''[b] == w2''[b], w2''[c] == 0, w1''''[b] == w2''''[b]\}, \{w1, w2\}, x]
```

\[
\begin{align*}
&w1 \rightarrow \text{Function}[\{x\}, \\
&\frac{1}{24 (-1 + c)} \left(-F + 4 c F - 3 c^2 F + 2 b^3 p - 6 b^4 c p + 6 b c^4 p - 2 c^6 p - 6 c F x + 6 c^3 F x - \\
&4 b^2 p x + 12 b^3 c p x - 12 b c^2 p x + 4 c^3 p x + 3 F x^2 - 3 c^2 F x^2 + 2 b^3 p x^2 - 6 b^4 c p x^2 + \\
&6 b c^4 p x^2 - 2 c^6 p x^2 - 2 F x^2 + 2 c F x^3\right)], \quad w2 \rightarrow \\
&\text{Function}[\{x\}, \frac{1}{24 (-1 + c)} \left(-F + 4 c F - 3 c^2 F + 2 b^3 p - 6 b^4 c p + b^4 c p + 6 b c^4 p - 2 c^6 p - \\
&6 c F x + 6 c^3 F x + 12 b^3 c p x - 4 b^4 c p x + 12 b c^2 p x + 4 c^3 p x + 3 F x^2 - 3 c^2 F x^2 - 6 b^4 p x^2 + \\
&2 b^3 p x^2 + 6 b c^4 p x^2 - 2 c^6 p x^2 - 2 F x^2 + 2 c F x^3 + 4 b p x^3 - 4 b c p x^3 - p x^4 + c p x^4\right)]]
\end{align*}
```

Membrane Profile within the cohesive zone

\[
w2 = \frac{1}{24 (-1 + c)} \left(b^4 (-1 + c) + 4 c^3 (-1 + x)^2 - x^4 + 6 b^2 (-c + 2 c x - x^2) + b^3 (2 - 4 c x + 2 x^2) + \\
b (-2 + 2 c (-6 - 12 x) + 6 x^2) - 4 c^2 (2 - 6 x + x^2) + c (2 - 6 x^2 + 4 x^3 + x^4)\right);
\]

Without cohesive zone

\[
w1 = \frac{1}{24 (1 - c)} F (1 - x)^2 \left((1 - c) (1 - 3 c + 2 x) - (b - c)^2\right);
\]

Punch Displacement

\[
w0 = \frac{1}{24} \left(b^4 + b (2 - 6 c) + 6 b^2 c - 2 b^3 (1 + c) + c (-2 + 6 c - 4 c^2 + c^3)\right) p
\]

Surface force range

\[
w (x + b) = \frac{(1 - b)^2 (b - c) \left(1 + 2 b - b^2 - 4 c + 2 c^2\right) p}{(12 (1 - c))}
\]

Clear[b, c, p, s]

\[
\text{FullSimplify}\left[\frac{1}{24} \left(b^4 + b (2 - 6 c) + 6 b^2 c - 2 b^3 (1 + c) + c (-2 + 6 c - 4 c^2 + c^3)\right) p - \\
((1 - b)^2 (b - c) \left(1 + 2 b - b^2 - 4 c + 2 c^2\right) p) / (12 (1 - c))\right]
\]

183
\[ y = \frac{(b - c)^3 \left(2 - b - c\right) (3 - 2 b - c) p}{24 (1 - c)} \]

**Elastic energy**

\[
F = 2 p (b - c) ;
\]

\[
w1[x] := \left(F (1 - x)^2 \left((1 - c) (1 - 3 c + 2 x) - (b - c)^2\right)\right)/(24 (1 - c));
\]

\[
w2[x] := \frac{p}{24 (1 - c)} \left(\left(\frac{b - x}{x}\right)^3 (b - 2 c + x)^2 (1 - c) + 2 \left(1 - b\right) (b - c) \left(\left(1 - c\right)^2 (1 - b - 2 c) - 3 (b - 2 c) (x - c)^2\right)\right);
\]

\[
UE1 = 2 \int \frac{1}{2} \left(w1'' [x]\right)^2 dx
\]

\[
UE2 = 2 \int \frac{1}{2} \left(w2'' [x]\right)^2 dx
\]

\[
\frac{1}{648 (1 - c)^2} (b - c)^3 \left(\left(-3 + b^2 - 2 b c - 2 (-3 + c) c\right)^2 - \left(3 + (6 + b) b + 4 b c - 2 c^3\right)^2\right) p^2
\]

\[
\frac{1}{180 (1 - c)^2} (b - c)^3 \left(45 + 5 b^4 + 20 b^3 (-2 + c) + 6 b^2 (19 + 2 c (-9 + 2 c)) + 4 c (-15 + c (5 + (-2 + c) c)) - 4 b (30 + c (-33 + 2 c (3 + c)))\right) p^2
\]

\[
UE = \left(\left(3 - b^2 + 2 b c - 2 (3 - c) c\right)^3 + \left(3 - (6 - b) b + 4 b c - 2 c^2\right)^3\right) /
\left(\left(1 - b\right)^4 (1 - c) (1 - (-2 + b) b + 2 (-2 + c) c)^2\right) \left(\text{w0} - \text{y}\right)^2 +
\left(16 \left(45 + 5 b^4 + 20 b^3 (-2 + c) + 6 b^2 (19 + 2 c (-9 + 2 c)) + 4 c (-15 + c (6 + (-2 + c) c)) - 4 b (30 + c (-33 + 2 c (3 + c)))\right) \text{y}^2\right) /
\left(5 (b - c)^2 (-2 + b + c)^2 (-3 + 2 b + c)^2\right)
\]

**Surface Energy**

\[
\text{Clear}[\text{w0}, \text{w2}, b, c, y, p, F, x]
\]

\[
w2 = \text{w0} \left(2 (1 - b) (b - c) \left((1 + b - 2 c) (1 - c) - (3 - b - 2 c) (c - x)^2\right) + (1 - c) (b - x)^2 (b - 2 c + x)^2\right) /
\left((1 - c) (b + 2 (6 - c) + 6 b^2 c - 2 b^3 (1 + c) + c (-2 + c (6 - (4 - c) c)))\right);
\]

\[
\text{FullSimplify}[\int p (y - (\text{w0} - \text{w2})) dx]
\]

\[
\left(p x \left(-3 w0 x^4 + 75 c^4 (w0 - y) + 15 b^4 (-1 + c) y + 15 c^6 (-w0 + y) + 10 b^3 (-3 c w0 x + w0 x^2 + 3 c^2 (w0 - y) + 3 y) - 15 c^5 \left(w0 x^4 (-6 + x^2) + 8 y\right) + 3 c \left(w0 x^3 (-10 + x (5 + x)) + 10 y\right) + 10 c^4 \left(w0 (-9 + 2 (-3 + x) x) + 15 y\right) - 30 b^2 \left(w0 (3 c^2 - 3 c x + x^2) - 3 (-1 + c) c y\right) + 30 b \left(w0 x^2 + 3 c^4 (w0 - y) - y + c (-3 w0 x + 4 y)\right)\right) /
\left(15 (-1 + c) (b + b (2 - 6 c) + 6 b^2 c - 2 b^3 (1 + c) + c (-2 + c (6 + (-4 + c) c)))\right)\right]
\]

184
Clear[{b, c, y, w0, p}]

\[ T[x_] := \]
\[ \left( p x \left( -3 w0 x^4 + 75 c^4 (w0 - y) + 15 b^4 (-1 + c) y + 15 c^5 (-w0 + y) + 10 b^3 \left( -3 c w0 x + w0 x^2 + 3 c^2 (w0 - y) + 3 y \right) - 15 c^2 \left( w0 x - 6 x^2 + 8 y \right) + 3 c \left( w0 x^2 (-10 + x (5 + x)) + 10 y \right) + 10 c^3 \left( w0 (-9 + 2 (-3 + x) x) + 15 y \right) - 30 b^2 \left( w0 \left( 3 c^2 - 3 c x + x^2 \right) - 3 (-1 + c) c y + 30 b \left( w0 x^2 + 3 c^2 (w0 - y) - y + c (-3 w0 x + 4 y) \right) \right) \right) / \left( 15 (-1 + c) \left( b^3 + b (2 - 6 c) + 6 h b^2 c - 2 b^2 (1 + c) + c (-2 + c (6 + (-4 + c) c)) \right) \right) \right) \]

\[ US1 = 2 \text{FullSimplify}[T[h] - T[c]] \]

\[ 2 \left( -\left( (b - c)^2 \left( 30 + 10 b^2 + c (-27 + 7 c) + b (-33 + 13 c) \right) p w0 \right) / \left( 15 (-1 + c) \left( -2 - b^3 + b (-4 + c) c + b^2 (2 + c) + c (6 + (-4 + c) c) \right) \right) + (b - c) p y \right) \]

\[ US = \]
\[ 2 c y + 2 \]
\[ - \left( (b - c)^2 \left( 30 + 10 b^2 + c (27 - 7 c) - b (33 - 13 c) \right) \right) / \left( 15 (1 - c) \left( 2 + b^3 + b (4 - c) c - b^2 (2 + c) - c (6 - (4 - c) c) \right) p w0 + y \right) (b - c) \]

Energy balance to get the equilibrium state

Clear[{b, c, p, P, w0, x, y, UE, US, UT}]

\[ y = 1; \]

\[ p = 10; \]

\[ w0 = \frac{1}{24} \left( b^4 + b (2 - 6 c) + 6 h b^2 c - 2 b^2 (1 + c) + c (-2 + 6 c - 4 c^2 + c^3) \right) p; \]

\[ UE = \frac{1}{548} (b - c)^2 \left( \left( -3 + b^2 - 2 b c - 2 (-3 + c) c \right)^3 - \left( 3 + (-6 + b) b + 4 b b c - 2 c^2 \right)^3 \right) p^2 + \]

\[ \frac{1}{180} (b - c)^5 \left( 45 + 5 b^4 + 20 b^3 (-2 + c) + 6 b^2 (19 + 2 c (-9 + 2 c)) + 4 c (-15 + c (6 + (-2 + c) c)) - 4 b (30 + c (-33 + 2 c (3 + c))) \right) p^2; \]

\[ US = \]
\[ 2 c y + 2 \]
\[ - \left( (b - c)^2 \left( 30 + 10 b^2 - c (27 - 7 c) - b (33 - 13 c) \right) \right) / \left( 15 (1 - c) \left( 2 + b^3 + b (4 - c) c - b^2 (2 + c) - c (6 - (4 - c) c) \right) p w0 + y \right) (b - c); \]

\[ UT = UE - US; \]

\[ \text{Minimize}\{\{UT, 0 < b < 1, 0 < c < 0.9999, w0 == 0.2\}, \{b, c\}\} \]

\[ \{-0.106286, \{b \rightarrow 0.521807, c \rightarrow 0.111957\}\} \]
Appendix 3: Mathematica Program for Circular Punch Test Model under Pure Bending

Clear[w1, w2, b, c, r, p, F]

DSolve[
{w1''''[r] + \frac{2}{r} w1''''[r] - \frac{1}{r^2} w1''[r] + \frac{1}{r^3} w1'[r] == 0,

w2''''[r] + \frac{2}{r} w2''''[r] - \frac{1}{r^2} w2''[r] + \frac{1}{r^3} w2'[r] == 2 p, w2'[c] == 0, w1'[1] == 0,

w1[1] == 0, w1''[b] + \frac{1}{b} w1''[b] - \frac{1}{b^2} w1'[b] == \frac{F}{h}, w1[b] == w2[b], w1'[b] == w2'[b],

w1''[b] == w2''[b], w1'''[b] == w2'''[b]} , \{w1, w2\}, r]

Membrane profile within the cohesive zone

w2 = \frac{1}{32 (-1 + c^2)} \left(-4 F + 4 c^2 F + 3 b^4 p - 5 b^4 c^2 p + 2 c^4 p + 4 F r^2 - 4 c^2 F r^2 - 4 b^2 p r^2 + 2 b^4 p r^2 + 4 b^2 c^2 p r^2 - 2 c^4 p r^2 - p r^4 + c^2 p r^4 - 4 b^4 p \log[b] + 8 b^2 c^2 p \log[b] + 4 b^4 c^2 p \log[b] - 8 b^2 p r^2 \log[b] + 8 c^2 F \log[c] - 8 b^2 c^2 p \log[c] - 8 c^2 F r^2 \log[c] + 8 b^2 c^2 p r^2 \log[c] - 4 b^4 c^2 p \log[r] + 4 c^4 p \log[r] - 8 F r^2 \log[r] + 8 c^2 F r^2 \log[r] + 8 b^2 c^2 p r^2 \log[r] + 16 b^2 c^2 p \log[b] \log[r] + 16 c^2 F \log[c] \log[r] - 16 b^2 c^2 p \log[c] \log[r] \right)

Without the cohesive zone

w1 = \frac{1}{16 (-1 + c^2)} \left(-2 F + 2 c^2 F - b^4 p + c^4 p + 2 F r^2 - 2 c^2 F r^2 + b^4 p r^2 - c^4 p r^2 + 4 b^2 c^2 p \log[b] - 4 b^2 c^2 p r^2 \log[b] + 4 c^2 F \log[c] - 4 b^2 c^2 p \log[c] - 4 c^2 F r^2 \log[c] + 4 b^2 c^2 p \log[c] - 2 b^4 p \log[r] + 2 c^4 p \log[r] - 4 F r^2 \log[r] + 4 c^2 F r^2 \log[r] + 8 b^2 c^2 p \log[b] \log[r] + 8 c^2 F \log[c] \log[r] - 8 b^2 c^2 p \log[c] \log[r] \right)

Punch Displacement

w0 = \frac{1}{32 (1 - c^2)} \left(p \left(1 - c^2 \right) \left(4 b^2 - 3 b^4 - 4 c^2 + 3 c^4 + 2 b^4 \log[b^2] \right) + 2 c^2 \left(b^4 - c^2 - 2 b^2 \log[b^2] \right) \log[c^2] + 16 c^4 \log[c^2] \right)
Surface force range

\[ y = \frac{1}{32 \left( -1 + c^2 \right)^4} \]

\[ \left( \frac{b - c}{b + c} \left( 2b^2 - 5c^2 + 3c^4 + b^3 \left( -1 + c^2 \right) \right) - 16b^2 c^2 \log[b]^2 - \\ 4c^2 \log[c] \left( b^4 + (-3 + 2b^2) c^2 + 4c^2 \log[c] \right) + \\ 4 \log[b] \left( -c^4 + 2b^2 c^2 \left(-2 + c^2\right) + b^4 \left(2 + c^2\right) + 4c^2 \left(b^2 + c^2\right) \log[c] \right) \right) \]

Elastic energy

Clear[b, c, p, F, r, w1, w2]

\[ F = p \left( b^2 - c^2 \right) \]

\[ w1[x_] := \frac{1}{16 \left( -1 + c^2 \right)} \left( -2F + 2c^2 F - b^4 p + c^4 p + 2F x^2 - 2c^2 F x^2 + b^4 p \right) x^2 - c^4 p x^2 + \\ 4b^2 c^2 p \log[b] - 4b^2 c^2 p \log[b] + 4c^2 F \log[c] - 4b^2 c^2 p \log[c] - \\ 4c^2 F x^2 \log[c] + 4b^2 c^2 p \log[c] - 2b^4 p \log[x] + 2c^4 p \log[x] - 4F x^2 \log[x] + \\ 4c^2 F x^2 \log[x] + 8b^2 c^2 p \log[b] \log[x] + 8c^2 F \log[c] \log[x] - \\ 8b^2 c^2 p \log[c] \log[x] \right) ; \\

w2[x_] := \\
\frac{1}{32 \left( -1 + c^2 \right)} \left( -4F + 4c^2 F + 3b^4 p - 5b^4 c^2 p + 2c^4 p + 4F x^2 - 4c^2 F x^2 - 4b^2 p x^2 + \\ 2b^4 p x^2 + 4b^2 c^2 p x^2 - 2c^4 p x^2 - 4b^2 p \log[b] + 8b^2 c^2 p \log[b] + \\ 4b^4 c^2 p \log[b] - 8b^2 p x^2 \log[b] + 8c^2 F \log[c] - 8b^2 c^2 p \log[c] - \\ 8c^2 F x^2 \log[c] + 8b^2 c^2 p x^2 \log[c] - 4b^4 c^2 p \log[x] + 4c^4 p \log[x] - \\ 8F x^2 \log[x] + 8c^2 F x^2 \log[x] + 8b^2 p x^2 \log[x] - 8b^2 c^2 p x^2 \log[x] + \\ 16b^2 c^2 p \log[b] \log[x] + 16c^2 F \log[c] \log[x] - 16b^2 c^2 p \log[c] \log[x] \right) ; \\

\[ \text{UE1} = \int \left( \frac{1}{2} \left( w1'[x] \right)^2 + \frac{1}{r} w1'[x] \right) \, dx \\
\text{UE2} = \int \left( \frac{1}{2} \left( w2'[x] \right)^2 + \frac{1}{r} w2'[x] \right) \, dx \]
\[ \text{Surface Energy} \]

\[ \text{Clear}[h, c, p, F, r, y, \psi_0, \psi_2] \]

\[ \psi_2 = \left( \frac{4 b^2 (-1 + c^2) - r^4 + c^2 (-2 + r^2)^2 + 2 c^4 (-1 + r^2) + b^4 (3 - 5 c^2 + 2 r^2)}{8 c^4 \log[c] (-1 + r^2 - 2 \log[r]) + 4 c^2 (-b^4 + c^2 - 2 (-1 + c^2) r^2) \log[r] + 4 b^2 \log[b] \left( b^2 (-1 + c^2) + 2 (c - r) (c + r) + 4 c^2 \log[r] \right)} \right) / \left( (-1 + c^2) \left( 4 b^2 - 3 b^4 - 4 c^2 + 3 c^4 \right) - 16 c^4 \log[c] \right) + 2 c^2 (-b^4 + c^2) \log[c^2] + 2 b^2 \log[b^2] \left( b^2 (-1 + c^2) + 2 c^2 \log[c^2] \right) \right) \psi_0; \]

\[ \text{US} - \gamma c^2 + \int_0^p (y - (\psi_0 - \psi_2)) \, dx \]

\[ \text{FullSimplify}[\text{US}] \]
Energy balance to get the equilibrium state

Clear\[b, c, p, F, w0, r, γ, UE, US, UT\]

\[γ = 1;\]
\[y = \frac{1}{p};\]
\[p = 8;\]
\[w0 = \]
\[
\frac{1}{32 \left(1 - c^2\right)} \left\{ 4 \ b^2 - 3 \ b^4 - 4 \ c^2 + 3 \ c^4 + 2 \ b^4 \ \text{Log}[b^2] \right\} + 2 \ c^2 \left( b^4 - c^2 - 2 \ b^2 \ \text{Log}[b^2] \right) \ \text{Log}[c^2] + \
16 \ c^4 \ \text{Log}[c^2]^2;\]

\[UE = \]
\[
\frac{1}{64 \left(1 + c^2\right)^2} \ b^2 \left(3 \ b^2 - 2 \ c^2 + 4 \ c^4 \ \text{Log}[b] \right) \left( b^4 - c^2 - 4 \ c^4 \ \text{Log}[c] \right) - \
\frac{1}{192 \left(1 + c^2\right)^2} \ b^2 \left(3 \ b^2 + 3 \ b^4 - 2 \ c^2 - 2 + 3 \ c^4 \right) + \
3 \ b^2 \left(4 - 8 \ c^2 + 5 \ c^4 \right) - 6 \ b^4 \left( c^2 - 4 \ c^4 + 2 \ c^6 \right) + \
48 \ b^2 \left( b^4 + c^4 \left(1 + c^2\right)^2 + 2 \ c^2 \left(-3 + 2 \ c^2\right) \ \text{Log}[b] \right) + \
24 \ c^4 \ \text{Log}[c] \left( b^6 + c^2 - b^2 \ c^4 - b^4 \left(-1 + c^2\right) \ \text{Log}[c] \right) - \
24 \ b^2 \ \text{Log}[b] \left( b^6 + c^4 - c^6 + b^4 \left(-1 + c^2 + c^4\right) + b^2 \left( c^2 - 3 \ c^4 + c^6\right) + \
4 \ c^4 \left(-1 + b^2 - c^2 + c^4 \right) \ \text{Log}[c] \right);\]

\[US = \]
\[
\frac{1}{192 \left(1 + c^2\right)^2} \ b^2 \left(3 \ b^2 + 3 \ b^4 - 2 \ c^2 - 2 + 3 \ c^4 \right) + \
3 \ b^2 \left(4 - 8 \ c^2 + 5 \ c^4 \right) - 6 \ b^4 \left( c^2 - 4 \ c^4 + 2 \ c^6 \right) + \
48 \ b^2 \left( b^4 + c^4 \left(1 + c^2\right)^2 + 2 \ c^2 \left(-3 + 2 \ c^2\right) \ \text{Log}[b] \right) + \
24 \ c^4 \ \text{Log}[c] \left( b^6 + c^2 - b^2 \ c^4 - b^4 \left(-1 + c^2\right) \ \text{Log}[c] \right) - \
24 \ b^2 \ \text{Log}[b] \left( b^6 + c^4 - c^6 + b^4 \left(-1 + c^2 + c^4\right) + b^2 \left( c^2 - 3 \ c^4 + c^6\right) + \
4 \ c^4 \left(-1 + b^2 - c^2 + c^4 \right) \ \text{Log}[c] \right);\]

\[UT = UE - US;\]

Minimize\[\{UT, 0.6 < b < 0.9999, 0.05 < c < 0.3, w0 :: 0.137, \{b, c\}\}\]
Appendix 4: Mathematica Program for Rectangular Pressurized Blister Model under Pure Stretching

Clear[w, w0, w1, w2, p, f, b, s, c, x]

FullSimplify[
  DSolve[{-s^2 w1''[x] == f, -s^2 w2''[x] == (f - p), w2[c] == 0, w1'[b] == w2'[b],
            w1[b] == w2[b], w1'[0] == 0}, {w1, w2}, x]
]

{w1 -> Function[{x}, c^2 f - b^2 p + 2 b c p - c^2 p - f x^2],
  w2 -> Function[{x}, c^2 f + 2 b c p - c^2 p - 2 b p x - f x^2 + p x^2]}

Membrane Profile without cohesive zone

w1 = \frac{c^2 f - b^2 p + 2 b c p - c^2 p - f x^2}{2 s^2};

Within cohesive zone

w2 = \frac{c^2 f + 2 b c p - c^2 p - 2 b p x - f x^2 + p x^2}{2 s^2};

Membrane stress without cohesive zone

Clear[w, w0, w1, w2, p, f, b, s, c, x]

w1 = \frac{c^2 f - b^2 p + 2 b c p - c^2 p - f x^2}{2 s^2};

dw1dx = \partial_x w1;

\int dw1dx^2 dx

f^2 x^3

3 s^4

Clear[p, b, c, d, s, x, y1]

y1[x_] := \frac{f^2 x^3}{3 s^4};

FullSimplify[6 (y1[b] - y1[0])]

\frac{2 b^2 f^3}{s^4}

Solve[s^2 == \frac{2 b^2 f^3}{s^4}, s]

s1 = (2 b^2 f^2)^{1/6}

s1^2 = \frac{b^2 f}{2 (w0 - y)}
\[
\left( \frac{b^2 f}{2 (w_0 - y)} \right)^3 = 2 b^2 f^2
\]
\[
f = \frac{16 (w_0 - y)^3}{b^4}
\]
\[
s_1 = \left( 2 b^2 f^2 \right)^{1/6}
\]
Clear\[w, w_0, w_1, w_2, p, F, b, s_1, c, x, w_0, y]\]
\[
f = \frac{16 (w_0 - y)^3}{b^4};
\]
\[
s_1 = \left( 2 b^2 f^2 \right)^{1/6};
\]
\[
UE_1 = 2 \text{FullSimplify}\left[ \frac{(s_1)^4}{24} (b - 0) \right]
\]
\[
\frac{16}{3} \frac{b}{(w_0 - y)^{\frac{2}{3}}}
\]
\[
UE_1 = \frac{16 (w_0 - y)^4}{3 b^3}
\]

Membrane stress within the cohesive zone

Clear\[w, w_0, w_1, w_2, p, f, b, s, c, x]\]
\[
w_2 = \frac{c^2 f + 2 b c p - c^2 p - 2 b p x - f x^2 + p x^2}{2 s^2};
\]
\[
dw2dx = \partial_x w_2:
\]
\[
\int dw2dx^2 \partial x
\]
\[
\frac{(b p + (f - p) x)^2}{3 (f - p) s^4}
\]
Clear\[p, b, c, x, y_2]\]
\[
y_2[x_] := \frac{(b p + (f - p) x)^3}{3 (f - p) s^4};
\]
\[
\text{FullSimplify}\left[ \frac{6 (y_2[c] - y_2[b])}{(c - b)} \right]
\]
\[
\frac{2 \left( c^2 (f - p)^2 + b c (f - p) (f + 2 p) + b^2 \left( f^2 + f p + p^2 \right) \right)}{s^4}
\]
\[
\text{Solve}\left[ s^2 = 2 \left( c^2 (f - p)^2 + b c (f - p) (f + 2 p) + b^2 \left( f^2 + f p + p^2 \right) \right), s \right]
\]
\[
s_2 = \left( 2 \left( c^2 (f - p)^2 + b c (f - p) (f + 2 p) + b^2 \left( f^2 + f p + p^2 \right) \right) \right)^{1/6}
\]
\[
s_2^2 = \frac{c^2 f - b^2 p + 2 b c p - c^2 p - f b^2}{2 y}
\]
\[
\left( \frac{c^2 f - b^2 p + 2 b c p - c^2 p - f b^2}{2 y} \right)^3 = 2 \left( c^2 (f - p)^2 + b c (f - p) (f + 2 p) + b^2 \left( f^2 + f p + p^2 \right) \right)
\]
\[ p = \frac{16}{b} \frac{c}{(b - c)^4} y^6; \]

Clear[\(w, w0, w1, w2, p, f, b, s2, c, x, w0, y\)]
\[ f = \frac{p}{c} (c - b); \]

\[ p = \frac{16}{b} \frac{c}{(b - c)^4} y^3; \]

\[ s2 = \left(2 \left(\frac{c^2 (f - y)^2 + b c (f - y) (f + 2 y) + b^2 (f^2 + f y + y^2)}{b - c} \right) \right)^{1/6}; \]

\[ \text{UE2} = 2 \text{FullSimplify} \left[\frac{(s2)^4}{24} (c - b)\right] \]
\[ \frac{16}{3} (-b + c) \left(\frac{y^6}{(b - c)^6}\right)^{2/3} \]

\[ \text{UE2} = \frac{16}{3} \frac{y^4}{(c - b)^3} \]

Elastic energy
\[ \text{UE} = \frac{16}{3} \frac{(w0 - y)^4}{b^3} + \frac{16}{3} \frac{y^4}{(c - b)^3} \]

Surface Energy

Clear[\(w, w0, w1, w2, p, f, b, s, c, x, y\)]
\[ f = \frac{p}{c} (c - b); \]

\[ w2 = \frac{(c - x) (2 b p + (f - y) (c + x))}{c^2 f - (b - c)^2 y} \left(\frac{2 b^2 f^2}{2 \left(\frac{c^2 (f - y)^2 + b c (f - y) (f + 2 y) + b^2 (f^2 + f y + y^2)}{b - c} \right) \right)^{1/3} w0; \]

\[ \int p (w - w2) \, dx \]
\[ p \left(-c w0 x^f + \frac{w0 x^3}{3} + c^2 x (w0 - y) + b c x y\right) \]
\[ \frac{(b - c) c}{(b - c) c} \]

Clear[\(b, c, p, f, x, y, w0, T, d\)]
\[ T[x_] := \frac{p \left(-c w0 x^f + \frac{w0 x^3}{3} + c^2 x (w0 - y) + b c x y\right)}{(b - c) c}; \]

\[ 2 \text{FullSimplify}[[T[c] - T[b]]] \]
\[ \frac{2 (b - c) p (b w0 - c w0 + 3 c y)}{(b - c) p (b w0 - c w0 + 3 c y)} \]

\[ \text{US2} = -\frac{2 (b - c) p (b w0 - c w0 + 3 c y)}{3 c} \]

192
\[ \text{US}^2 = \frac{2}{3c} \left(- (c - b) p w_0 + 3c \gamma \right) \]

\[ \text{US} = \frac{2}{3c} \left(- (c - b)^2 p w_0 - 2 \gamma b \right) \]

**Energy balance to get the equilibrium state**

**Beginning state is the same as the standard pressurized blister without delamination**

\[
\text{Clear} \left[ w, w_0, w_1, w_2, p, f, b, s, c, x \right] \\
\text{FullSimplify} \left[ \text{DSolve} \left[ \left\{ -s^2 w''[x] = f, w[1] = 0, w'[0] = 0 \right\}, w, x \right] \right] \\
\left\{ \left[ w \rightarrow \text{Function} \left[ (x), \frac{f - f x^2}{2 s^2} \right] \right] \right\} \\
\]

\[ w_0 = \left( \frac{f}{16} \right)^{1/3} \]

\[
\text{Clear} \left[ w, w_0, y, w_2, p, f, b, s, c, r \right] \\
p = 0; \\
\text{Solve} \left[ 0.121 = \left( \frac{f + p}{16} \right)^{1/3}, f \right] \\
\left\{ \left[ f \rightarrow 0.028345 \right] \right\} \\
\]

**This is the delamination beginning state, but b keeps 1, c increases from 1**

\[
\text{Clear} \left[ b, c, p, f, w_0, y, x, y, s, \text{UE}, \text{US}, \text{UT} \right] \\
\gamma = 1; \\
b = 1; \\
p = 100; \\
f = \frac{p (c - b)}{c}; \\
y = \frac{\gamma}{p}; \\
s = \left( 2 b^2 f^2 \right)^{1/6}; \\
w_0 = \frac{c^2 f - b^2 p + 2 b c p - c^2 p}{2 s^2}; \\
\text{UE} = \frac{16}{3} \frac{(w_0 - \gamma)^4}{b^2} + \frac{16}{3} \frac{\gamma^4}{(c - b)^2}; \\
\text{US} = \frac{2}{3c} \left(- (c - b)^2 p w_0 - 2 \gamma b \right); \\
\text{UT} = \text{UE} - \text{US}; \\
\text{Minimize} \left[ \left\{ \text{UT}, 1 < c < 3, w_0 = 0.35 \right\}, c \right] \\
\left\{ 2.4231, \left[ c \rightarrow 1.01336 \right] \right\} \\
\]

193
The further state with delamination occuring and b increases from 1

Clear[{b, c, p, f, w0, y, r, γ, s, UE, US, UT}]

γ = 1;
p = 100;
f = \frac{p (c - b)}{c};
y = \frac{γ}{p};
s = \left(2 \cdot b^2 \cdot f^2\right)^{1/6};
\nu0 = \frac{c^2 \cdot f - b^2 \cdot p + 2 \cdot b \cdot c \cdot p - c^2 \cdot p}{2 \cdot s^2};
UE = \frac{16 \cdot (\nu0 - y)^4}{3 \cdot b^2} + \frac{16 \cdot y^4}{3 \cdot (c - b)^2};
US = -\frac{2 \cdot (c - b)^2}{3 \cdot c} \cdot p \cdot w0 - 2 \cdot γ \cdot b;
UT = UE - US;

Minimize[{\{UT, 1 < b < 4, 1 < c < 4, w0 = 1.0001\}, \{b, c\}}]

{4.46287, \{b -> 1.6962, c -> 1.72781\}}
Appendix 5: Mathematica Program for Rectangular Pressurized Blister Model under Pure Bending

Clear[w1, w2, b, c, x, p, f]
DSolve [{w1''''[x] == f, w2''''[x] == (-p), w2'[c] == 0, w2'[0] == 0, w1''''[b] == f b, 
  w1[b] == w2[b], w1'[b] == w2'[b], w1''[b] == w2''[b], w1'''[b] == w2'''[b], w1'[0] == 0}, 
  {w1, w2}, x]

Membrane Profile without cohesive zone

w1[x_] :=
  1/24 c (c^5 f + b^4 c p - 2 b^3 c^2 p + 2 b c^4 p -
  c^5 p - 2 c^3 f x^2 - 2 b^3 p x^4 + 6 b^4 c p x^4 - 6 b c^4 p x^4 + 2 c^3 p x^4 + c f x^4),

Within the cohesive zone

w2[x_] :=
  1/24 c (c^5 f - 2 b^3 c^2 p + 2 b c^4 p - c^5 p + 4 b^3 c p x - 2 c^3 f x^2 - 2 b^3 p x^4 - 6 b c^2 p x^2 +
  2 c^3 p x^2 + 4 b c p x^3 + c f x^4 - c p x^4);

Clear[b, c, p, f, x, w1, w2, w0]

f = p (c - b) / c;

w1[x_] :=
  1/24 c (c^5 f + b^4 c p - 2 b^3 c^2 p + 2 b c^4 p - c^5 p - 2 c^3 f x^2 - 2 b^3 p x^2 + 6 b^2 c p x^2 -
  6 b c^2 p x^2 + 2 c^3 p x^2 + c f x^4),

w2[x_] :=
  1/24 c (c^5 f - 2 b^3 c^2 p + 2 b c^4 p - c^5 p + 4 b^3 c p x - 2 c^3 f x^2 - 2 b^3 p x^2 - 6 b c^2 p x^2 +
  2 c^3 p x^2 + 4 b c p x^3 + c f x^4 - c p x^4);

w[x_] := Piecewise[{{w1[x], 0 <= x <= b}, {w2[x], b <= x <= c}}];

Simplify[Limit[w1[x], x -> 0]]
Simplify[w2[b]]
Simplify[w1[0] - w2[b]]
Central Displacement
\[ w_0 = \frac{1}{24} \left( b^3 - 2 b^2 c + c^3 \right) p \]

Surface force range
\[ y = \frac{b \left( c - b \right)^3 (3b + c) p}{24c} \]
\[ w_0 - y = \frac{b^3 \left( 3b^2 - 7bc + 4c^2 \right) p}{24c} \]

Elastic energy
Clear[{b, c, p, f, x, w1, w2}]

\[ w1[x_] := \frac{1}{24c} \left( c^5 f + b^4 c p - 2 b^3 c^2 p + 2 b c^4 p - c^5 p - 2 c^3 f x^2 - 2 b^3 p x^2 + 6 b^2 c p x^2 - 6 b c^2 p x^2 + 2 c^3 p x^2 + c f x^4 \right) \]

\[ w2[x_] := \frac{1}{24c} \left( c^5 f - 2 b^3 c^2 p + 2 b c^4 p - c^5 p + 4 b^3 c p x - 2 c^3 f x^2 - 2 b^3 p x^2 - 6 b^2 c p x^2 + 2 c^3 p x^2 + 4 b c p x^3 + c f x^4 - c f x^4 \right) \]

\[ UE1 = 2 \int_0^1 \frac{1}{2} \left( w1'[x]^2 \right) dx \]

\[ UE2 = 2 \int_0^1 \frac{1}{2} \left( w2'[x]^2 \right) dx \]

\[ UE1 = \frac{b \left( c^2 \left( 9b^4 - 10b^2c^2 + 5c^4 \right) f^2 - 10 \left( b - c \right)^4 c \left( b + c \right) f p + 5 \left( b - c \right)^6 b^2 \right)}{180c^2} \]

\[ UE2 = \frac{1}{180c^2} \left( c^2 \left( -9b^5 + 10b^3c^2 - 5bc^4 + 4c^5 \right) f^2 + (b - c)^5 c \left( 10b^3 + 3b^2c - bc^2 + 8c^3 \right) fp + (-b + c)^5 \left( 5b^2 + 4c^2 \right) f^2 \right) \]

Without the cohesive zone
Clear[{b, c, p, f, x, T1, T2}]

\[ D = \frac{24c}{b^2 \left( 3b^2 - 7bc + 4c^2 \right)} \left( w_0 - y \right) \]

\[ \text{FullSimplify} \left[ \frac{b \left( c^2 \left( 9b^4 - 10b^2c^2 + 5c^4 \right) f^2 - 10 \left( b - c \right)^4 c \left( b + c \right) f p + 5 \left( b - c \right)^6 b^2 \right)}{180c^2} \right] \]
\[ \frac{64 \left( 6b^4 - 10bc + 5c^4 \right) (w_0 - y)^2}{5b^2 \left( 3b^2 - 4c \right)^2} \]
\[ UE1 = \frac{64 \left( 6b^2 - 10bc + 5c^2 \right)}{5b^3 \left( 3b - 4c \right)^2} (w_0 - y)^2 \]
Within the cohesive zone

\[ D = \frac{24}{b} \frac{Y}{(c - b)^3 (3b + c)} \]

\[ \text{FullSimplify} \left[ -\frac{b^2 (b - c)^3 \left(6b^2 - 2bc + c^2\right)p^2}{45c^2} \right] \]

\[ -\frac{64}{5} \frac{\left(6b^2 - 2bc + c^2\right)Y^2}{(b - c)^3 (3b + c)^2} \]

\[ UE = \frac{64}{5} \frac{\left(6b^2 - 10bc + 5c^2\right)}{b^2 (3b - 4c)^2} (w_0 - y)^2 + \frac{64}{5} \frac{\left(6b^2 - 2bc + c^2\right)}{(b - c)^3 (3b + c)^2} Y^2 \]

Surface Energy

\[ \text{Clear}[b, c, p, f, x, y, T2] \]

\[ w_2 = \frac{(c - x)^2 \left(-2b^2 + c^2 + 2cx - x^2\right)}{c \left(b^2 - 2b^2c + c^2\right)} w_0; \]

\[ \text{FullSimplify} \left[ \int p (y - w_2) \, dx \right] \]

\[ \frac{1}{15c \left(b^2 - 2b^2c + c^2\right)} \left[ \frac{1}{15c \left(b^2 - 2b^2c + c^2\right)} \right] \]

\[ 3w_0 x^4 + 10b^2 \left(-3cw_0 x + w_0 x^2 + 3c^2 \left(w_0 - y\right)\right) + 15b^3c y + 15c^4 \left(-w_0 + y\right) \]

\[ \text{Clear}[b, c, p, f, x, y, w_0, T] \]

\[ T[x] := \frac{1}{15c \left(b^2 - 2b^2c + c^2\right)} \]

\[ p \left[ 20c^2 w_0 x^2 - 15cw_0 x^3 + 3w_0 x^4 + 10b^2 \left(-3cw_0 x + w_0 x^2 + 3c^2 \left(w_0 - y\right)\right) + 15b^3c y + 15c^4 \left(-w_0 + y\right) \right]; \]

\[ 2 \text{FullSimplify}[T[c] - T[b]] \]

\[ 2 \left( \frac{(b - c)^3 (13b + 7c)}{15c \left(-b^2 + bc + c^2\right)} \right) \]

\[ US = -2Yo + 2 \frac{(b - c)^3 (13b + 7c)}{15c \left(-b^2 + bc + c^2\right)} w_0 \]

197
Initially, no delamination occurs and the film just bulges up. It looks like a blister fixed at the periphery. \( b = c = 1 \)

```math
\begin{align*}
&\text{Clear[\( w1, w2, b, c, x, p, f \)]} \\
&\text{\( b = 1 \);} \\
&\text{\( DSolve[\{\{w1''[x] == f, w1[1] == 0, w1'[1] == 0, w1''[b] == f b, w1'[0] == 0\},\]
\{w1, x\}]} \\
&\quad \left\{\left\{w1 \to \text{Function[\((x), \frac{1}{24} \left(f - 2 f x^2 + f x^4\right)\)]}\right\}\right. \\
&\text{\( w[x_\_] := \frac{1}{24} f \left(1 - x^2\right)^2 \)} \\
&\text{\( w0 = \frac{1}{24} f \)}
\end{align*}
```

At a critical point, delamination begins to propagate, but cohesive edge keeps 1. \( b = 1, c > 1 \)

```math
\begin{align*}
&\text{Clear[\( b, c, p, f, w0 \)]} \\
&\text{\( b = 1 \);} \\
&\text{\( w0 = \frac{1}{24} b \left(b^3 - 2 b^2 c + c^3\right) p \)} \\
&\quad \frac{1}{24} \left(1 - 2 c + c^3\right) p \\
&\text{\( w0 = \frac{1}{24} \left(1 - 2 c + c^3\right) p \)}
\end{align*}
```

```math
\begin{align*}
&\text{Clear[\( b, c, p, f, w0, x, \gamma, UE, US, UT \)]} \\
&\text{\( \gamma = 1 \);} \\
&\text{\( b = 1 \);} \\
&\text{\( p = 100 \);} \\
&\text{\( w0 = \frac{1}{24} \left(1 - 2 c + c^3\right) p \);} \\
&\text{\( UE = \frac{b^2 \left(-2 b^4 + 6 b^3 c - 5 b^2 c^2 + c^4\right) p^2}{45 c} \);} \\
&\text{\( US = -2 \gamma b + 2 \frac{(b - c)^3 (13 b + 7 c)}{15 c \left(-b^2 + b c + c^2\right)} p w0 \);} \\
&\text{\( UT = UE - US \);} \\
&\text{\( \text{Minimize[\([UT, 0.2 < c < 2, w0 == 0.25\], c\]} \)} \\
&\text{\( \{2.69388, \{c \to 1.05181\}\} \)}
\end{align*}
```
Clear\[b, c, p, f, y\]
\[p = 100;\]
\[b = 1;\]
\[c = 1.0518084790658975;\]
\[f = \frac{p (c - b)}{c};\]
\[y = \frac{b (c - b)^3 (3 b + c) p}{24 c};\]
\[4.92566;\]
\[0.00223205;\]

The third stat is the general case with \(b > 1\) and \(c > 1\)

Energy balance to get the equilibrium state

Clear\[b, c, p, F, w0, r, χ, UE, US, UT\]
\[r = 1;\]
\[p = 10;\]
\[w0 = \frac{1}{24} b \left(b^3 - 2 b^2 c + c^3\right) p;\]
\[UE = \frac{b^2 \left(-2 b^4 + 6 b^3 c - 5 b^2 c^2 + c^4\right) p^2}{45 c};\]
\[US = -2 χ b + 2 \frac{(b - c)^3 (13 b + 7 c)}{15 c \left(-b^2 + b c + c^2\right)} p w0;\]
\[UT = UE - US;\]
\[\text{Minimize}\left[\{UT, 0.1 < b < 10, 0.2 < c < 10, w0 == 1\}, \{b, c\}\right]\]
\{5.11191, \{b \rightarrow 1.71976, c \rightarrow 2.02243\}\}

Clear\[b, c, p, f, y\]
\[p = 100;\]
\[b = 2.0477550841930823;\]
\[c = 2.0746411484853864;\]
\[f = \frac{p (c - b)}{c};\]
\[1.29594;\]
Appendix 6: Mathematica Program for Circular Pressurized Blister Model under Pure Stretching

Clear[\(w, w0, w1, w2, p, f, b, s, c, r\)]

FullSimplify[
  DSolve[
    \[-s^2 \left( \frac{\partial}{\partial r} \left( r \left( \frac{\partial}{\partial r} w1[r] \right) \right) \right) = 2 f, \quad -s^2 \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \left( \frac{\partial}{\partial r} w2[r] \right) \right) \right) = 2 \left( f - p \right), \quad w2[0] = 0, \quad w1'[0] = w2'[0], \quad w1[0] = w2[0] \], \{w1, w2, r\}]
]

\[\{\{w1 \to \text{Function}[\{r\}, \frac{c^2 f + b^2 p - c^2 p - f r^2 - 2 b^2 p \text{Log}[b] + 2 b^2 p \text{Log}[c]}{2 s^4}], \quad w2 \to \text{Function}[\{r\}, \frac{c^2 f - c^2 p - f r^2 + p r^2 + 2 b^2 p \text{Log}[c] - 2 b^2 p \text{Log}[c]}{2 s^4}]\}\]

Central displacement

\[w0 = \frac{c^2 f + b^2 p - c^2 p - 2 b^2 p \text{Log}[b] + 2 b^2 p \text{Log}[c]}{2 s^2}\]

Intersurface force range

\[Y = w1[0] = \frac{c^2 f + b^2 p - c^2 p - f b^2 - 2 b^2 p \text{Log}[b] + 2 b^2 p \text{Log}[c]}{2 s^2}\]

Without the cohesive zone

Clear[\(w, w0, w1, w2, p, f, b, s, c, r\)]

\[w1 = \frac{c^2 f + b^2 p - c^2 p - f r^2 - 2 b^2 p \text{Log}[b] + 2 b^2 p \text{Log}[c]}{2 s^2} ;\]

\[\text{dw1dr} = \frac{\partial}{\partial r} w1; \quad \int (\text{dw1dr})^2 r \, dr\]

\[\frac{f^2 r^4}{4 s^4}\]

Clear[\(p, b, c, d, s, r, y1\)]

\[y1[x_] := \frac{f^2 r^4}{4 s^4};\]

FullSimplify[\[6 (y1[b] - y1[0]) \right]\]

\[\frac{3 b^2 f^2}{2 s^4}\]

Solve[\[s^2 = \frac{3 b^2 f^2}{2 s^4}, s\]

\[s = \left( \frac{3 b^2 f^2}{2} \right)^{1/6}\]
\[ s_1^2 = \frac{b^2 f}{2 (w_0 - y)} \]

\[
\left( \frac{b^2 f}{2 (w_0 - y)} \right)^3 = \frac{3b^2 f^2}{2}
\]

\[ f = \frac{12(w_0 - y)^3}{b^4} \]

\[ s_1 = \left( \frac{3b^2 f^2}{2} \right)^{1/6} \]

Clear\[w, w_0, w_1, w_2, p, F, b, s_1, c, r, w_0, y\]

\[ f = \frac{12(w_0 - y)^3}{b^4} ; \]

\[ s_1 = \left( \frac{3b^2 f^2}{2} \right)^{1/6} ; \]

\[ \text{UE1 = FullSimplify}\left[ \frac{(s_1)^4}{24} (b^2 - 0^2) \right] \]

\[
\frac{3}{2} b^2 \left( \frac{(w_0 - y)^4}{b^4} \right)^{1/3} \]

\[ \text{UE1} = \frac{3}{2} b^2 (w_0 - y)^4 \]

**Within the cohesive zone**

Clear\[w, w_0, w_1, w_2, p, f, b, s, c, r\]

\[ w_2 = \frac{c^2 f - c^2 p - f r^2 + \frac{1}{4} (-f + p)^2 r^4 + b^4 p^2 \log[c] - 2b^2 p \log[r]}{2 s^2} ; \]

\[ \text{dw2dr = \partial_r w_2} ; \]

\[ \int \left( \text{dw2dr}^2 \right) r \, dr \]

\[
-\frac{b^2 p (-f + p) r^2 + \frac{1}{4} (-f + p)^2 r^4 + b^4 p^2 \log[r]}{s^4}
\]

Clear\[p, b, c, s, r, y_2\]

\[ y_2[x_] := \frac{-b^2 p (-f + p) r^2 + \frac{1}{4} (-f + p)^2 r^4 + b^4 p^2 \log[r]}{s^4} ; \]

\[ \text{FullSimplify} \left[ \frac{6(y_2[c] - y_2[b])}{(c^2 - b^2)} \right] \]

\[
3 \left( \left( b^2 - c^2 \right) (f - p) \left( c^2 (f - p) + b^2 (f + 3p) \right) + 4b^4 p^2 \left( \log[b] - \log[c] \right) \right) \]

\[
2 \left( b^2 - c^2 \right) s^4
\]

\[ \text{Solve} \left[ s^2 = \frac{3 \left( \left( b^2 - c^2 \right) (f - p) \left( c^2 (f - p) + b^2 (f + 3p) \right) + 4b^4 p^2 \left( \log[b] - \log[c] \right) \right)}{2 \left( b^2 - c^2 \right) s^4} \right] , \]

\[ s \]
\[
\begin{align*}
s_2 &= \left( \frac{3 \left( (c^2 - b^2) \left( f - p \right) + h^2 \left( f + 3 \ p \right) \right) + 2 h^4 p^2 \log \left[ \frac{c^2}{h^2} \right]}{2 \left( c^2 - b^2 \right)} \right)^{1/6} \\
s_2 &= \frac{c^2 f + h^2 p - c^2 p - f h^2 - 2 h^2 p \log [b] + 2 h^2 p \log [c]}{2 y} \\
&\left( \frac{c^2 f + h^2 p - c^2 p - f h^2 - 2 h^2 p \log [b] + 2 h^2 p \log [c]}{2 y} \right)^3 \\
&= \frac{3 \left( (c^2 - b^2) \left( f - p \right) (c^2 (f - p) + h^2 (f + 3 \ p)) + 2 h^4 p^2 \log \left[ \frac{c^2}{h^2} \right] \right)}{2 \left( c^2 - b^2 \right)} \\
p &= \frac{12}{h^2 \left( b^2 - c^2 \right)} \left( b^2 - c^2 - 2 \ \log b + 2 \ \log c \right) Y^3; \\
f &= \frac{p \left( c^2 - b^2 \right)}{c^2}; \\
p &= \frac{12}{h^2 \left( b^2 - c^2 \right)} \left( b^2 - c^2 - 2 \ \log b + 2 \ \log c \right) Y^3; \\
s_2 &= \left( \frac{3 \left( (c^2 - b^2) \left( f - p \right) (c^2 (f - p) + h^2 (f + 3 \ p)) + 2 h^4 p^2 \log \left[ \frac{c^2}{h^2} \right] \right)}{2 \left( c^2 - b^2 \right)} \right)^{1/6}; \\
UE_2 &= \text{FullSimplify} \left[ \frac{(s_2)^4}{24} \left( c^2 - b^2 \right) \right] \\
&= \frac{3}{2} \left( -b^2 + c^2 \right) \left( \frac{\left( b^4 - 4 b^2 c^2 + 3 \ c^4 - 2 \ c^4 \log \left[ \frac{c^2}{b^2} \right] \right)^3}{\left( b^2 - c^2 \right)^3 \left( b^2 - c^2 + 2 \ \log (- \log b + \log c) \right)} \right)^{2/3} \\
UE_2 &= \frac{3}{2} \left( b^4 - 4 b^2 c^2 + 3 \ c^4 - 2 \ c^4 \log \left[ \frac{c^2}{b^2} \right] \right)^2 Y^4 \\
\text{Elastic energy} \quad \text{UE} &= \frac{3}{2 h^2} \left( w_0 - y \right)^4 + \frac{3}{2} \left( b^4 - 4 b^2 c^2 + 3 \ c^4 - 2 \ c^4 \log \left[ \frac{c^2}{b^2} \right] \right)^2 \ \left( b^2 - c^2 + 2 \ \log \left[ \frac{c^2}{b^2} \right] \right)^4 Y^4
\end{align*}
\]
Surface Energy

Clear[w, w0, w1, w2, p, f, b, s, c, r, y]

\( f = \frac{p (c^2 - b^2)}{c^2} \);

\( w2 = \frac{c^2 f - c^2 p - f x^2 + p x^2 + 2 b^2 p \Log[c] - 2 b^2 p \Log[r]}{c^2 f + b^2 p - c^2 p - 2 b^2 p \Log[b] + 2 b^2 p \Log[c]} \)

\[ 1^{1/3} \begin{pmatrix} \frac{3 b^2 c^2}{2} \\ \frac{1}{2} (c^2 - b^2) (\Log[p] - \Log[b]) + \frac{1}{2} (c^2 - b^2) (\Log[p] - \Log[c]) \end{pmatrix} \]

\( w0; \)

\( \int_{0}^{\infty} p (y - w2) 2 x \, dx \)

\( US = -c^2 y + \)

\[ \frac{1}{4} - \frac{b^4 w0}{c^2 (\Log[b] - \Log[c])} \left( \frac{(b^2 - c^2)^3}{b^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 - 2 c^4 \Log\left[ \frac{c^2}{b^2} \right] \right)} \right)^{1/3} \]

\[ + 4 b^2 \left( y - w0 \left( \frac{(b^2 - c^2)^3}{b^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 - 2 c^4 \Log\left[ \frac{c^2}{b^2} \right] \right)} \right)^{1/3} \right) \]

\[ + c^2 \left( y + \frac{w0}{\Log[b] - \Log[c]} \left( \frac{(b^2 - c^2)^3}{b^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 - 2 c^4 \Log\left[ \frac{c^2}{b^2} \right] \right)} \right)^{1/3} \right) \]
\[ US = \left( \frac{(b^2 - c^2)^3}{b^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 - 2 c^4 \log \left( \frac{c^2}{b^2} \right) \right)} \right)^{1/3} = \frac{h^4}{2 c^2 \log \left( \frac{c^2}{b^2} \right)} - p w0 + b^2 y + \]

\[ \frac{b^2}{h^2} \left( \frac{(b^2 - c^2)^3}{b^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 - 2 c^4 \log \left( \frac{c^2}{b^2} \right) \right)} \right)^{1/3} = p w0 + c^2 y - \]

\[ \left( \frac{(b^2 - c^2)^3}{b^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 - 2 c^4 \log \left( \frac{c^2}{b^2} \right) \right)} \right)^{1/3} = \frac{c^2}{2 \log \left( \frac{c^2}{b^2} \right)} p w0 \]

\[ US = \left( \frac{(c^2 - h^2)^3}{h^2 \left( -h^4 + 4 h^2 c^2 - 3 c^4 + 2 c^4 \log \left( \frac{c^2}{b^2} \right) \right)} \right)^{1/3} = \frac{b^2}{2 c^2 \log \left( \frac{c^2}{b^2} \right)} - \frac{(c^4 - h^4)}{p w0 - y h^2} \]

**Energy balance to get the equilibrium state**

**Beginning state is the same as the constrained blister under the pressure**

```
Clear[w, w0, w1, w2, p, f, b, s, c, r]

FullSimplify[DSolve[{-s^2 \[PartialD][w[r], r] (r \[PartialD][w[r], r])} == 2 (f), w[0] == 0, w'[0] == 0}, w, r]]

{\{w \[RightArrow] Function[r, \(f - f \frac{r^2}{2 s^2}\)]\}}

w0 = \(f \frac{1}{12}\)^{1/3}
```

```
Clear[w, w0, y, w2, p, f, b, s, c, r]

p = 0;

Solve[0.1 == (\(f + b\) \(\frac{1}{12}\))^{1/3}, f]

{(f \[Rule] 0.012)}
```

204
This is the delamination beginning state, but b keeps 1, c increases from 1

Clear[{h, c, p, f, w0, y, r, y, s, UE, US, UT}]

γ = 1;

b = 1;

\[ p = 100; \]

\[ f = \frac{p \left( c^2 - b^2 \right)}{c^2}; \]

\[ y = \frac{\gamma}{p}; \]

\[ w_0 = \frac{h^2 \, \rho \, \log\left[ \frac{c^2}{y^2} \right]}{2^{2/3} \, 3^{1/3} \, \left( \frac{b^2 \left( b^2 - 2 \right)^2 \, y^2}{3^2} \right)^{1/3}}; \]

\[ UE = \frac{3}{2} \, \frac{h^2 \, (w_0 - y)^4}{2} + 3 \, \frac{b^4 - 4 \, b^2 \, c^2 + 3 \, c^4 - 2 \, c^4 \, \log\left[ \frac{c^2}{b^2} \right]}{2 \left( c^2 - b^2 \right) \left( b^2 - c^2 + c^2 \, \log\left[ \frac{c^2}{b^2} \right] \right)^2} \, y^4; \]

\[ US = \frac{\left( c^2 - b^2 \right)^3}{2 \, b^2 \left( b^4 - 4 \, b^2 \, c^2 - 3 \, c^4 + 2 \, c^4 \, \log\left[ \frac{c^2}{b^2} \right] \right)^{1/3}} \left( \frac{b^2 - \left( c^4 - b^4 \right)}{2 \, c^2 \, \log\left[ \frac{c^2}{b^2} \right]} \right) \, p \, w_0 - y \, b^2; \]

\[ UT = UE - US; \]

Minimize[{UT, 1 < c < 3, w0 == 0.15}, c]

\{1608.18, {c -> 1.0002} \}

\[ p = 100; \]

\[ b = 1; \]

\[ c = 1.0002024305501642; \]

\[ \frac{p \left( c^2 - b^2 \right)}{c^2} \]

\[ 0.0404754 \]
Further delamination makes $b$ larger than 1

Clear [$h, c, p, f, w_0, y, r, \gamma, s, UE, US, UT$]

$\gamma = 1$;
$p = 100000; 
\begin{align*}
   f &= \frac{p (c^2 - h^2)}{c^2}; \\
   y &= \frac{c}{p}; \\
   s &= \left(\frac{3 \ h^2 \ f^2}{2}\right)^{1/6}; \\
   w_0 &= \frac{h^2 \ p \ \text{Log} \left[ \frac{c^2}{b^2} \right]}{2^{2/3} \ 3^{1/3} \ \left( \frac{b^2 (b^2 - 2 c^2)^{2/3}}{c^4} \right)^{1/3}}; \\
   UE &= \frac{3}{2 \ h^2} \ (w_0 - y)^4 + \frac{3}{2} \ \left( \frac{b^4 - 4 \ h^2 \ c^2 + 3 \ c^4 - 2 \ c^4 \ \text{Log} \left[ \frac{c^2}{b^2} \right]}{c^2 - h^2} \right)^2 \ \left( h^2 - c^2 + \frac{c^2 \ \text{Log} \left[ \frac{c^2}{b^2} \right]}{c^2} \right)^4 - y^4; \\
   US &= \left( \frac{(c^2 - h^2)^3}{h^2 \left[ b^4 + 4 \ h^2 \ c^2 - 3 \ c^4 + 2 c^4 \ \text{Log} \left[ \frac{c^2}{b^2} \right] \right]} \right)^{1/3} \ \left( h^2 - \frac{(c^4 - h^4)}{2 c^2 \ \text{Log} \left[ \frac{c^2}{b^2} \right]} \right) \ p \ w_0 - y \ h^2; \\
   UT &= UE - US; \\
   \text{Minimize} \{(UT, 1 < b < 1.05, 1 < c < 1.1, w_0 = 1.2), \ (b, c)\} \\
   (3.92436, (b \to 1.05, c \to 1.05009))
\end{align*}
Appendix 7: Mathematica Program for Circular Pressurized Blister Model under Pure Bending

Clear[w1, w2, b, c, r, p, f]

DSolve[
{w1''''''[r] + \frac{2}{r} w1''''[r] - \frac{1}{r^2} w1''''[r] + \frac{1}{r^3} w1'[r] == 2 f,
    w2''''''[r] + \frac{2}{r} w2''''[r] - \frac{1}{r^2} w2''''[r] + \frac{1}{r^3} w2'[r] == 2 (f - p),
    w2[c] == 0,
    w1''''''[b] + \frac{1}{b} w1''''[b] - \frac{1}{b^2} w1'[b] == f b, w1[b] == w2[b],
    w1''[b] == w2''[b], w1''''[b] == w2''''[b], w1''''''[b] == w2''''''[b], w1'[0] == 0},
{w1, w2}, r
]

\{(w1 \rightarrow \text{Function}[r, \frac{1}{32 c^2} (6 f - 3 b^4 c^2 p + 4 b^2 c^4 p - c^6 p - 2 c^4 f r^2 - 2 b^4 p r^2 + 2 c^4 p r^2 + c^6 f r^4 + 4 b^4 c^2 p \log[b] + 8 b^2 c^4 p r^2 \log[b] - 4 b^4 c^2 p \log[c] - 8 b^2 c^4 p r^2 \log[c])],
    (w2 \rightarrow \text{Function}[r, \frac{1}{32 c^2} (6 f + 2 b^4 c^2 p + 4 b^2 c^4 p - c^6 p - 2 c^4 f r^2 - 2 b^4 p r^2 - 2 c^4 p r^2 + c^6 f r^4 - 4 b^4 c^2 p \log[c] - 8 b^2 c^4 p r^2 \log[c] + 4 b^4 c^2 p \log[r] + 8 b^2 c^2 p r^2 \log[r]))\}

Membrane Profile without cohesive zone

w1 = \frac{1}{32 c^2} (6 f - 3 b^4 c^2 p + 4 b^2 c^4 p - c^6 p - 2 c^4 f r^2 - 2 b^4 p r^2 + 2 c^4 p r^2 + c^6 f r^4 + 4 b^4 c^2 p \log[b] + 8 b^2 c^4 p r^2 \log[b] - 4 b^4 c^2 p \log[c] - 8 b^2 c^2 p r^2 \log[c]);

Within cohesive zone

w2 = \frac{1}{32 c^2} (6 f + 2 b^4 c^2 p + 4 b^2 c^4 p - c^6 p - 2 c^4 f r^2 - 2 b^4 p r^2 - 4 b^2 c^2 p r^2 + 2 c^4 p r^2 + c^6 f r^4 - c^2 p r^4 - 4 b^4 c^2 p \log[c] - 8 b^2 c^2 p r^2 \log[c] + 4 b^4 c^2 p \log[r] + 8 b^2 c^2 p r^2 \log[r]);
Central Displacement

\[ w_0 = \frac{1}{32} \left( c^4 f - 3 b^4 p + 4 b^2 c^2 p - c^4 p + 4 b^4 p \Log[b] - 4 b^4 p \Log[c] \right) \]

\[ = \frac{1}{32} b^2 p \left( -3 b^2 + 3 c^2 - 4 b^2 \Log\left[ \frac{c}{b} \right] \right) \]

Surface force range

\[ y = -\frac{\left( b^2 - c^2 \right) \left( -b^2 c^2 \left( f - 5 p \right) + c^4 \left( f - p \right) + 2 b^4 p \right) - 12 b^4 c^2 p \Log[b] + 12 b^4 c^2 p \Log[c]}{32 c^2} \]

\[ = \frac{3 b^2 p \left( -b^4 + c^4 - 4 b^2 c^2 \Log\left[ \frac{c}{b} \right] \right)}{32 c^2} \]

\[ w_0 - y = \frac{b^2 \left( -b^2 c^2 f + 2 c^4 f - 2 b^4 p - 2 c^4 p - 8 b^2 c^2 p \Log[b] + 8 b^2 c^2 p \Log[c] \right)}{32 c^2} \]

\[ = \frac{b^4 p \left( 3 b^2 - 3 c^2 + 8 c^2 \Log\left[ \frac{c}{b} \right] \right)}{32 c^2} \]

Elastic energy

Clear[{b, c, p, f, r, w1, w2}]

\[ w1[x] := \frac{1}{32 c^2} \left( c^6 f - 3 b^4 c^2 p + 4 b^2 c^4 p - c^6 p - 2 c^4 f x^2 - 2 b^4 p x^2 + 2 c^4 p x^2 + c^2 f x^4 + 4 b^4 c^2 p \Log[b] + 8 b^2 c^2 p x^2 \Log[b] - 4 b^4 c^2 p \Log[c] - 8 b^2 c^2 p x^2 \Log[c] \right); \]

\[ w2[x] := \frac{1}{32 c^2} \left( c^6 f + 2 b^4 c^2 p + 4 b^2 c^4 p - c^6 p - 2 c^4 f x^2 - 2 b^4 p x^2 - 4 b^2 c^2 p x^2 + 2 c^4 p x^2 + c^2 f x^4 - c^2 p x^4 - 4 b^4 c^2 p \Log[c] - 8 b^2 c^2 p x^2 \Log[c] + 4 b^4 c^2 p \Log[x] + 8 b^2 c^2 p x^2 \Log[x] \right); \]

\[ UE1 = \int_0^\infty \left( \frac{1}{2} \left( w1''[x] - \frac{1}{r} \Log[r] \right) \right)^2 r \, dr \]

\[ UE2 = \int_0^\infty \left( \frac{1}{2} \left( w2''[x] - \frac{1}{r} \Log[r] \right) \right)^2 r \, dr \]
Clear\[b, c, p, f, r, UE1, UE2, UE\]
\[f = \frac{p \left(c^2 - b^2\right)}{c^2};\]

\[UE1 = \frac{1}{32 c^4} \left(\frac{2}{3} b^6 c^4 f^2 - b^4 c^2 f \left(c^4 (f - p) + b^4 p + 4 b^2 c^2 p \left(-\log[b] + \log[c]\right)\right) + \frac{1}{2} b^2 \left(c^4 (f - p) + b^4 p + 4 b^2 c^2 p \left(-\log[b] + \log[c]\right)\right)^2\right);\]

\[UE2 = \frac{1}{192 c^4} \left(-b^2 - c^2\right) \left(-2 b^2 c^6 (f - p) (f - p) + c^8 (f - p)^2 + 3 b^8 p^2 + 6 b^6 c^2 p (-f + p) + 2 b^4 c^4 \left(2 p^2 - f p + 5 p^2\right)\right) \cdot 24 b^4 c^2 p \left(\log[b] - \log[c]\right) \left(c^4 (f - p) + b^4 p + b^2 c^2 (-f + p) + 2 b^2 c^2 p \left(-\log[b] + \log[c]\right)\right)\];

FullSimplify\[UE1 + UE2\]
\[\frac{b^4 p^4 \left(-5 b^4 - 2 b^4 c^2 + 7 c^4 + 24 b^4 c^2 \left(\log[b] - \log[c]\right)\right)}{192 c^2}\]

**Surface Energy**

Clear\[b, c, p, f, r, y, w0, w2\]
\[w2 = \frac{\left(c^2 - r^2\right) \left(2 b^2 + 3 c^2 + r^2\right) - 4 c^2 \left(b^2 + 2 r^2\right) \log\left[\frac{c}{r}\right]}{c^2 \left(-3 b^2 + 3 c^2 - 4 b^2 \log\left[\frac{c}{b}\right]\right)};\]

\[US = -\gamma c^2 + \int_c^r p \left(y - w2\right) 2 r \, dr\]

FullSimplify\[US\]
\[US = -\gamma b^2 + \left\{2 b^2 + \frac{2 \left(2 b^6 - 6 b^4 c^2 + 3 b^2 c^4 + c^6\right)}{3 c^2 \left(3 (b - c) (b + c) + 4 b^2 \log\left[\frac{c}{b}\right]\right)}\right\} p \, w0\]
Initially, no delamination occurs and the film just bulges up. It looks like a blister fixed at the periphery. \( b = c = 1 \)

Clear\([w1, w2, b, c, r, p, f] \)
\( b = 1; \)
\( DSolve \left[ \left( \frac{\text{w1['''[r]} + \frac{2}{r} \text{w1''[r]} - \frac{1}{r^2} \text{w1''''[r]} + \frac{1}{r^3} \text{w1'''[r]}}{2} = f, \text{w1[1]} = 0, \text{w1'[1]} = 0, \text{w1''[b]} + \frac{1}{b} \text{w1'''[b]} - \frac{1}{b^2} \text{w1''[b]} = f b, \text{w1'[0]} = 0 \right), \text{w1, r} \right] \)
\( \{ \text{w1} \rightarrow \text{Function} \left[ \{r\}, \frac{1}{32} \left( f - 2 f r^2 + f r^4 \right) \right] \} \)
\( w[r_] := \frac{1}{32} f \left( 1 - r^2 \right)^2 \)
\( w_0 = \frac{1}{32} f \)

At a critical point, delamination begins to propagate, but cohesive edge keeps 1. \( b = 1, c > 1 \)

Clear\([b, c, p, f, w_0] \)
\( b = 1; \)
\( w_0 = \frac{1}{32} b^2 p \left( -3 b^2 + 3 c^2 + 4 b^2 \log \left[ \frac{C}{b} \right] \right) \)
\( \frac{1}{32} p \left( -3 + 3 c^2 - 4 \log [c] \right) \)
\( w_0 = \frac{1}{32} p \left( 3 c^2 - 3 - 4 \log [c] \right) \)

Clear\([b, c, p, F, w_0, r, \gamma, \text{UE, US, UT}] \)
\( \gamma = 1; \)
\( b = 1; \)
\( p = 20; \)
\( w_0 = \frac{1}{32} b^2 p \left( -3 b^4 + 3 c^2 - 4 b^2 \log \left[ \frac{C}{b} \right] \right); \)
\( \text{UE} = \frac{b^4 p^2 \left( 5 b^4 - 2 b^2 c^2 + 7 c^4 - 24 b^2 c^2 \log \left[ \frac{C}{b} \right] \right)}{192 c^2} ; \)
\( \text{US} = -\gamma b^2 + \left( 2 b^2 + \frac{2 \left( 2 b^6 - 6 b^4 c^2 + 3 b^2 c^4 + c^6 \right)}{3 c^2 \left( 3 \left( b - c \right) \left( b + c \right) + 4 b^2 \log \left[ \frac{C}{b} \right] \right)} \right) p w_0; \)
\( \text{UT} = \text{UE} - \text{US}; \)
\( \text{Minimize} \left[ \{ \text{UT}, 0.2 < c < 10, w_0 = 0.15 \}, c \right] \)
\{1.10349, \{c \rightarrow 1.09703\} \}
Clear[b, c, p, f, y]

p = 20;
b = 1;
c = 1.060479064474932;
f = \frac{p (c^2 - b^2)}{c^2}

y = \frac{3 b^2 p (-b^4 + c^4 - 4 b^2 c^2 \log\left[\frac{2}{b}\right])}{32 c^2}
2.48148
0.00145429

The third stat is the general case with b > 1 and c > 1

Energy balance to get the equilibrium state
Clear[b, c, p, f, w0, r, x, u0, us, ut]

\chi = 1;
p = 50;
w0 = \frac{1}{32} b^2 p \left(-3 b^2 + c^2 - 4 b^2 \log\left[\frac{b}{b}\right]\right);
ue = \frac{b^4 p^2 (-5 b^4 - 2 b^2 c^4 + 7 c^4 - 24 b^2 c^2 \log\left[\frac{c}{b}\right])}{192 c^2} 

us = -\chi b^2 + \frac{2 \left(2 b^6 - 6 b^4 c^2 + 3 b^2 c^4 + c^6\right)}{3 c^2 \left(3 (b - c) (b + c) + 4 b^2 \log\left[\frac{c}{b}\right]\right)} p \ w0;

ut = ue - us;

Minimize[{ut, 0.1 < b < 10, 0.2 < c < 10, w0 == 1.5}, {b, c}]

{6.67815, {b -> 1.76578, c -> 1.84433}}

Clear[b, c, p, f, x]
p = 50;
b = 1.765781266832909;
c = 1.8443291091973981;
f = \frac{p (c^2 - b^2)}{c^2}
4.16819
Appendix 8: Mathematica Program for Circular Constrained Blister Model under Pure Stretching

Clear[w, w0, w1, w2, p, f, b, s, c, r]

FullSimplify[
    DSolve[
        \(-s^2 \left( \frac{1}{r} \partial_r r \partial_r w1[r] \right) \right) \rightarrow 2 f, -s^2 \left( \frac{1}{r} \partial_r r \partial_r w2[r] \right) \right) \rightarrow 2 \left( f + p \right), w1[1] \rightarrow 0,
        w1'[b] == w2'[b], w1[b] == w2[b], w2'[c] == 0, \{w1, w2, r\}]]

\[ \{\{w1 \rightarrow \text{Function}\left[r, \frac{\frac{f - fr^2}{2} + 2 c^2 f \log[r] - 2 b^2 p \log[r] + 2 c^2 p \log[r]}{2 s^2}\right],
    w2 \rightarrow \text{Function}\left[r, \frac{\frac{f + b^2 p - fr^2 - pr^2}{2} + 2 b^2 p \log[b] + 2 c^2 f \log[r] + 2 c^2 p \log[r]}{2 s^2}\right]\}\}\]

**Membrane profile without cohesive zone**

\[ w1 = \frac{f - fr^2 + 2 c^2 f \log[r] - 2 b^2 p \log[r] + 2 c^2 p \log[r]}{2 s^2}; \]

**Within cohesive zone**

\[ w2 = \frac{f + b^2 p - fr^2 - pr^2 - 2 b^2 p \log[b] + 2 c^2 f \log[r] + 2 c^2 p \log[r]}{2 s^2}; \]

**Blister height**

\[ w0 = \frac{f + b^2 p - fc^2 - pc^2 - 2 b^2 p \log[b] + 2 c^2 f \log[c] + 2 c^2 p \log[c]}{2 s^2}; \]

**Without the cohesive zone**

Clear[w, w0, w1, w2, p, f, b, s, c, r]

\[ w1 = \frac{f - fr^2 + 2 c^2 f \log[r] - 2 b^2 p \log[r] + 2 c^2 p \log[r]}{2 s^2}; \]

\[ dwdr = \partial_r w1; \]

\[ \int (dwdr^2) \, r \, dr \]

\[-f \left( c^2 f - b^4 p + c^2 p \right) \frac{r^4}{4} + \left( c^4 f^2 - 2 b^4 c^2 f + 2 c^4 f p + 2 b^4 p^2 + 2 b^2 c^2 p i + c^4 p f \right) \log[r] \]

\[ s^4 \]
\[ y_1[x_] := \frac{1}{s^4} \left( -f (c^2 f - b^2 p + c^2 p) x^2 + \frac{f^2 x^4}{4} + \left( c^2 f^2 - 2 b^2 c^2 f p + 2 c^4 f p + b^4 p^2 - 2 b^2 c^2 p^2 + c^4 p^2 \right) \log[x] \right); \]

\[ \text{FullSimplify}\left[ \frac{6 (y_1[1] - y_1[0])}{(1^2 - b^2)} \right] \]

\[
\frac{3 \left( -1 + b^2 \right) f \left( \left( 1 + b^2 - 4 c^2 \right) f + 4 \left( b^2 - c^2 \right) p \right) + 4 \left( b^2 p - c^2 \left( f + p \right) \right)^2 \log[b]}{2 \left( -1 + b^2 \right) s^4}
\]

\[ \text{Solve}\left[ s^2 = \frac{3 \left( -1 + b^2 \right) f \left( \left( 1 + b^2 - 4 c^2 \right) f + 4 \left( b^2 - c^2 \right) p \right) + 4 \left( b^2 p - c^2 \left( f + p \right) \right)^2 \log[b]}{2 \left( -1 + b^2 \right) s^4}, s \right] \]

\[ s_1 = \left( \frac{3 \left( 1 - b^2 \right) f \left( \left( 1 + b^2 - 4 c^2 \right) f + 4 \left( b^2 - c^2 \right) p \right) - 4 \left( b^2 p - c^2 \left( f + p \right) \right)^2 \log[b]}{2 \left( 1 - b^2 \right)} \right)^{1/6} \]

**Within the cohesive zone**

\[ w_2 = \frac{f + b^2 p - f r^2 - p r^2 - 2 b^2 p \log[h] + 2 c^2 f \log[r] + 2 c^2 p \log[p]}{2 s^2}; \]

\[ \frac{\partial w_2}{\partial x} = \int (\partial w_2/\partial x) \, \text{d}x \]

\[
\left( f + p \right)^2 \left( -c^2 x^2 + \frac{x^4}{4} + c^4 \log[r] \right)
\]

\[ \text{Solve}\left[ s^2 = \frac{3 \left( f + p \right)^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 \log[h] - \log[c] \right)}{2 \left( b^2 - c^2 \right) s^4}, s \right] \]

\[ s_2 = \left( \frac{3 \left( f + p \right)^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 \log[h] - \log[c] \right)}{2 \left( b^2 - c^2 \right)} \right)^{1/6} \]
Clear[w, w0, w1, w2, p, f, b, s, c, r]

\[ s = \left( \frac{3 (f + p)^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\text{Log}[b] - \text{Log}[c]) \right)}{2 (b^2 - c^2)} \right)^{1/6} ; \]

\[ w2[x_] := \frac{f + b^2 p - f x^2 - p x^2 - 2 b^2 p \text{Log}[b] + 2 c^2 f \text{Log}[x] + 2 c^2 p \text{Log}[x]}{2 s^2} ; \]

FullSimplify[w2[c]]

FullSimplify[w2[c] - w2[b]]

\[ f - c^2 f + (b^2 - c^2) p - 2 b^2 p \text{Log}[b] + 2 c^2 (f + p) \text{Log}[c] \]

\[ 2^{1/3} \cdot \frac{3^{1/3}}{\left( \left( f + p \right)^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\text{Log}[b] - \text{Log}[c]) \right) \right)^{1/3}} \]

\[ (f + p) \left( b^2 - c^2 + 2 c^2 (\text{Log}[b] + \text{Log}[c]) \right) \]

\[ 2^{1/3} \cdot \frac{3^{1/3}}{\left( \left( f + p \right)^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\text{Log}[b] - \text{Log}[c]) \right) \right)^{1/3}} \]

\[ w0 = \frac{f - c^2 f + (b^2 - c^2) p - 2 b^2 p \text{Log}[b] + 2 c^2 (f + p) \text{Log}[c]}{2^{1/3} \cdot \frac{3^{1/3}}{\left( \left( f + p \right)^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\text{Log}[b] - \text{Log}[c]) \right) \right)^{1/3}}} \]

\[ w0 = \left( \frac{b^2 - c^2}{12 \left( f + p \right)^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\text{Log}[b] - \text{Log}[c]) \right)} \right)^{1/3} \]

\[ (f - c^2 f + (b^2 - c^2) p - 2 b^2 p \text{Log}[b] + 2 c^2 (f + p) \text{Log}[c]) \]

\[ \frac{\left( f + p \right) \left( b^2 - c^2 + 2 c^2 (\text{Log}[b] + \text{Log}[c]) \right)}{2^{1/3} \cdot \frac{3^{1/3}}{\left( \left( f + p \right)^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\text{Log}[b] - \text{Log}[c]) \right) \right)^{1/3}}} \]

\[ y = \left( \frac{b^2 - c^2}{12 \left( f + p \right)^2 \left( b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\text{Log}[b] - \text{Log}[c]) \right)} \right)^{1/3} \]

\[ (f + p) \left( b^2 - c^2 + 2 c^2 (\text{Log}[b] + \text{Log}[c]) \right) \]
Solve the cohesive zone radius and contact radius

Clear[w, w0, w1, w2, p, f, b, s, c, r]

\( \chi = 0.8 \);

\( p = 100 \);

\( f = 1.5633 \);

\[
Y = \left( \frac{b^2 - c^2}{12 (f + p)^2 \left[ b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\log(b) - \log(c)) \right]} \right)^{1/3} (f + p) \left( b^2 - c^2 + 2 c^2 (-\log(b) + \log(c)) \right);
\]

\[
w0 = \left( \frac{b^2 - c^2}{12 (1 + p)^2 \left[ b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\log(b) - \log(c)) \right]} \right)^{1/3} \left( f - c^2 f + \left( b^2 - c^2 \right) p - 2 b^2 p \log(b) + 2 c^2 (f + p) \log(c) \right);
\]

FindRoot[{Y == Y, w0 == 0.8}, {b, 0.28}, {c, 0.27}]

\( \{b \to 0.238486, c \to 0.226493\} \)

Without adhesion

Clear[w, w0, w1, w2, p, f, b, s, c, r]

\( b = 1 \);

\( p = 0 \);

\[
w0 = \left( \frac{b^2 - c^2}{12 (f + p)^2 \left[ b^4 - 4 b^2 c^2 + 3 c^4 + 4 c^4 (\log(b) - \log(c)) \right]} \right)^{1/3} \left( f - c^2 f + \left( b^2 - c^2 \right) p - 2 b^2 p \log(b) + 2 c^2 (f + p) \log(c) \right)
\]

\[
= \frac{\left( \frac{1-c^2}{f^2 \left[ 1 + b^2 c^4 + 4 b^2 \log(c) \right]} \right)^{1/3} \left( f - c^2 f + 2 c^2 f \log(c) \right)}{2^{2/3} 3^{1/3}}
\]

Clear[c, f, w0, b, \( \chi \)]

Solve\[w0 == \frac{\left( \frac{1-c^2}{f^2 \left[ 1 + b^2 c^4 + 4 b^2 \log(c) \right]} \right)^{1/3} \left( f - c^2 f + 2 c^2 f \log(c) \right)}{2^{2/3} 3^{1/3}}, f\]

\[
\{\{f \rightarrow \frac{12 w0^2 \left( -1 + 4 c^4 - 3 c^4 + 4 c^4 \log(c) \right)}{(-1 + c^2) (1 - c^2 + 2 c^2 \log(c))}\}\}\]

\[
f = \frac{12 w0^2 \left( -1 + 4 c^4 - 3 c^4 + 4 c^4 \log(c) \right)}{(-1 + c^2) (1 - c^2 + 2 c^2 \log(c))^{1/3}}
\]
Appendix 9: Mathematica Program for Circular Constrained Blister Model under Pure Bending

Clear[w1, w2, b, c, \[Gamma], p, f, w0]

DSolve \[\left\{\begin{array}{l}
w1''''[x] + \frac{2}{x} w1''[x] - \frac{1}{x^2} w1'''[x] + \frac{1}{x^3} w1''[x] = 2 f, \\
w2''''[x] + \frac{2}{x} w2''[x] - \frac{1}{x^2} w2'''[x] + \frac{1}{x^3} w2''[x] = 2 (f + p), \\
w1[b] = w2[b], w1'[b] = w2'[b], w1''[b] = w2''[b], w1'''[b] = w2'''[b], w1''''[b] = w2''''[b], \\
w1[1] = 0, w1'[1] = 0, \end{array}\right\} \}

Without adhesion

\[f = \frac{32 w0 \left(-1 + c^2 - 2 \log[c]\right)}{\left(-3 + c^2\right)^2 - 2 \log[c] \left(1 + 2 c^2 - 3 c^4 + 4 c^4 \log[c]\right)}\]

With adhesion

Clear[b, c, f, w0, \[Gamma], p, \[Gamma], w2]

\[v2[x_] := \frac{1}{32 \left(1 - 2 c^2 + c^4 - 4 c^2 \log[c]^2\right)}\]

\[
\left\{c^2 f - c^4 f + c^6 f - 4 b^2 c^2 p + 5 b^4 c^2 p - c^4 p + 4 b^2 c^4 p - 5 b^4 c^4 p + c^6 p - f x^2 + c^4 f x^2 + c^6 f x^2 - c^4 f x^2 + 4 b^2 p x^2 - 5 b^4 p x^2 + 4 b^2 c^2 p x^2 + 5 b^4 c^2 p x^2 + c^4 p x^2 - c^4 p x^2 + c^4 f x^2 + 4 b^2 p x^2 - 2 c^2 p x^2 + c^4 p x^2 + 32 w0 - 32 c^2 w0 - 32 x^2 w0 + 32 c^2 w0 - 8 b^2 c^2 p \log[b] - 4 b^4 c^2 p \log[b] + 8 b^2 c^4 p \log[b] + 4 b^4 c^4 p \log[b] + 8 b^2 p x^2 \log[b] + 4 b^4 p x^2 \log[b] - 8 b^2 c^2 p x^2 \log[b] - 4 b^4 c^2 p x^2 \log[b] - 2 c^2 f \log[c] + 4 c^4 f \log[c] - 2 c^6 f \log[c] + 8 b^2 c^2 p \log[c] - 10 b^4 c^2 p \log[c] + 4 c^4 p \log[c] - 2 c^6 p \log[c] + 2 c^2 f x^2 \log[c] - 4 c^4 f x^2 \log[c] + 2 c^6 f x^2 \log[c] - 8 b^2 c^2 p x^2 \log[c] + 10 b^4 c^2 p x^2 \log[c] - 4 b^4 p x^2 \log[c] + 2 c^6 p x^2 \log[c] - 64 c^2 w0 \log[c] + 64 c^2 x^2 w0 \log[c] + 16 b^2 c^2 p \log[b] \log[c] + 8 b^4 c^2 p \log[b] \log[c] - 16 b^4 c^2 p \log[b] \log[c] - 16 b^4 c^2 p \log[b] \log[c] - 16 b^4 c^2 p x^2 \log[b] \log[c] - 16 b^4 c^2 p x^2 \log[b] \log[c] - 16 b^4 c^2 p x^2 \log[b] \log[c] - 16 b^4 c^2 p x^2 \log[b] \log[c] - 4 c^2 f x^2 \log[c] + 8 c^4 f x^2 \log[c] + 8 b^4 c^2 p x^2 \log[b] \log[c] - 32 b^2 c^2 p x^2 \log[b] \log[c] - 4 c^2 f \log[x] - 8 c^4 f \log[x] + 4 c^6 f \log[x] + 4 b^4 c^2 p \log[x] - 4 c^4 p \log[x] - 4 b^4 c^2 p \log[x] + 4 c^6 p \log[x] - 2 c^4 f x^2 \log[x] + 2 c^6 f x^2 \log[x] - 2 c^4 f x^2 \log[x] - 8 b^2 p x^2 \log[x] + 6 b^4 p x^2 \log[x] + 8 b^2 c^2 p x^2 \log[x] - 64 c^2 x^2 \log[x] - 64 c^2 x^2 w0 \log[x] - 16 b^2 c^2 p \log[b] \log[x] - 16 b^2 c^2 p \log[b] \log[x] + 4 c^6 p \log[c] \log[x] + 8 b^4 c^2 p x^2 \log[b] \log[x] + 4 c^2 f \log[c] \log[x] - 4 c^6 f \log[c] \log[x] + 12 b^2 c^2 p \log[c] \log[x] - 8 b^4 c^2 p x^2 \log[b] \log[x] + 8 c^2 f x^2 \log[c] \log[x] + 8 c^4 f x^2 \log[c] \log[x] - 8 b^4 c^2 p x^2 \log[c] \log[x] + 8 c^4 p x^2 \log[c] \log[x] - 16 b^2 c^2 p \log[b] \log[c] \log[x] + 32 b^2 c^2 p x^2 \log[b] \log[c] \log[x] \right\}\}

FullSimplify[Solve[v2''[c] == 0, f]]

FullSimplify[w2[c] - w2[b]]

216
\[
\left\{ f \rightarrow \left( (1 + c^4) \ (b - c) \ (b + c) \ (-4 + b^2 + c^2) \ p + 32 \ w_0 \right) + \\
4 b^2 \ p \ \log[b] \left( (1 + b^2) \ (-1 + c^2) + 2 \ (b^2 - 2 c^2) \ \log[c] \right) + \\
2 \ \log[c] \left( 4 b^2 \ p - 3 c^4 \ p + b^4 \ (-3 + 2 c^2) \ p - 32 \ w_0 + 4 c^4 \ p \ \log[c] \right) / \\
\left( (-3 + c^2) \ (-1 + c^2)^2 - 2 \ \log[c] \left( 1 + 2 c^2 - 3 c^4 + 4 c^4 \ \log[c] \right) \right) \right\}
\]

\[
\frac{1}{32 \ ( (1 + c^2)^2 - 4 c^2 \ \log[c]^2 )} \\
\left( b^2 - c^2 \ ( -1 + c^2 ) \ ((-1 + b^2) \ (1 + c^2) f + (5 b^2 + c^2) p) + 32 \ w_0 \right) + \\
4 b^2 \ p \ \log[b] \left( (1 + b^2) \ (-1 + c^2) + 2 \ (b^2 - 2 c^2) \ \log[c] \right) + \\
2 \ \log[c] \left( 4 b^2 \ p - 3 c^4 \ p + b^4 \ (-3 + 2 c^2) \ p - 32 \ w_0 + 4 c^4 \ p \ \log[c] \right) / \\
\left( (-3 + c^2) \ (-1 + c^2)^2 - 2 \ \log[c] \left( 1 + 2 c^2 - 3 c^4 + 4 c^4 \ \log[c] \right) \right) \}
\]

\[
\left\{ y \rightarrow - \frac{1}{32 \ ( (1 + c^2)^2 - 4 c^2 \ \log[c]^2 )} \\
\left( b^2 - c^2 \ ( -1 + c^2 ) \ ((-1 + b^2) \ (1 + c^2) f + (5 b^2 + c^2) p) + 32 \ w_0 \right) + \\
4 b^2 \ p \ \log[b] \left( (1 + b^2) \ (1 + c^2) + 2 \ (b^2 - 2 c^2) \ \log[c] \right) + \\
2 c^2 \ \log[c] \left( (1 + b^2) \ ((-1 + c^2)^2 f + (-4 b^2 + 5 b^4 - 2 c^2 + c^4) p) + 32 \ w_0 \right) - \\
2 \ \left( (1 + b^2)^2 f - 2 b^4 \ ( -2 + b^2 + b^4) p - 32 \ w_0 \ \log[c] \right) - \\
2 \ \log[b] \left( (1 + c^2) \ (5 b^6 p - 2 c^2 \ ( -1 + c^2 ) f + c^2 p) + b^2 \ (( -1 + c^2) f + c^2 \ ( -4 + c^2 ) p + 32 \ w_0 ) \right) + \\
2 c^2 \ \log[c] \left( (1 + b^2) \ (1 - 2 b^2 + c^2) f + (5 b^4 + 4 b^6 + c^4 - 2 b^2 (4 + c^2)) p + 32 \ w_0 + 12 b^4 \ p \ \log[c] \right) \}
\]

217
Solve cohesive zone radius and the contact radius

Clear[w, w0, w1, w2, p, f, b, s, c, r]

\( \chi = 0.22; \)

\( p = 20; \)

\( w_0 = 0.055; \)

\[
Y = -\frac{1}{32 \left( (-1 + c^2)^2 - 4 c^2 \log[c]^2 \right) + 8 b^2 \log[b]^2 \left( (-1 + c^2)^2 \left( b^4 + 2 c^2 \right) + 6 b^2 c^2 \log[c] \right) + 2 c^2 \log[c] \left( (-1 + b^2)^2 \left( (-1 + c^2)^2 f + (-4 b^2 + 5 b^4 - 2 c^2 + c^4) p + 32 w_0 \right) - 2 \left( (-1 + b^2)^2 f - 2 b^2 (-2 + b^2 + b^4) p - 32 w_0 \right) \log[c] \right) + 2 \log[b] \left( (-1 + c^2)^2 \left( 5 b^6 p - 2 c^2 \left( (-1 + c^2) f + c^2 p \right) + b^2 \left( (-1 + c^4) f + c^2 (-4 + c^2) p + 32 w_0 \right) \right) + 2 c^2 \log[c] \left( (-1 + c^2)^2 (1 - 2 b^2 + c^2) f + (5 b^4 + 4 b^6 + c^4 - 2 b^2 (4 + c^2)) p + 32 w_0 + 12 b^4 p \log[c] \right) \right)};\]

\[
f = \left( (-1 + c^2) \left( b - c \right) \left( b + c \right) \left( -4 + b^2 + c^2 \right) p + 32 w_0 \right) + 4 b^2 \log[b] \left( (-2 + b^2) (-1 + c^2) + 2 \left( b^2 - 2 c^2 \right) \log[c] \right) + 2 \log[c] \left( 4 b^2 p - 3 c^4 p + b^4 \left( -3 + 2 c^2 \right) p - 32 w_0 + 4 c^4 p \log[c] \right) \right) / \left( (-3 + c^2)^2 (-1 + c^2)^2 - 2 \log[c] \left( 1 + 2 c^2 - 3 c^2 - 4 c^4 \log[c] \right) \right);\]

FindRoot[v:\ \frac{Y}{p} = \chi, \{f, 8\}, \{b, 0.8\}, \{c, 0.4\}]

(b \to 0.617446, c \to 0.395343)
Appendix 10: Mathematica Program for Rectangular Constrained Blister Model under Pure Stretching

Clear[w, w0, w1, w2, p, f, b, s, c, x]
FullSimplify[
DSolve[{ -s^2 w1''[x] == f, -s^2 w2''[x] == f + p, w1'[1] == 0, w1'[b] == w2'[b], w1[b] == w2[b], w2'[c] == 0},
{w1, w2}, x]]

Membrane profile without cohesive zone

\[ w1 = \frac{(1 - x) (f (1 + x - 2 c) + 2 (b - c) p)}{2 s^2} \]

Without cohesive zone

\[ w2 = \frac{(1 - x) (f (1 + x) - 2 c f - 2 c p) + p (2 b - b^2 - x^2)}{2 s^2} \]

Blister height

\[ w0 = \frac{(-1 + c)^2 f + (-b + c) (-2 + b + c) p}{2 s^2} \]

Without the cohesive zone

Clear[w, w0, w1, w2, p, f, b, s, c, x]
\[ w1 = \frac{f - 2 c f + 2 b p - 2 c p + 2 c f x - 2 b p x + 2 c p x - f x^2}{2 s^2} \]
\[ \frac{\text{d}w1}{\text{d}x} = \frac{(b p - c (f + p) + f x)^3}{3 f s^4} \]
\[ \int \frac{(b p - c (f + p) + f x)^3}{3 f s^4} \text{d}x \]

Clear[w, w0, w1, w2, p, f, b, s, c, x]
\[ y1[x_] := \frac{(b p - c (f + p) + f x)^3}{3 f s^4} ; \]

FullSimplify[\[ \frac{6 (y1[1] - y1[b])}{(1 - b)} \]
\[ \frac{2 (1 + b + b^2 - 3 b c + 3 (-1 + c) c) f^2 + 6 (1 + b - 2 c) (b - c) f p + 6 (b - c)^2 p^2}{s^4} \]

219
\[
S_2 = \frac{2 \left( (1+b)^2 - 3bc + 3(1+c)f^2 + 3(1+b-2c)(b-c)fp + 3(b-c)^2p^2 \right)}{s^4}, s
\]

\[
s_1 = \left( \left( (1+b)^2 - 3bc + 3(1+c)f^2 + 3(1+b-2c)(b-c)fp + 3(b-c)^2p^2 \right)^{3/6} \right)
\]

**Within the cohesive zone**

Clear \([w, w0, w1, w2, p, f, b, s, c, x]\)

\[
w_2 = \frac{f - 2cf + 2bp - b^2p + 2cp + 2f + 2cp + f - f^2 - p - x^2}{2s^2};
\]

\[
dw1dx = \partial_x w_2;
\]

\[
\int dw1dx^2 \, dx
\]

Clear \([p, b, c, s, x, y_2]\)

\[
y_2[x_] := -\frac{(f+p)^2(c-x)^3}{3s^4};
\]

FullSimplify \(6(y_2(b) - y_2(c))/\)(b-c))

\[
S_2 = \left( \frac{2(b-c)^2(f+p)^2}{s^4}, s \right)
\]

\[
s_2 = \left( 2(b-c)^2(f+p)^2 \right)^{1/6}
\]

Clear \([w, w0, w1, w2, p, f, b, s, c, x]\)

\[
s = \left( 2(b-c)^2(f+p)^2 \right)^{1/6};
\]

\[
w_2[x_] := \frac{f - 2cf + 2bp - b^2p + 2f + 2cp + f - f^2 - p - x^2}{2s^2};
\]

FullSimplify \([w2[c]]\)

FullSimplify \([w2[c] - w2[b]]\)

\[
w_0 = \frac{(-1+c)^2f + (-b+c)(-2+b+c)p}{2 \cdot 2^{1/3} \left( (b-c)^2(f+p)^2 \right)^{1/3}}
\]

\[
y = \frac{(b-c)^{4/3}(f+p)^{1/3}}{2 \cdot 2^{1/3}}
\]

220
Solve the variables of cohesive zone radius and contact radius

Clear[w, w0, w1, w2, p, f, b, s, c, x]
γ = 0.8;
p = 1000;
f = 2.00;

\[ y = \frac{(b - c)^{4/3} (f + p)^{1/3}}{2 \times 2^{1/3}}; \]
\[ w0 = \frac{(-1 + c)^2 f + (-b + c) (-2 + b + c) p}{2 \times 2^{1/3} ((b - c)^2 (f + p)^2)^{1/3}}; \]

FindRoot[[y == γ, w0 == 1.5], {b, 0.6}, {c, 0.5}]

No adhesion

Clear[w, w0, w1, w2, p, f, b, s, c, r]
b = 1;
p = 0;

\[ w0 = \frac{(-1 + c)^2 f + (-b + c) (-2 + b + c) p}{2 \times 2^{1/3} ((b - c)^2 (f + p)^2)^{1/3}}; \]

\[ \frac{(-1 + c)^2 f}{2 \times 2^{1/3} ((1 - c)^2 f^2)^{1/3}} \]

Clear[c, f, w0, b, γ]

Solve[w0 == \frac{(-1 + c)^2 f}{2 \times 2^{1/3} ((1 - c)^2 f^2)^{1/3}}, f]

\[ \left\{ \left\{ f \rightarrow \frac{16 \, w0^3}{(-1 + c)^4} \right\} \right\} \]

f = \frac{16 \, w0^3}{(-1 + c)^4}
Clear[{b, c, y, w0, y, s, p}]

\[ w_0 = 0.8; \]

0 >> c.txt; 0 >> f.txt;

cmin = 0.000000001; cmax = 0.4; cinc = (cmax - cmin) / 50;

Do[
    \[ f = N\left[\frac{16 w_0^3}{(-1 + c)^4}\right] \rightarrow f.txt; \]
    N[c] >>> c.txt:, {c, cmin, cmax, cinc}]

X = Import["C:\Documents and Settings\Ga.Li\My Documents\f.txt", "List"];
Y = Import["C:\Documents and Settings\Ga.Li\My Documents\c.txt", "List"];
XYtable = {X[[1]], Y[[1]]}:

Do[XYtable = Append[XYtable, {X[[i]], Y[[i]]}], {i, 2, Length[X]}];
g1 = ListPlot[XYtable, PlotRange -> {{0, 30}, {0, 1}}]

DMT-limit

Clear[{w, w0, w1, w2, p, f, b, s, c, r}]

b = 1;

\[ w_0 = \frac{(-1 + c)^2 f + (-b + c)(-2 + b + c) p}{2 \times 2^{1/3} (b - c)^2 (1 + p)^2}; \]

\[ f = \frac{(-1 + c)^4 f + (-1 + c)^4 p}{2 \times 2^{1/3} (1 - c)^2 (1 + p)^2}; \]

\[ f = -p + \frac{16}{(1 - c)^4} w_0^3; \]

Clear[{b, c, y, w0, y, s, p}]

\[ w_0 = 0.8; \]

p = 1;

0 >> c.txt; 0 >> f.txt;

cmin = 0.000000001; cmax = 0.5; cinc = (cmax - cmin) / 20;

Do[
    \[ f = N\left[-p + \frac{16}{(1 - c)^4} w_0^3\right] \rightarrow f.txt; \]
    N[c] >>> c.txt:, {c, cmin, cmax, cinc}]

X = Import["C:\Documents and Settings\Ga.Li\My Documents\f.txt", "List"];
Y = Import["C:\Documents and Settings\Ga.Li\My Documents\c.txt", "List"];
XYtable = {X[[1]], Y[[1]]}:

Do[XYtable = Append[XYtable, {X[[i]], Y[[i]]}], {i, 2, Length[X]}];
g1 = ListPlot[XYtable, PlotRange -> {{0, 30}, {0, 1}}]
\[ w_0 = \frac{f - c f^2 + 2 c^2 f \log[x] - 2 c q \log[x]}{2 s^2}; \]

1. Calculate \( dw_2 dx \) and \( dw_2 dr \) by integrating the expressions.
2. Simplify the expressions using the `FullSimplify` function.
3. Solve for \( w \) using the `Solve` function with the given initial conditions.

\[
\begin{align*}
\text{Clear} \{w, w0, w1, w2, p, f, b, s, c, r, q\} \\
\text{FullSimplify}\left[\text{DSolve}\left[\left\{\left[-s^2 \frac{r}{(w0 w1[r])} = f \left(r^2 - c^2\right) + q c, \quad w1[1] = 0\right], w1, r\right]\right]\right] = \left\{\left[w1 \rightarrow \text{Function}\left[r, \frac{f - f \frac{r^2}{4} + \frac{c f^2}{4} + \left(c^4 \frac{r^2}{4} - 2 c^3 f q + c^2 q^2\right) \log[x]}{s^4}\right]\right]\right\} \\
\text{Clear} \{w, w0, w1, w2, p, f, b, s, c, r\} \\
w2 = \frac{f - f r^2 + 2 c^2 f \log[x] - 2 c q \log[x]}{2 s^2}; \\
\int \left( dw2 dr \right) dx \\
-c f (c f - q) r^2 + \frac{f s^4}{4} + \left(c^4 f^2 - 2 c^3 f q + c^2 q^2\right) \log[x] \\
\frac{1}{s^4} \\
\text{Clear} \{p, b, c, s, r, y2\} \\
y2[x_] := \frac{-c f (c f - q) r^2 + \frac{f s^4}{4} + \left(c^4 f^2 - 2 c^3 f q + c^2 q^2\right) \log[x]}{s^4} \\
\text{FullSimplify}\left[\frac{6 (y2[1] - y2[c])}{(1^2 - c^2)}\right] \\
3 \left(f \left(f - 3 c^2 f + 4 c q\right) \right) + \frac{4 c^2 (c f^2 - q)}{-1 - c^2} \log[x] \right) \\
\frac{2 s^4}{s^4} \\
s = \left(3 \left(f \left(f - 3 c^2 f + 4 c q\right) \right) + \frac{4 c^2 (c f^2 - q)}{-1 - c^2} \log[x] \right) \right)^{1/6} \\
\text{Clear} \{w, w0, w1, w2, p, f, b, s, c, r, q\} \\
s = \left(\frac{3 \left(f \left(f - 3 c^2 f + 4 c q\right) \right) + \frac{4 c^2 (c f^2 - q)}{-1 - c^2} \log[x]}{2}\right) \right)^{1/6}; \\
w[x_] := \frac{f - f r^2 + 2 c^2 f \log[x] - 2 c q \log[x]}{2 s^2}; \\
\text{FullSimplify}\left[w[c]\right] \\
\frac{f - c^4 f + 2 c (c f - q) \log[c]}{2^{1/3} 3^{1/3} \left(f \left(f - 3 c^2 f + 4 c q\right) + \frac{4 c^2 (c f^2 - q)}{-1 - c^2} \log[x] \right)^{1/3}} \\
\text{Clear} \{w, w0, w1, w2, p, f, b, s, c, r, q\} \\
q = 0.5; \quad c = 0.09; \quad w0 = 0.4; \\
\text{Solve} \left[w0 \rightarrow \frac{f - c^2 f + 2 c (c f - q) \log[c]}{2^{1/3} 3^{1/3} \left(f \left(f - 3 c^2 f + 4 c q\right) + \frac{4 c^2 (c f^2 - q)}{-1 - c^2} \log[x] \right)^{1/3}} \right] \\
\{(f \rightarrow -0.0384635 - 0.142482 \, \text{i}), (f \rightarrow -0.0384635 + 0.142482 \, \text{i}), (f \rightarrow 0.261265)\} \]
Appendix 11: Mathematica Program for Rectangular Constrained Blister Model under Pure Bending

Clear[w1, w2, b, c, x, p, f, w0]
D Solve [{w1''''[x] == f, w2''''[x] == f + p, w2''[c] == 0, w2[c] == w0, w1[b] == w2[b], 
  w1''[b] == w2''[b], w1''[b] == w2''[b], w1''''[b] == w2''''[b], w1[1] == 0, w1'[1] == 0}, 
  {w1, w2}, x]

w1 gives the membrane profile without cohesive zone
w2 gives the membrane profile within cohesive zone

JKR-limit
Clear[b, c, p, f, w, w0, x]
b = c;
w[x_] := 
  1/(24 (-1 + c)^3) (-c^2 f + 3 c^3 f - 3 c^4 f + c^5 f + b^4 p - 3 b^4 c p - 6 b^2 c^2 p + 8 b^3 c^2 p + 8 b c^3 p - 
               6 b^2 c^3 p - 3 c^4 p + 3 c^5 p - 24 w0 + 72 c w0 + 2 c f x - 4 c^2 f x + 4 c^4 f x - 2 c^5 f x - 4 b^3 p x + 
               12 b^2 c^2 p x + 12 b^2 c^3 p x + 4 c^4 p x - 2 c^5 p x - 144 c w0 x - f x^2 - c f x^2 + 8 c^2 f x^2 - 8 c^3 f x^2 + 
               c^4 f x^2 + c^5 f x^2 + 8 b^3 p x^2 - 3 b^4 p x^2 - 3 b^4 c p x^2 + 8 b^3 c p x^2 + 8 b^3 c p x^2 + 3 b^4 c p x^2 - 
               12 b c^2 p x^2 + 8 b^3 c^2 p x^2 - 8 c^3 p x^2 - 6 b^2 c^2 p x^2 - 6 b^2 c^3 p x^2 + 4 c^4 p x^2 + c^5 p x^2 + 72 w0 x^2 + 72 c w0 x^2 + 
               2 f x^3 - 4 c f x^3 + 4 c^3 f x^3 - 2 c^4 f x^3 - 4 b^3 p x^3 + 2 b^4 p x^3 + 12 b^2 c^2 p x^3 - 
               4 b^3 c p x^3 - 
               12 b c^2 p x^3 + 4 c^3 p x^3 - 2 c^4 p x^3 - 48 w0 x^3 - 3 c f x^4 + 3 c f x^4 + c^4 f x^4, 
               FullSimplify[w[x]]

w[x_] := 
  (-1 + x)^2 (-24 w0 + c ((-1 + c)^3 c f + 72 w0) - 2 ((-1 + c)^3 c f + 24 w0) x + (-1 + c)^2 f x^2) 
  24 (-1 + c)^3

Clear[b, c, p, f, w, x, y, w0]
w[x_] := 
  (-1 + x)^2 (-24 w0 + c ((-1 + c)^3 c f + 72 w0) - 2 ((-1 + c)^3 c f + 24 w0) x + (-1 + c)^2 f x^2) 
  24 (-1 + c)^3

2 Integral[w''[x]^2, x]
(-1 + c)^6 f^2 + 8640 w0^2
24 (-1 + c)^3

UE = 2 Integral[w''[x]^2, x] = 1/(720) (-1 + c)^5 f^2 + 12 w0^2
(1 - c)^3
Clear\[b, c, p, f, w, x, \gamma, UE, US, w0\]

\[UE = \frac{1}{720} (1 - c)^5 f^2 + \frac{12 w0^2}{(1 - c)^3};\]

\[US = 2 \gamma c;\]

\text{FullSimplify[Solve[\partial_\gamma UE == 0, US, f]]}

\[\begin{align*}
\{\{\xi \to \frac{12 \pm \sqrt{-\frac{36 w0^2}{(-1 + c)^4} + 2 \gamma}}{(-1 + c)^3}\}, \\
\{\xi \to \frac{12 \pm \sqrt{-\frac{36 w0^2}{(-1 + c)^4} + 2 \gamma}}{(-1 + c)^3}\}\}\end{align*}\]

\[f = \frac{12 \sqrt{\frac{36 w0^2}{(1 - c)^4} - 2 \gamma}}{(1 - c)^2}\]

\text{DMT - limit}

\text{In this case, } b = 1

Clear\[w1, w2, b, c, x, p, f, w0\]

\text{Simplify[DSolve [[w2 \[RightArrow] \{x[[i]] == f + p, w2[[i]] == c == 0, w2[c] == w0, w2[1] == 0, w2'[1] == 0], w2, x]]}

\[\{\{w2 \to \}
\]

\text{Function}\[\{x\}, \frac{1}{24 (-1 + c)^3} \left(-c^2 f + 3 c^3 f - 3 c^4 f + c^5 f - c^6 f + c^7 f + c^8 f - c^2 p + 3 c^3 p - 3 c^4 p + c^5 p + c^6 p + 24 w0 + 72 c w0 + 2 c f x - 4 c^2 f x - 4 c^3 f x + 4 c^4 f x - 2 c^5 f x + 2 c p x - 4 c^2 p x - 4 c^3 p x + 4 c^4 p x - 2 c^5 p x + 2 c^6 p x - 4 c^7 p x + 8 c^8 p x + 4 c^5 f x^2 + c^6 f x^2 + 8 c^7 f x^2 - c^8 f x^2 + 8 c^9 f x^2 + 4 c^5 p x^2 + 4 c^6 p x^2 + 4 c^7 p x^2 + 4 c^8 p x^2 - 8 c^9 p x^2 - 4 c^10 p x^2 - 4 c^2 f x^3 + 4 c^3 f x^3 - 2 c^4 f x^3 - 2 c^5 f x^3 + 2 c^6 f x^3 - 8 c^7 f x^3 + 4 c^8 f x^3 - 8 c^9 f x^3 + 8 c^10 f x^3 + 4 c^5 p x^3 + 4 c^6 p x^3 + 4 c^7 p x^3 + 4 c^8 p x^3 - 8 c^9 p x^3 - 4 c^10 p x^3 - 8 c^11 p x^3 + 4 c^5 f x^4 - 4 c^6 f x^4 + 4 c^7 f x^4 - 4 c^8 f x^4 + 4 c^9 f x^4 - 4 c^{10} f x^4 + 4 c^5 p x^4 - 4 c^6 p x^4 + 4 c^7 p x^4 - 4 c^8 p x^4 + 4 c^9 p x^4 - 4 c^{10} p x^4 + 4 c^{11} p x^4\}\}\}

Clear\[b, c, p, f, x, w1, w2, w0\]

\[w2[[x]] = 1 = \frac{1}{24 (-1 + c)^3} \left(-c^2 f + 3 c^3 f - 3 c^4 f + c^5 f - c^6 f + c^7 f + c^8 f - c^2 p + 3 c^3 p - 3 c^4 p + c^5 p + c^6 p + 24 w0 + 72 c w0 + 4 c^2 f x + 4 c^3 f x - 2 c^4 f x + 2 c p x - 4 c^2 p x + 4 c^3 p x - 4 c^4 p x - 2 c^5 p x + 144 c w0 x - f x^2 - c f x^2 + 8 c^2 f x^2 - 8 c^3 f x^2 + c^4 f x^2 + 8 c^5 f x^2 - c p x^2 + 8 c^2 p x^2 - 8 c^3 p x^2 + 4 c^4 p x^2 + 8 c^5 p x^2 + 4 c^6 p x^2 - 8 c^7 p x^2 + 8 c^8 p x^2 + 4 c^6 p x^2 + 4 c^7 p x^2 + 4 c^8 p x^2 - 8 c^9 p x^2 - 4 c^{10} p x^2 - 8 c^{11} p x^2 + 4 c^5 f x^3 - 4 c^6 f x^3 + 4 c^7 f x^3 - 2 c^8 f x^3 + 2 c^9 f x^3 - 4 c^{10} f x^3 + 4 c^5 p x^3 - 4 c^6 p x^3 + 4 c^7 p x^3 - 4 c^8 p x^3 + 4 c^9 p x^3 - 4 c^{10} p x^3 + 4 c^{11} p x^3\right}\]

\text{FullSimplify[Solve[w2 [[c]] == 0, f]]}

\[\{\{\xi \to -p + \frac{72 w0}{(-1 + c)^4}\}\}\]

\[f = -p + \frac{72 w0}{(-1 + c)^4}\]
Clear[{b, c, f, w0, χ, p}]

w0 = 0.055;

p = 4;

f = N[-p + 72 w0 / (-1 + c)^4]

N[c] >>> c.txt; {c, cmin, cmax, cinc}

X = Import["C:\Documents and Settings\Gu. Li\My Documents\f.txt", "List"];

Y = Import["C:\Documents and Settings\Gu. Li\My Documents\c.txt", "List"];

XYtable = {{X[[1]], Y[[1]]}}, {i, 2, Length[X]};

Do[XYtable = Append[XYtable, {X[[i]], Y[[i]]}], {i, 2, Length[X]}];

q1 = ListPlot[XYtable, PlotRange -> {{0, 30}, {0, 1}}];

No adhesion

f = 72 w0 / (-1 + c)^4

Clear[{b, c, f, w0, χ, p, x, w2}]

w2[x_] :=

1 / 24 (-1 + c)^3 (-c^2 f + 3 c^3 f - 3 c^4 f + c^5 f - 6 b^2 c^2 p + 8 b^3 c^2 p - 3 b^4 c^2 p + 8 b c^3 p - 6 b^2 c^3 p +

b^4 c^3 p - 3 c^4 p + c^5 p - 24 w0 + 72 c w0 + 2 c f x - 4 c^2 f x + 4 c^4 f x - 2 c^5 f x + 12 b^2 c p x -

16 b^3 c p x + 6 b^4 c p x - 12 b^5 c p x + 12 b^2 c^2 p x - 4 b^3 c^2 p x + 4 c^3 p x - 12 b c^3 p x +

12 b^2 c^3 p x - 4 b^3 c^3 p x + 4 c^4 p x - 2 c^5 p x - 144 c w0 - f x^2 - c f x^2 + 8 c^2 f x^2 - 8 c^3 f x^2 +

c^4 f x^2 + c^5 f x^2 - 8 b^2 c p x^2 - 6 b^3 c p x^2 + 8 b^2 c p x^2 - 3 b^3 c p x^2 +

24 b c p x^2 - 24 b^2 c^2 p x^2 + 8 b^3 c^2 p x^2 - 8 c^3 p x^2 + c^4 p x^2 + c^5 p x^2 + 72 w0 x^2 + 72 c w0 x^2 +

2 f x^3 - 4 c f x^3 + 4 c^3 f x^3 - 2 c^4 f x^3 + 4 b p x^3 - 4 b^3 p x^3 + 2 b^4 p x^3 - 12 b c p x^3 + 12 b c p x^3 -

4 b^2 c p x^3 + 4 c^2 p x^3 - 2 c^4 p x^3 - 48 w0 x^3 - f x^4 + 3 c f x^4 - 3 c^2 f x^4 + c^3 f x^4 - p x^4 +

3 c p x^4 - 3 c^2 p x^4 + c^3 p x^4);

FullSimplify[Solve[w2''[c] == 0, f]]

FullSimplify[w2[c] - w2[b]]
Solve the variables of contact radius and cohesive zone radius

Clear[\[w, w0, w1, w2, p, f, b, s, c, \]

\[\gamma = 0.22;\]

\[p = 7;\]

\[w0 = 0.055;\]

\[y = \frac{(b - c)^2 \left((-1 + b)^2 (1 + c)^3 f + (-3 + 2 b + c) \left((-1 + b)^2 (b - c)^2 p - 24 w0\right)\right)}{24 (-1 + c)^3};\]

\[f = \frac{-(b - c)^2 \left(6 + 3 b^2 + 2 b (-4 + c) + (-4 + c) c\right) p + 72 w0}{(-1 + c)^4};\]

FindRoot[[\[y = \frac{y}{p}; f = 9\], \{b, 0.85\}, \{c, 0.3\}]\]

\{b \rightarrow 0.746414, c \rightarrow 0.284432\}
VITA

Guangxu Li was born on August 20th 1984 in Xiangyang City, Hubei Province, P. R. China, where he lived until graduation from Xiangyang No. 5 Middle School in July, 2002. He then attended Huazhong University of Science and Technology and received the bachelor degree majoring in Engineering Mechanics in June, 2006. During the undergraduate period, he was awarded several times of scholarship and earned admission to graduate study in the senior year because of the academic excellence. After achieving the master degree in Fluid Mechanics from Huazhong University of Science and Technology in June, 2008, he joined Professor Kai-tak Wan’s group for PhD program in Northeastern University in Boston, Massachusetts, USA in September, 2008. He was held a Graduate Research Assistantship from Department of Mechanical and Industrial Engineering in Northeastern University during the PhD study. He is a member of Adhesion Society, Material Research Society and American Physical Society. In May 2012, he received his PhD in Mechanical Engineering from Northeastern University.