CONTACT MODELING OF AN

RF MEMS SWITCH

A Thesis Presented

by

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Abstract

A contact model is built to understand the contact mechanics of ohmic contact RF MEMS microswitches. To adequately predict the complicated phenomena which occur in a plastically deforming adhesive contact, a finite element model is developed to study adhesion of elastic-plastic microcontacts. This model differs from existing models, in that it includes the effect of adhesion on the deformation and stresses field, making it applicable to a wide range of material properties. It shows two distinct separation modes - brittle separation and ductile separation.

A series of simulations are conducted using this model to determine the influence of the four non-dimensional parameters on the contact and on the separation modes. The results show that the parameter $S$ (the ratio of the theoretical stress to the hardness) and $\delta_f/\delta_c$ (the ratio of the final loading interference to the critical interference for initial yielding) are the most important. Small values of $S$ always lead to brittle separation, while both separation modes are consistent with large values of $S$, depending on $\delta_f/\delta_c$; ductile separation occurs at small $\delta_f/\delta_c$ and brittle separation at great $\delta_f/\delta_c$. The transition between the two separation modes occurs at about $S=1.2$ for $\delta_f/\delta_c=30$ which corresponds to the theoretical stress being 20% greater than the hardness. This result is qualitatively similar to the existing simplified analytical models, in that the adhesion energy, the
hardness, and the loading level play important roles in the occurrence of ductile separation.

When the surface is rough, there are many nano asperities on the top of the sphere. The contact at the macroscopic level is often actually a cascade of many nanocontacts. Using the same procedure as for the microcontacts, instead of considering the physics of the nucleation and motion of dislocations at this nanoscale, a series of simulations were performed for nano-scale hemispheres with the adhesion energy varying from $0.3 - 1.5\, J/m^2$. Our preliminary results are in accordance with published molecular dynamics simulation results, which demonstrate that under loading conditions well beyond the elastic limit, different adhesion energies have a significantly different effect on the unloading.
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Nomenclature

I. Material properties:

\( E \) Young’s modulus

\( E^* \) Effective Young’s modulus,
\[
\frac{1}{E^*} = \frac{1 - v_1^2}{E_1} + \frac{1 - v_2^2}{E_2}
\]

\( K \) Effective modulus of elasticity, \( K = \frac{4}{3}E^* \)

\( H \) Hardness, \( H = 3\sigma_y \)

\( Z_0 \) Equilibrium molecular distance

\( \gamma \) Surface energy

\( \Delta\gamma \) Work of adhesion (adhesion energy)
\[
\Delta\gamma = \gamma_1 + \gamma_2 - \gamma_{12}
\]

\( v \) Poisson’s ratio

\( \sigma_{th} \) Theoretical stress (maximum Lennard-Jones’ attractive stress)
\[
\sigma_{th} = 1.026 \frac{\Delta\gamma}{Z_0}
\]

\( \sigma_y \) Yielding strength
Nomenclature

II. Other parameters:

- $a_c$: Critical contact radius for initial yielding
- $a_f$: Final (maximum) contact radius
- $a_p$: Transition contact radius from elasto-plastic to fully plastic contact
- $F$: Contact force, $F = F_e + F_s$
- $F_{adh}$: Adherence force (pull-off force)
- $F_e$: External force
- $F_f$: Final (maximum) external force
- $F_s$: Adhesion force
- $p_m$: Mean pressure
- $R$: Radius of curvature of the spherical bump
- $R_{res}$: Residual radius of curvature
- $\delta$: Interference
- $\delta_c$: Critical interference for initial yielding $\delta_c = \frac{a_c^2}{R}$
- $\delta_f$: Final (maximum) interference
Chapter 1

Introduction

1.1 RF MEMS switches

MEMS (Micro Electro Mechanical Systems) are small integrated devices or systems that combine electrical and mechanical components. Although this term first appeared in 1987, its history can be traced to the late 1960’s. After the invention of the transistor at Bell Telephone Laboratories in 1947 and the production of the first integrated circuit (IC) at Texas Instruments in 1958 using germanium (Ge) devices, a gold resonating MOS gate device was fabricated in 1967 [Nathanson 1967] which is generally accepted as the first MEMS device. The turning point for MEMS was the beginning of the 1990s with the development of integrated circuit (IC) fabrication processes where sensors, actuators, and control functions were co-fabricated in silicon. Since then MEMS has rapidly emerged and found broad applications in biotechnology, communications, and inertial sensing. It has the potential to change our daily lives as the computer has. However its
reliability is a major problem which limits its application at this preliminary stage. A thorough understanding of the properties of existing MEMS materials is just as important as the development of new MEMS materials.

Traditional MEMS can be divided into two classes: MEMS actuators and MEMS sensors. MEMS actuators are moving mechanism activated by an electrical signal like a micromotor. Micro sensors are the devices used to detect changes in the system’s environment by measuring mechanical, thermal, magnetic, chemical or electromagnetic information or phenomena. This thesis is a part of a project about High Reliability, One-Watt Contact-Type RF MEMS Switches which belongs to the first category.

MEMS switches show special promise in radio frequency (RF) applications. The term RF MEMS refers to the design and fabrication of MEMS for switching and manipulation of RF signals. RF, or radio frequency signals have a broad range from 300 kHz to 300 GHz which covers a significant portion of the electromagnetic radio spectrum in Figure 1.1.

Among the switch technologies presently used in RF systems, electromechanical (EM) relays offer the best high frequency performance in terms of low insertion loss, high isolation, and good power handling (up to several watts), but are large, slow, expensive, and lack durability. Solid state (SS) switches, e.g., PIN diodes and GaAs MESFETs offer chip level integration, small size, fast switching times, excellent durability, and low cost, but generally do not perform well in broadband applications, because of high insertion loss, and poor isolation. The attraction of MEMS switches is that they offer the performance of EM switches with the size and low cost of SS switches. Their advantages include: (1) high linearity; (2) low insertion loss; (3) low power
Figure 1.1 Electromagnetic radio frequency spectrum (©1996 Encyclopedia Britannica Inc). RF covers a significant portion of the frequency spectrum ranging from 300 kHz to 300 GHz.

Table 1.1 Comparisons of the performance of Solid State switches and MEMS switches

<table>
<thead>
<tr>
<th>Switch Type</th>
<th>Isolation</th>
<th>Insertion loss</th>
<th>Power handling</th>
<th>Power consumption</th>
<th>Cost</th>
<th>Switching speed</th>
<th>Reliability</th>
</tr>
</thead>
<tbody>
<tr>
<td>PIN diodes</td>
<td>Good</td>
<td>Good</td>
<td>Good</td>
<td>Poor</td>
<td>Good</td>
<td>Good</td>
<td>Good</td>
</tr>
<tr>
<td>GaAs FETs</td>
<td>Good</td>
<td>Good</td>
<td>Poor</td>
<td>Good</td>
<td>Poor</td>
<td>Excell</td>
<td>Good</td>
</tr>
<tr>
<td>MEMS switches</td>
<td>Excell</td>
<td>Excell</td>
<td>Excell</td>
<td>Excell</td>
<td>Good</td>
<td>Poor</td>
<td>Poor</td>
</tr>
</tbody>
</table>

consumption; (4) reduced size; (5) high shock resistance; (6) wider temperature range; (7) good isolation; and (8) low cost. However, high switching voltage, relatively slow switching speeds (compared to SS, although it is not so important for some applications),
low power handling, concerns about packaging, and questionable reliability are areas of concern. Comparisons of the performance in the areas above are listed in Table 1.1. A lot of effort has gone into MEMS switches in industry, government, and academia, but many issues need to be solved for it to be commercially viable.

MEMS switches technologies can be categorized based on the following aspects. (1) Fabrication: bulk micromachining, surface micromachining, and LIGA; (2) Material: silicon, GaAs, quartz, silicon dioxide, silicon nitride, and various metals; (3) Actuation: electrostatic, magnetic, and thermal; (4) Contact type: ohmic and capacitive; (5) Physical shape: beam, membrane, rotary, and plate; (6) Contact direction: vertical and lateral.

Failures of electrostatically actuated microrelays have been observed in the contact, the actuator, and in the package. By improving the microfabrication process, many failures in the actuator and in the package can be effectively limited. However, failures at the contact are not yet well understood. They can only be solved by more knowledge of the causes.

**Capacitive switches are often built using a membrane.** The active element is a thin metallic membrane movable through the application of a DC electrostatic field. Application of a DC electrostatic field results in deflection of the membrane. The membrane snaps onto the dielectric below and is therefore capacitively coupled to the bottom metal trace. So the contact is metal-to-dielectric, typically Au-on-silicon nitride. The most critical limitation results from stiction between dielectrics because of adhesion due to large area, self-actuation (above $2W$ RF power), and dielectric charging effects (for instance, even it has a lower dielectric constant, SiO$_2$ is better than Si$_3$N$_4$ from this angle).
point of view), limiting the switch lifetime to about 100 million to 1 billion switching cycles.

The failure of resistive contact switches is associated with the resistive failure caused by damage, pitting, hardening or contamination, and resulting in contact resistance over 4 - 5 Ω. Some experimental results including adhesion, welding, melting and an unexplained increase in contact resistance (Figure 1.2) were found which may lead to the switch failure ([Peterson 1979], [Wright 1998], [Majumder 2001], [Schiele 1999], [Becher 2002]).

Figure 1.2 Variation in contact resistance over first $10^6$ switching cycles of seven switches belonging to a single die [Majumder 2001].

In Figure 1.2 the test was done on a Northeastern University fabricated switch [Majumder 2001]. The current through the switch is between 4 and 20 mA. Cycling the switches results in a reduction in the contact resistance over the first $10^4$-$10^5$ switching
cycles, to less than 0.1 $\Omega$. Beyond $10^5$-$10^7$ cycles, contact resistance is typically found to increase progressively. Switches eventually fail in one of two modes – they either stay closed permanently, or their resistance increases progressively as they are cycled.

RF switches employing the cantilever beam type design are the most widely reported. Figure 1.3 is a cross-section of a MEMS device of the type designed by MicroAssembly, Inc. after bonding. The outlined portion shows the actuation of the cantilever. The horizontal bar is the cantilever beam made of SOI. A flat surface coated with a metal such as gold is fabricated on it. The corresponding contact on the cantilever beam is a microbump coated with metal as well. When a voltage is applied between the beam and the substrate, due to the electrostatic force, the beam is attracted downward to the substrate which causes metal-to-metal (ohmic) contact and the switch is on. Then the voltage is removed, and due to the restoring force of the beam, the beam is pulled away from the substrate, and the switch is off.

![Diagram of MEMS device](image)

Figure 1.3. The cross-section of package and MEMS device of the type designed by MicroAssembly, Inc. after bonding. The outlined portion shows the actuation of the cantilever.
Chapter 1 Introduction

It is desired to have a contact resistance of less than $1 \sim 2 \ \Omega$. Low contact resistance of MEMS switches requires contact material with superior electrical, mechanical and chemical properties, such as low resistivity, low hardness and high chemical resistance to corrosion. To achieve a low contact resistance, it requires a relatively bigger contact area which can be produced by a large force applied to the contact. Thus, gold-on-gold electric contact has been typically used in MEMS switches due to its low electric resistivity, and resistance to surface oxide. The low hardness and high adhesion energy (clean surface) of gold, however, lead to adhesion problems in MEMS switches – stuck-closed failure due to the pull-off force exceeding the restoring force of the cantilever beam.

The results in Figure 1.4 were obtained by a SPM-based contact test station. The change of the adhesion forces on gold contacts can be divided into three phases of evolution. In the first phase, contact adhesion increases after a small number (< 10) of cycles and becomes relatively stable. In the second phase the adhesion changes and mostly increases. The piezo-control movement always forces the contact to separate which won’t cause stiction problem in the test station. But consider in the real switch, when the increased the adhesion force exceeds the actuator’s restoring force - “stuck-closed” failure happens. With continued cycling, the adhesion becomes more stable. It is necessary to build a contact model to help understand this behavior and improve the reliability of the device.

The focus of this thesis will be on the reliability, and failure mechanisms of ohmic contact-type switches with Au or Ru contacts. Finally, it should be mentioned that long term reliability assessment is still an open point for RF MEMS.
Figure 1.4: Change in adhesion in a hemispherical/flat contact with cycling for Au contacts at 200 µN. A “stuck-closed” failure was found since the adhesion force dramatically increase with continued cycling [Chen 2007].

1.2 Related work

There are two switching modes (i.e., hot or cold). In hot switching, the signal flows through the contact until the contact breaks mechanically. In cold switching, the signal is turned on and off only when the electrodes are engaged. The analysis of hot switching is more complicated because the effect of current may cause melting and/or softening of metallic contact, affecting the switch lifetime. In this thesis, we consider contact with zero current.

It is useful to build a contact model to understand the failures mechanisms discussed above and help find solutions to improve the reliability of the device. A lot of
attention has been paid to this subject. I focus on the research on mechanical effects such as the effect of separation modes and pull-off forces from different material properties and loading conditions. Although the problem is on the micro or even smaller scale, classical theories are still valid. The well-known Hertz theory very successfully explains the elastic contact without adhesion. The following JKR and DMT theories are good extensions of Hertz theory to include the effect of adhesion.

When the contact with adhesion goes into the plastic deformation regime with more pressure and more strain, the case is more complicated. A simple analytical model (SAM) of elasto-plastic and fully plastic deformation with adhesion was developed by Majumder et al. [Majumder 2003] for use in a microswitch, using techniques from [Maugis 1984] and [Johnson 1985]. The SAM model made the assumption that for the first cycle of unloading and all the following cycles of loading and unloading only elastic deformation may occur. By investigation, we found that the assumption is correct only for certain conditions, such as weak adhesion energy, or hard materials. Most time the failure mechanisms are associated with plastic deformation during unloading. If it is not negligible, the plastic deformation produced by adhesion alters the local separation of the surfaces which in turn affects the adhesion force. As early thoughts, Maugis and Pollock (MP) [Maugis 1984] and Johnson [Johnson 1976] mentioned the two separation modes which are ductile and brittle separation as early as 1976. These ideas came from the field of fracture mechanics. It should be a correct categorization, and it is also observed experimentally. But thirty years have passed, and the criteria to distinguish these two separation modes are still not clear.
Chapter 1 Introduction

It is more straightforward to treat this problem by numerical methods, especially when much faster computation is available nowadays. For example, Kogut and Etsion (KE) have built a finite element model (FEM) with ANSYS® to study elastic-plastic contact between a sphere and a flat surface without [Kogut 2002] and with [Kogut 2003] adhesion. The results allowed simple curve-fit equations to be developed for the relations among force, displacement and contact area. Subsequent work by Jackson and Green [Jackson 2005] without adhesion using more nodes agreed well with [Kogut 2002] and allowed for greater displacements. Etsion and his colleagues (EKK) [Etsion 2005] gave the details of unloading such as the curve-fit equations for the residual radius of curvature and residual interference after the sphere is completely unloaded. Note that the EKK model does not include adhesion. It is also found that plastic deformation occurs even during the first cycle of unloading and during the following unloading [Kadin 2006]. But neither of those models considered the effect of adhesion on the deformation of the sphere outside contact, so it is a sort of DMT type model. In addition they did not predict different separation modes.

Another good method applied to this problem is by Professor Srolovitz and his students from Princeton University based on Molecular Dynamics (MD) simulations [Song 2006]. Compared with the finite element continuum model, the MD method concentrates on the interactions of individual atoms within nano scale structures. It starts from the potential between atoms within the same body, or different bodies, so it can give a clear clue how the atoms interact and where the atoms go. They found the magnitude of plasticity increases during unloading with an increase of adhesion energy. A large amount of atom transfer occurs, mostly from the side with the bump to the flat substrate
Chapter 1 Introduction

when the adhesion energy is larger than a certain value. Also a very small number of atoms may move from the flat side to the side of the bump. These models help us better understand the separation modes. So far the connection between the atomic level model and continuum model hasn’t been built. From MD, we still do not know what the key parameters are to cause different separation modes except for the one case studied.

In this thesis a modified finite element model with implemented using ANSYS® is presented to study the effect of adhesion in an elastic-plastic microcontact. That model differs from previous FEM models such as the KE model in that it includes the coupled effects of adhesion on the deformation and stress fields, thus making it applicable to a wide range of material properties. Ductile and brittle separation can be distinguished and the criteria for different separation modes can be determined which is anticipated to be helpful in selecting MEMS contact materials.

As a complement to the modeling work, an SPM-based test station has been established to study the fundamentals of contacts in a microswitch by another Ph.D student (Lei Chen) working in the same project. The evolution of the contact force, the contact adhesion, and the contact resistance is measured and evolution of the contact shape is observed with SPM and SEM [Chen 2007]. Figure 1.5(a) and Figure 1.5(b) are SEM images of an Au contact bump taken before and after several cycles at a force of 200 \( \mu N \). Figure 1.5(c) is a zoom-in picture of Figure 1.5(b) taken at a tilted angle of 85 degrees which shows the details of the damaged surface. The shape of the center apparent contact area was changed and some sharp protuberances were formed which are a result of the occurrence of a ductile separation.
Figure 1.6 is the AFM image of a contact bump of a real microswitch used in our project taken by Lei Chen. It is coated with plated gold with thickness of about 1 \( \mu m \). The
Figure 1.5, SEM images of an Au contact bump cycled at a force of 200 \( \mu N \). (a) The original bump before cycling; (b) The bump after several cycles; (c) The zoom-in image of (b) tilted at 85 degree. The surface was damaged due to ductile separation. The radius of curvature at its summit is about 4 \( \mu m \) and the height about 157 nm. The substrate is a SOI coated with SiO\(_2\).

Figure 1.6, The AFM image of a contact bump of a real microswitch used in our project (taken by Lei Chen). The bump is coated with plated gold with thickness of about 1 \( \mu m \). The radius of curvature at its summit is about 4 \( \mu m \) and the height about 157 nm.

1.3 Organization of this thesis
Chapter 1 Introduction

The rest of this thesis is organized into five chapters. In Chapter 2, I will first introduce the basics of contact mechanics with adhesion for both the loading and unloading phases which can provide qualitative insight into the general contact problem. The predicted behavior of real switches is calculated based on the existing theories. In Chapter 3 a finite element model with ANSYS® is introduced. It includes the coupled effects of adhesion on the deformation and stress fields, thus making it applicable to a wide range of material properties. Simulations were performed during a single load-unload cycle at four different maximum loading levels for both Ruthenium (Ru) and Gold (Au). These metals are two popular materials used in MEMS switches and are expected to exhibit different contact properties.

For small loading, the results of our model for Ru are consistent with the Maugis elastic model [Maugis 1992] and the KE model [Kogut 2003], but show significant differences with those models for Au. During unloading two distinct separation modes, i.e. brittle separation and ductile separation were observed for Ru and Au, respectively. Understanding the unloading of a contact is very important because the failure mechanisms in a microswitch, can be attributed to ductile separation resulting from too high an adherence force [McGruer 2006]. Therefore the impact of four possible key parameters on the separation modes is studied completely in Chapter 4. The nanoscale contact with continuum FEM is presented in Chapter 5 where comparisons are made with the results of the molecular dynamics model by Srolovitz. Chapter 6 presents conclusions and future work, such as building a multi-asperity model based on the results for individual nano contacts.
Chapter 2

Asperity contact models with adhesion

This chapter presents a brief but complete introduction to the theories of contact deformation with the adhesion effect. A microswitch contact can be modeled as a flat surface in contact with a hemisphere. Depending on the magnitude of the loading force, the first cycle of loading can be elastic, elasto-plastic or fully plastic. Without adhesion, for the first cycle of unloading and the following cycles of loading and unloading, a frequently used assumption is that only elastic deformation occurs and that it follows the Hertzian contact model. Unloading following elastic loading is a totally reversible process. Unloading following plastic loading shows some permanent deformation of the contact bodies. When adhesion is involved, theories are well developed for elastic
Chapter 2

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loading with different material properties, such as the JKR and the DMT model, but they are not applicable for plastic loading. The phenomena are more complicated considering the combination of the effect of adhesion and plasticity. A simple analytical model (SAM) with adhesion is developed by Majumder [2003] using techniques from the existing theories which can provide qualitative insight into the general contact problem. Maugis and Pollock built an unloading model with adhesion which described three separation modes. Finally calculations with real switch material properties are made based on the above theories. First let us discuss the origin of the adhesion.

2.1 Surface energy and the Lennard-Jones potential

More details about this topic can be found in the first chapter of “Contact, Adhesion and Rupture of Elastic Solids” written by Maugis [Maugis 2000]. Bonds between atoms can be divided into strong bonds (whose rupture corresponds to a large absorption of energy, around one hundred kcal/mole) and weak bonds (a few kcal/mole). The ionic bond, covalent bond and metallic bond are examples of strong bonds. The hydrogen bond and the van der Waals forces are weak bonds. The surface energy is the work needed to create reversibly and isothermally a unit area of a new surface, expressed in J/m². It reflects the nature of the bonds between the atoms which constitute it. Metals and covalently bonded materials have high surface energies (1000-3000 mJ/m²). The surface energies of ionic crystals are weaker (100-500 mJ/m²), and those of molecular crystals still weaker (less than 100 mJ/m²). When two clean metal surfaces 1 and 2 are in intimate contact, the bond between them is the metallic bond. The ideal surface energy is high. But if they are
Asperity contact models with adhesion

contaminated, the surface energy will decrease, corresponding to van der Waals interaction energies. Evidence of the existence of adhesion is seen in that a mechanical force which is called the pull-off force or adherence force is needed to separate the two parts. Combined with the material properties and geometries, sometimes the effect of the adhesion could be significant, especially at small scales.

The work to separate two solids reversibly and isothermally is termed Dupré’s adhesion energy $\Delta \gamma$, sometimes denoted by the symbol $\gamma$. It is determined by the surface energy of two solids $\gamma_1, \gamma_2$ and their interfacial energy $\gamma_{12}$,

$$\Delta \gamma = \gamma_1 + \gamma_2 - \gamma_{12}, \quad (0.1)$$

When the two solids form a single crystal, the interfacial energy $\gamma_{12}$ is zero, and the energy $\Delta \gamma = 2\gamma$ represents the theoretical cohesive energy.

One of the more usual empirical equations for the energy of interaction between two atoms or two molecules separated by a distance $r$ is the Lennard-Jones potential,

$$U = 4U_0[(\frac{a}{r})^{12} - (\frac{a}{r})^{6}], \quad (0.2)$$

where $a$ is intermolecular equilibrium distance between two individual molecules at which the Lennard-Jones potential is zero. Based on Eq. (2.2) the Lennard-Jones potential between two parallel plates separated by a distance $Z$ is,

$$U(Z) = -\frac{4\Delta \gamma}{3}[(\frac{Z_0}{Z})^2 - \frac{1}{4} (\frac{Z_0}{Z})^8], \quad (0.3)$$

and the interaction force per unit area is

$$\sigma(Z) = \frac{8}{3} \frac{\Delta \gamma}{Z_0} [(\frac{Z_0}{Z})^3 - (\frac{Z_0}{Z})^5], \quad (0.4)$$

where $Z$ is the separation between the two surfaces and $Z_0$ is the equilibrium distance between two surfaces at which the stress is zero. The LJ surface force law as given in Eq. (2.4) is widely accepted and used in modeling adhesive contacts. Examples include
Asperity contact models with adhesion

Maugis theory [Maugis 1992], Greenwood’s numerical solution for a single sphere [Greenwood 1997], and Chang et al. adhesion model for surfaces [Chang 1988]. However, the value of $Z_0$ used in Eq. (2.4) is a somewhat arbitrarily chosen number between 0.3 and 0.6 nm ([Muller 1980], [Chang 1988], [Attard 1992]). The lack of clear understanding and specific knowledge of the equilibrium distance $Z_0$ limits the applicability and accuracy of continuum-based adhesion models. Yu and Polycarpou proposed a method to calculate $Z_0$ based on the nearest neighbor distance $r_N$ [Yu 2004],

$$Z_0 = (15)^{1/6} r_N$$

(0.5)

They gave the value $Z_0 = 0.184$ nm for Au which is going to be used in this thesis. Using the same method, we obtained $Z_0 = 0.169$ nm for Ru, using $r_N = 0.265$ nm from [Kittle 1976]. However it needs to be mentioned that the effect of different crystal planes chosen on $Z_0$ is not included in Yu’s paper.

From Figure 0.1(a) we can see when $Z < Z_0$, the stress is negative representing a compressive stress, while positive means an attractive stress with $Z > Z_0$. The magnitude of compressive stress increases dramatically with closer distance, and it goes to infinity, as the separation approaches zero. A simplified model is shown in Figure 0.1(b). $Z_0$ is the closest possible distance between two surfaces. Therefore the stresses at smaller distances than $Z_0$ are calculated in other way (such as using contact element in finite element model) while the stresses at larger distances than $Z_0$ are still defined as in Eq. (2.4). From Eq. (2.4) we can introduce a couple of useful material properties. The slope at $Z = Z_0$ allows us to define Young’s modulus,

$$E = Z_0 \left( \frac{d\sigma}{dZ} \right)_{Z=Z_0} = 16 \frac{\Delta \gamma}{Z_0} = 32 \frac{\gamma}{Z_0},$$

(0.6)
Chapter 2

Asperity contact models with adhesion

(b)

Lennard Jones Stresses ($\sigma/\sigma_{th}$)

-1
-0.5
0
0.5
1

Separation ($Z/Z_0$)

1
2
3
4
5

Attractive - Adhesive Zone

Repulsive - Contact Zone
Chapter 2

Asperity contact models with adhesion

Figure 2.1 Lennard-Jones’ Stress distribution between two half-space as a function of the distance. (a) general case; (b) simplified case with the minimum separation is limited at \( Z_0 \).

and the maximum stress (termed theoretical stress) at which \( \frac{d\sigma}{dz} = 0 \) is,

\[
\sigma_{th} = 0.06E = 2.04 \frac{\gamma}{Z_0} = 0.36 \sqrt{E\gamma \over Z_0},
\]

( 0.7 )

at \( Z_n = 3^{1/6} Z_0 \approx 1.2Z_0 \). For example, for clean gold with \( Z_0 = 0.184 \text{ nm} \), Young’s Modulus \( E = 91 \text{ GPa} \), Eq. (2.6) gives \( \gamma = 0.52 \text{ J/m}^2 \), and Eq. (2.7) gives \( \sigma_{th} = 5.46 \text{ GPa} \). It is higher than normal elastic limit which is due to the existence of defects and impurities.

The derivation of Eq. (2.4) treats the solid as a continuum; it can work not only for two parallel surfaces, but also for two spheres or one flat surface and one sphere. For one flat surface with one sphere case, the slope of the sphere around its summit is almost flat and can be treated as approximately parallel with the flat surface. Away from the summit, where the slope of the sphere is large, the distance between the sphere and the flat is large enough to neglect the effect of adhesion. The same reasoning holds for the case of two spheres. In Maugis’ book [Maugis 2000] he also describes calculation of the interaction potential between two surfaces in the range of metallic bonds and obtains the theoretical stress as,

\[
\sigma_{th} = 0.5 \sqrt{E\gamma \over Z_0},
\]

( 0.8 )

We can see it is larger compared with that of Eq. (2.7) because of the difference between the Lennard-Jones potential and metallic bonding. Generally the theoretical stress for rupture is of the order of \( E/10 \) to \( E/5 \) for metals.
2.2 Introduction of a single asperity contact

Since there are a lot of parameters associated with the models in this thesis, it is necessary to introduce the definition for most of them first to help understand the contact model.

Depending on the fabrication process, the topography of the bump of the microswitch can be rough and the contact should be treated at the nanoscale, where single asperity contacts first occur. Majumder in his thesis [Majumder 2003] treated the multi-scale contact as the 10-100 small asperities with the same radius of curvature at 0.1 μm and a Gaussian height distribution (Figure 0.2). The nanocontact is going to be discussed in Chapter 5. Here let us assume the surface of the micro bump is smooth, the loading force is large enough to bring all the small asperities into contact. So the contact is a single asperity contact between a round micro bump and the flat surface. Although the whole bump is not in a perfect round shape, the variation of the radius of curvature is small in the contact area which is very small in dimensions compared with the radius of curvature. The more general case is the contact of two spheres of radii $R_1$ and $R_2$. Contact with a flat surface is a special case where the radius of curvature of the flat surface is infinite.

Based on the above analysis, the contact of a microswitch can be simply represented as a hemisphere in adhesive contact with a flat surface as shown in Figure 2.3. Both sides of the contact are covered with metals such as Gold (Au) or Ruthenium.
Asperity contact models with adhesion (Ru). As a preliminary study, the flat is taken as rigid. The contact radius under the external load $F_e$ is denoted by $a$. The interference $\delta$ is defined as the distance between

Figure 0.2 Appearance of rough surface (left); Schematic of multi-scale single asperity contacts (right).

Figure 0.3 Forces acting between a sphere and a rigid flat. The contact radius under the external load is denoted $a$. The interference $\delta$ is defined as the distance between the
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The contact force $F$ is the sum of the external force $F_e$ and the adhesion force $F_s$, i.e.

$$ F = F_e + F_s $$

The final (maximum) values of the external force, contact radius and interference are denoted by $F_f$, $a_f$, and $\delta_f$ respectively.

Figure 2.4 describes the contact during a single cycle of loading and unloading. First let us ignore the effect of adhesion. Before loading the two bodies are close but not touching each other. The bump has an original radius of curvature $R$. During loading, due to the electrostatic force acting on the cantilever of a MEMS switch, for example, the bump is pulled down to touch the flat surface which is equivalent to an external compressive force $F_e$ exerted on the bump. The bump is deformed to a bigger radius of curvature $R'$ on contact. With the increase of the magnitude of the external force, the contact radius $a$, the radius of curvature $R'$, and the interference $\delta$ increase accordingly.

During unloading, the restoring force of the cantilever starts to pull the bump apart from the flat surface due to the withdrawal of the electrostatic force.

Based on the magnitude of loading force, the deformation of the contact can be elastic, elasto-plastic or fully plastic. When the contacting bodies experience sufficient pressure, a plastic zone first appears below the surface and causes some permanent deformation. According to the von Misés yield criterion, the initiation of plastic
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deformation occurs when the second invariant of the deviatoric stress tensor reaches a
critical value which is related to the yield strength ($\sigma_Y$). This state, in which some material
is plastic, while the surrounding material is elastic, is called elasto-plastic deformation.

With increasing loading force, the plastic zone grows until it reaches the surface.
Eventually the entire contact area undergoes plastic deformation and the contact pressure
is equal to the hardness. Although elastic loading is a reversible process, plastic loading is
irreversible, and some permanent deformation remains after unloading. So the final
geometry could be the last picture in Figure 0.4 with the new radii of $R_1$ and $R_2$. 

Figure 0.4 Three contact phases – before loading, during loading and after unloading.

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Experimentally a mechanical force called the pull-off force or adherence force $F_{adh}$ is required to separate two bodies which proves the existence of the adhesion ([Majumder 2001], [Chen 2005]). Its effect is connected with some failure mechanisms of the microswitch, especially for gold due to its low hardness and lower probability of being contaminated. When the effect of adhesion is not negligible, the Lennard-Jones stress described in Figure 0.1 is used. Figure 0.5 shows the schematic crystal lattice which doesn’t represent the real relation between $Z_0$ and $r_N$ as in Eq. (2.5). We need to build a connection between models at the molecular level as in Figure 0.5 and at continuum level shown in Figure 0.3. The solid straight line represents the interface of the bodies 1 and 2. When the separation between two bodies is equal to $Z_0$, they are within contact, while those with separation larger than $Z_0$ are out of contact. Therefore an addition of $Z_0$ should be added on the separation $Z$ at continuum level for adjustment.

Figure 0.5 Crystal lattice to describe the connection between separation distance for the continuum model and molecular model.
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Asperity contact models with adhesion

When the contact radius is \( a \), adhesion force is the integration of adhesive stresses

\[
F_a = 2\pi \int_a^\infty p(Z + Z_0) r dr,
\]

(0.10)

When two surfaces are in contact only at a point and the adhesion does not affect the shape of the bump, the adhesion force is,

\[
F_{ad} = 2\pi \int_0^\infty p(Z) r dr = 2\pi \gamma R,
\]

(0.11)

This is a result from the DMT model which is going to be discussed more in the following section.

In the loading phase, we can study the relationships among the external force \( F_e \), contact radius \( a \), interference \( \delta \), as well as the mean pressure \( p_{\text{avg}} = \frac{F}{\pi a^2} \). During unloading, we can study the adherence force \( F_{\text{adh}} \) and determine the criteria for separation modes to help understand some failure mechanisms.

2.3 Elastic loading with adhesion

Since the first satisfactory analysis of the stresses at the contact was worked out by Hertz in 1882, elastic contact of two solid bodies without adhesion has been well developed. Hertz calculated the deformation at contact between isotropic, homogeneous bodies with spherical surfaces in the static, linear, elastic approximation. If two spheres of radii \( R_1 \) and \( R_2 \) with Young’s modulus and Poisson’s ratio \( E_{1,1} \), \( v_1 \) and \( E_{2,2} \), \( v_2 \), respectively are placed in contact, the contact can be predicted as follows,
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\[ a = \left( \frac{3FR}{4E^*} \right)^{1/3}, \]  \hspace{1cm} (0.12)

\[ \delta = \frac{a^2}{R}, \]  \hspace{1cm} (0.13)

\[ p_n = \frac{F}{\pi a^2} = \left( \frac{6FE^*}{\pi^3 R^2} \right)^{1/3}, \]  \hspace{1cm} (0.14)

where, \( R \) is the equivalent radius \( \frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2} \) and \( E^* \) is the effective Young’s modulus.

\[ \frac{1}{E} = \frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2}, \] and the contact modulus of elasticity \( K \) is defined as \( K = (4/3)E^* \).

The above results are based on the following assumptions:

1. \( a << R \);
2. There is no friction at the interface;
3. There is no tensile stress in the area of the contact.

The JKR and DMT models successfully extended the Hertz model by considering adhesion in two limiting regimes. The first is by Johnson, Kendall, and Roberts (JKR) who neglected the adhesion forces outside the contact area, so that both compressive stresses and tensile stresses can only exist in the contact area [Johnson 1971]. The JKR model showed by a Griffith energy argument [Griffith 1920] (assuming that contact over a circle of radius \( a \) introduces a surface energy \( \pi a^2 \Delta \gamma \) that the adherence force is \( 1.5 \pi \Delta \gamma R \). Another model is by Derjaguin, Muller, and Toporov (DMT), in which adhesion forces act in an annular zone around the contact but without deforming the profile, which remains Hertzian. The main results of their theory were that the adherence force between two rigid spheres is \( 2\pi \Delta \gamma R \) [Derjaguin 1975].
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The expressions from the JKR and DMT models are independent of the elastic modulus and so appear to be universally applicable and therefore there is a conflict between these two models. The discrepancy was explained by Tabor who introduced a parameter [Tabor 1977]

\[
\mu = \left( \frac{R \Delta \gamma^2}{E \sigma^2 Z_0^3} \right)^{1/3}
\] (0.15)

governing the transition from DMT model to JKR model. In the contact of an elastic sphere with a rigid and flat surface, \( R \) is the radius of curvature of the sphere. Generally the JKR model is applicable for \( \mu > 3 \), and the DMT model is applicable for \( \mu < 0.1 \). Therefore the JKR model applies for soft solids, large radius of curvature, and large adhesion energy, and the DMT model for hard solids, small radius of curvature, and weak adhesion energy. Tabor pointed out that the defect of the JKR model is to neglect the adhesion outside of contact, while the DMT model neglects the effect of adhesion on the deformation. Subsequently Muller et al. [Muller 1980] performed a complete numerical solution in terms of the Lennard-Jones potential, and got a smooth transition from the JKR model towards the DMT model when the Tabor parameter \( \mu \) decreases. Analytical solutions for various Tabor parameters have also been given by Maugis under simplified assumptions [Maugis 1992].

The results of the JKR and DMT theories are listed in Table 2.1. To ensure that the \( F_e \sim a \) expression has real solutions, a minimum contact radius \( a_{\text{min}} \) is required in the JKR theory, whereas there is no limit on that in the DMT theory. \( a_0 \) is the contact radius under zero loading, that is at \( F_e = 0 \). By taking the dimensionless coordinates defined in Table 2.2 we can see the difference of Hertz, JKR and DMT on the plot of \( F_e \sim a \) in
Chapter 2

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The normal pressure distributions for Hertz, JKR, DMT, and Maugis’ model are shown in Figure 0.7. As we can see in both the JKR model and DMT model, the pressure distribution has a discontinuity at the edge of contact radius $a$. The Maugis model postulates an annular cohesive zone outside the contact zone, where the adhesive tensile stress is constant and equal to the theoretical stress $\sigma_{th}$.

Figure 0.6. The JKR theory predicts a greater contact radius than DMT or Hertz.

<table>
<thead>
<tr>
<th>JKR</th>
<th>DMT</th>
<th>Hertz</th>
</tr>
</thead>
</table>

Table 2.1 Main formulas of the JKR and DMT models
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\[
\frac{a^3 K}{R} = F_e + 3\pi\Delta\gamma R + \sqrt{6\pi\Delta\gamma R F_e + (3\pi\Delta\gamma R)^2}
\]

\[
\delta = a^2 \frac{8\pi\Delta\gamma}{3K} \sqrt{6\pi\Delta\gamma R F_e + (3\pi\Delta\gamma R)^2}
\]

\[
\delta = a^2 \frac{8\pi\Delta\gamma}{3K} \sqrt{6\pi\Delta\gamma R F_e + (3\pi\Delta\gamma R)^2}
\]

\[
F_{min} = -\frac{3\pi\Delta\gamma R}{2}
\]

\[
a_{min} = \left(\frac{3\pi\Delta\gamma R^2}{2K}\right)^{1/3}
\]

\[
\delta_{min} = -\frac{a_{min}^2}{3R}
\]

\[
a_0 = \left(\frac{6\pi\Delta\gamma R^2}{K}\right)^{1/3}
\]

\[
\frac{a_0}{a} = \left(\frac{2\pi\Delta\gamma R^2}{K}\right)^{1/3}
\]

Table 2.1 Dimensionless symbols used in Maugis’ transition model

<table>
<thead>
<tr>
<th>Dimensional Symbol</th>
<th>Dimensionless Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact Radius</td>
<td>( A )</td>
</tr>
<tr>
<td>( a = \frac{a}{(\pi\Delta\gamma R^2 / K)^{1/3}} )</td>
<td></td>
</tr>
<tr>
<td>External Force</td>
<td>( F_e )</td>
</tr>
<tr>
<td>( \bar{F}_e = \frac{F_e}{\pi\Delta\gamma R} )</td>
<td></td>
</tr>
<tr>
<td>Adhesion Force</td>
<td>( F_s )</td>
</tr>
<tr>
<td>( \bar{F}_s = \frac{F_s}{\pi\Delta\gamma R} )</td>
<td></td>
</tr>
<tr>
<td>Interference</td>
<td>( \delta )</td>
</tr>
<tr>
<td>( \Delta = \frac{\delta}{(\pi^2\Delta\gamma^2 R / K^2)^{1/3}} )</td>
<td></td>
</tr>
<tr>
<td>Radial Position</td>
<td>( r )</td>
</tr>
<tr>
<td>( \rho = r / a )</td>
<td></td>
</tr>
</tbody>
</table>

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Asperity contact models with adhesion

The normal pressure distributions for Hertz, JKR, DMT, and Maugis’ model are shown in Figure 0.7. As we can see in both the JKR model and DMT model, the pressure distribution has a discontinuity at the edge of contact radius $a$. The Maugis model postulates an annular cohesive zone outside the contact zone, where the adhesive tensile stress is constant and equal to the theoretical stress $\sigma_{th}$.

![Plot of dimensionless contact radius vs. applied force for Hertz, JKR and DMT models.](image)

By defining dimensionless parameters as in

---

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Table 2.1, Maugis presented the following results. Maugis’ parameter $\lambda$ is related to $\mu$ by

$$\lambda = \sigma_m \left( \frac{9R}{2\pi\lambda E^2} \right)^{1/3} \approx 1.16\mu,$$  \hspace{1cm} (0.16)

$$F_e = A^3 - \lambda A^2 \left( \sqrt{m^2 - 1} + m^2 \tan^{-1} \sqrt{m^2 - 1} \right),$$  \hspace{1cm} (0.17)

$$\Delta = A^2 - \frac{4}{3} A \lambda \sqrt{m^2 - 1},$$  \hspace{1cm} (0.18)

where $m = c/a$. $c$ and $a$ are demonstrated in Fig. 2.7(d). $a$ is the contact radius. $c-a$ is the width of the cohesive zone with a constant stress $\sigma_{th}$. 

Comment: What is m??

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Asperity contact models with **adhesion**

![Normal pressure distributions for Hertz, JKR, DMT, and Maugis’ models.](image)

Positive represents compressive stresses, and negative for adhesive stresses.

**The rate of decrease of stored elastic energy in the system per unit area of crack advance is called the strain energy release rate** $G$. According to the Griffith theory [Griffith 1920], a sharp crack will advance when $G = \Delta \gamma$, that is, the energy per unit area required to create two free surfaces. Maugis derived the following based on the Griffith Equilibrium Equation.

**Comment:** You need to explain the significance of this.
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\[
\frac{\lambda A^2}{2} \left[ \sqrt{m^2 - 1} + (m^2 - 2) \tan^{-1} \sqrt{m^2 - 1} \right] \\
+ \frac{4\lambda^2 A}{3} \left[ (\sqrt{m^2 - 1} \tan^{-1} \sqrt{m^2 - 1}) - m + 1 \right] = 1
\]  

(0.19)

The stress distribution in the area of contact (positive value means tensile stress, negative value means compressive stress) is given by

\[
\sigma_z (\rho, 0) = \frac{3aK}{2\pi R} \sqrt{1 - \rho^2} + \frac{2\sigma_{th}}{\pi} \tan^{-1} \left( \frac{m^2 - 1}{1 - \rho^2} \right), \quad \rho < 1,
\]

(0.20)

\[
\sigma_z (\rho, 0) = \sigma_{th}, \quad \rho = 1,
\]

\[
\sigma_z (\rho, 0) = 0, \quad \rho = d < 1,
\]

where \(d\) is the radial position in the contact region at which the stress is zero. So there exist tensile stresses within the contact. This stress distribution outside the area of contact is given by

\[
\sigma_z (\rho, 0) = \sigma_{th}, \quad 1 < \rho < m,
\]

(0.21)

This internal loading acting in the air gap (the external crack) leads to a stress intensity factor, which is cancelled with the stress intensity factor due to the external loading. The adhesion force \(F_a\) is the integration of the tensile stresses existing both within the contact and outside the contact,

\[
F_a = 2\pi a^2 \left( \int_1^m \sigma_z (\rho, 0) \rho d\rho + \int_0^d \sigma_{th} \rho d\rho \right),
\]

(0.22)

The comparison of Maugis’ analytical model with finite element model results will be given in Chapter 3. His main results are shown in Figure 0.8 - Figure 0.10.
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Figure 2.8: Relation between radius of contact and penetration for various λ.

Figure 2.9: Relation between radius of contact and applied force for various λ.
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2.4 Plastic contact with adhesion – The Simplified Analytical Model (SAM)

All the above models are only applicable for elastic contact. When the contact bodies experience more pressure or strain, the contact is elasto-plastic or fully plastic. A simple analytical model (SAM) of elasto-plastic and fully plastic deformation with adhesion was developed by Majumder et al. [Majumder 2003] for use in a microswitch, using techniques from [Maugis 1992] and [Johnson 1985]. According to the von Misés yield criterion, the initiation of plastic deformation occurs when the second invariant of the deviatoric stress tensor reaches a critical value which is related to the yield strength ($\sigma_Y$). This state, in which some material is plastic, while the surrounding material is elastic, is
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called elasto-plastic deformation. The transition for the mean pressure from elastic to
elasto-plastic deformation is [Johnson 1985]

\[ p_n = 1.1\sigma_y , \] (0.23)

Note that Eq. (2.23) is only applicable for \( \nu = 0.3 \), though it depends weakly on \( \nu \).

Combining Eq. (2.23) with Eq. (2.12) and Eq. (2.14), the critical contact radius
for initial yielding without adhesion for a rigid indenter with \( \nu = 0.3 \) is

\[ a_c = 2.3 \frac{R\sigma_y}{E} , \] (0.24)

The critical interference can be arrived by substituting Eq. (2.24) into Eq. (2.13) which is

\[ \delta_c = \left(\frac{2.3\sigma_y}{E}\right)^2 R , \] (0.25)

and similarly the critical contact force can be arrived by substituting Eq. (2.24) into Eq. (2.12).

Chang et al. developed a plastic contact model (CEB) which approximated elasto-
plastic contact by modeling a plastically deformed portion of a hemisphere using volume
conservation [Chang 1987]. The critical interference used in CEB model is given by

\[ \delta_c^{CEB} = \left(\frac{\pi K_H H}{2E'}\right)^2 R \] (0.26)

where the hardness coefficient is given by \( K_H = 0.454 + 0.41\nu \) and \( H \) is the hardness. It is
noted that Eq. (2.26) is formulated somewhat differently than Eq. (2.25) by including
Poisson’s ratio and the relationship between the hardness and the yield strength. However
from an engineering perspective the corresponding values given by Eqs. (2.25) and (2.26)
are very close. The critical contact radius \( a_c \) and the critical contact force \( F_c \)
corresponding to the critical interference in Eq. (2.26) given in the CEB model are
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\[ a_{\text{CEB}}^c = (\delta R)^{1/2}, \quad (0.27) \]

\[ F_{\text{CEB}}^c = (2/3)K_H \pi \delta R. \quad (0.28) \]

But the critical interference with adhesion is not given by any existing theories.

With the increase of the loading force, the mean pressure keeps increasing and the plastic zone keeps growing till it reaches the surface, and the mean pressure becomes constant \( H \) (material hardness) where it is fully plastic contact.

\[ p_n = \frac{F}{\pi a^2} = 2.8\sigma_Y = H, \quad (0.29) \]

It is widely accepted that \( H/\sigma_Y = 3 \) such as in [Tabor 1951] and [Maugis 1984]. But recently theoretical and numerical results have shown that the ratio should be 2.8 ([William 1994], [Jackson 2005]). So Eq. (2.29) is used in this thesis.

Not like the Hertzian mean pressure in Eq. (2.14) which is achieved by a strict derivation, that of elasto-plastic contact is semi-empirical. Earlier work on the rigid sphere of radius \( R \) in contact with flat metallic surface was done by Studman ([Studman 1976], [Studman 1977]). For \( \nu = 0.5 \), mean pressure is,

\[ p_n = \frac{F}{\pi a^2} = \sigma_Y (1 + \frac{2}{3} \ln \frac{Ea}{3\sigma_Y R}), \quad (0.30) \]

Actually the effect of Poisson’s ratio \( \nu \) is very small, here we assume Eq. (2.30) is applicable for different \( \nu \). The critical contact radius of full plasticity by experiments is,

\[ a_p = 60 \frac{R\sigma_Y}{E}, \quad (0.31) \]

In order to obtain smooth elastic/elasto-plastic and elasto-plastic/fully plastic transitions, a slightly modified form of Eq. (2.30) was made by Maugis [Maugis 1984],
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\[ p_m = \sigma_y (1.1 + 0.58 \ln \frac{Ea}{2.3 \sigma_y R}), \quad (0.32) \]

Note that \( H/\sigma = 3 \) was used to obtain Eq. (2.32). Equation (2.32) is derived for a rigid sphere in contact with a deformable flat. It is also applicable for the case of a deformable sphere in contact with a rigid flat. If both bodies are identical materials, Eq. (2.31) is modified as

\[ p_m = \frac{F}{\pi a^2} = \sigma_y (1.1 + 0.58 \ln \frac{Ea}{4.6 \sigma_y R}), \quad (0.33) \]

The derivation for mean pressure distribution of different conditions from Eq. (2.31) to Eq. (2.33) can be found in Appendix A.

The approximate \( \delta \sim a \) relationship under fully plastic conditions was stated by Abbott and Firestone [Abbott 1933] by truncating the sphere as the rigid flat translates with an interference \( \delta \),

\[ \delta = \frac{a^2}{2R}, \quad (0.34) \]

When the adhesion is not negligible, there is no accurate analytical model for plasticity. Normally in the fully plastic regime, because the ratio of the adhesion force to the contact force is relatively small, it is reasonable to take adhesion force as a constant [Roy 1981],

\[ F = F_c + 2 \pi \gamma R = \pi a^2 H, \quad (0.35) \]

If it is also a good approximation in the elasto-plastic regime, Eq. (2.35) is still applicable and can be modified as,

\[ F = F_c + 2 \pi \gamma R = \pi a^2 p_m, \quad (0.36) \]

To derive the \( \delta \sim a \) relationship, we need consider the continuity on both extreme ends. Under sufficiently large loading forces, the effect of the adhesion force becomes
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small. Therefore the $\delta \sim a$ relationship should tend towards $\delta = \frac{a^2}{2R}$ in Eq. (2.34) of the adhesionless contact model. The other one is at the elastic limit where the $\delta \sim a$ relation of JKR model in

\[ \delta = \frac{a^2}{2R} + \frac{a_e^2}{2R} - \frac{8\pi a_e \Delta \gamma}{3K}, \quad (0.37) \]

Table should be approached. Based on these considerations, the following relationship in the elasto-plastic and fully plastic regimes are assumed [Majumder 2003],

2.5 Existing unloading model

Unloading as a follow-up stage of loading plays an important role on the reliability of microswitch since its separation modes may determine the magnitude of the adherence force and the subsequent topography. As in plastic loading, plasticity may also occur during unloading for large loading plasticity. For example, Kadin found plastic unloading during both the first and the following cycles of loading and unloading when $\delta_f / \delta_e$ is up to 150 [Kadin 2006]. Figure 0.11 is the equivalent von Misès stress field after the first loading. Yielding was found near the edge of the contact. This discussion is for the case without adhesion.
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Unloading plasticity may also be caused by high adhesion energy, as shown in Figure 2.12. A molecular dynamics model showed that the adhesion can cause ductile

![Equivalent von Mises stress field](image)

Figure 0.11, Equivalent von Mises stress field after the first unloading from $\frac{\delta_f}{\delta_c} = 150$ [Kadin 2006].
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Figure 0.12. Morphology of the nano contact after unloading with adhesion energy equal to 1 J/m$^2$ from MD simulation [Song 2006].

separation in contact bumps as small as 2.5 nm in radius [Song 2006]. Material transfer was also found from one side to the other. More details will be presented in the next chapter.

Although unloading plasticity is widely observed in experiments and numerical simulations, it is hard to predict theoretically the unloading plasticity in detail because of the complex combinations of many phenomena, such as elasticity, plastic deformation, chemical reactions, adhesion, material transfer, etc. And it is even more complicated when multi-scale effects are involved.

In this section we talk only about elastic unloading. The assumption that the unloading is purely elastic is widely used by a lot of analytical work to simplify the problem ([Maugis 1984], [Mesarovic 2000]). First let us think about the case without adhesion. If the loading is elastic (Hertzian), then the unloading is simply Hertzian. If the loading is plastic, a generally accepted assumption is that plastic deformation only occurs within the first cycle of loading. The following cycles of loading and unloading only have elastic deformation, and follow Hertz theory. So to achieve the same mean pressure at the same loading force and contact radius, the radius of the bump should be replaced by residual radius of curvature,

$$R_{res} = \frac{a^3 K}{F} = \frac{a^3 K}{\pi a^2 p_m} = \frac{aK}{\pi p_m}, \quad (0.38)$$

The force-displacement curve is like those in Figure 0.13 [Etsion 2005].
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The bump is flattened after contact due to plastic deformation in Figure 0.14 and its residue interference is given by Etsion [Etsion 2005] as

\[
\frac{\delta_{res}}{\delta_f} = (1 - \frac{1}{(\delta_f / \delta_c)^{0.28}})(1 - \frac{1}{(\delta_f / \delta_c)^{0.07}}),
\]  

(0.39)

Figure 0.13. Dimensionless contact load vs. dimensionless interference without adhesion [Etsion 2005].
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Figure 0.14 Three different elastic-plastic stages of the unloading problem.

which was shown to agree well with the theoretical results,

\[
\frac{\delta_{\text{res}}}{\delta_f} = 1 - \frac{a^2}{R_{\text{res}}\delta_f}, \quad (0.40)
\]

\[ R_{\text{res}} \] is a useful parameter. But in reality, the residue profile of the sphere after unloading is not an ideally round bump with radius of \( R_{\text{res}} \). The EKK model gives a curve-fit to the finite element simulations for \( R_{\text{res}} \) [Etsion 2005],

\[
\frac{R_{\text{res}}}{R} = 1 + 1.275\left(\frac{E}{\sigma_y}\right)^{-0.216}\left(\frac{\delta}{\delta_y} - 1\right), \quad (0.41)
\]

Although the EKK model did not consider adhesion, it can be used for the DMT type of adhesion model with plastic deformation since the adhesion does not change the deformation in the DMT model. Note that in Eq. (2.41) \( R_{\text{res}} \) is called the residual radius of curvature at the summit of the deformed and fully unloaded sphere. This value is found to be greater at the summit than at other radial positions indicating that the sphere
Asperity contact models with adhesion has been flattened more at its apex than elsewhere. The discrepancy between the numerical $R_{res}$ in Eq. (2.41) and the $R_{res}$ in Eq. (2.38) from the SAM model is enlarged with larger penetration and smaller ratio of $E/\sigma_y$.

When the adhesion is included in unloading, the behavior is more complicated. $R_{res}$ is affected which will in turn affect the adherence force. For unloading following an elastic loading, the Maugis’ transition model for a wide range of Tabor parameter $\mu$ (Maugis used $\lambda = 1.16 \mu$ instead) is still applicable. So the path is going to follow the curves in Figure 0.8 - Figure 0.10 back and the separation occurs at the unstable equilibrium point. The adherence force (pull-off force) required to separate the contact at fixed force or at fixed grips corresponds to a horizontal or vertical tangent, when it exists in Figure 0.10. Its value is plotted as a function of $\lambda$ in Figure 0.15.
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Figure 2.15. Adherence force at fixed load and at fixed grips as a function of $\lambda$. At fixed load there is always a jump; at fixed grips the jump appears at $\lambda > 0.938$ [Maugis 2000].

Fixed grip is that a force is applied with infinite spring stiffness. Fixed force is that a force is applied with a weight. Separation with fixed load always has a jump out of contact, while separation with fixed grip only have jump with $\lambda > 0.938$ when the curve in Figure 2.10 becomes $S$-shaped. Otherwise separation occurs at contact radius equal to zero. Therefore the adherence force for fixed load can be expressed as

$$ F_{adh} = \alpha \pi \Delta \gamma R $$

in which the coefficient $\alpha$ can vary from 2 to 1.5 with the increase of Tabor parameter $\mu$ from the DMT region to the JKR region. For $\mu > 1.7$, the coefficient is close to 1.5. The adherence force for finite stiffness should be located between the two curves.

Maugis has another contribution in collaboration with Pollock (the MP model) to the unloading following plastic loading by modifying JKR theory and deriving three separation modes, and when they exist [Maugis 1984].

JKR theory in its original form applies only to the elastic loading case. But it can also be used to explain unloading by replacing $R$ with $R_{res}$. More details can be found in [Maugis 1984] and [Majumder 2003]. The initiation of unloading is equivalent to the elastic unloading of a flat punch at constant contact radius, until a force $F_m$ is reached where the equilibrium condition that strain energy release rate is equal to adhesion energy ($G = \Delta \gamma$) is met.

$$ F_m = -\left\{ (6\pi \Delta \gamma K a^3)^{1/2} - \pi a^2 p_w \right\}, $$

(0.43)
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If the contact radius $a$ is already less than the minimum stable radius,

$$a_{\text{min}} = \left( \frac{3}{2} \frac{\pi \gamma R_{\text{res}}}{2K} \right)^{1/3},$$

permitted by the JKR theory, this equilibrium is unstable and separation occurs. Thus in this case $F_m$ is in fact the adherence force. If $a > a_{\text{min}}$, the contact radius starts to decrease till $a_{\text{min}}$ and separates, the adherence force is the minimum allowed applied force $F_e$, which is

$$F_b = -\frac{3}{2} \frac{\pi \gamma R_{\text{res}}}{2K},$$

There exist both an analytically derived expression Eq. (2.38), and a numerically derived expression Eq. (2.41) for the effective radius of curvature $R_{\text{res}}$ in Eq. (2.45).

The above two kinds of separations at the interface can be called brittle separation, while ductile separation occurs within the softer body of the contact when the average tensile stress becomes equal to the hardness. Here only constant contact radius is considered for ductile separation. The adherence force then is,

$$F_d = \pi a^2 H,$$

The criteria for these three separation modes were first studied by the MP model [Maugis 1984] and further summarized in [Majumder 2003],

**Ductile ($F_d$) mode:** following elasto-plastic loading - $a < \frac{6K\Delta\gamma}{\pi(H + p_n)^2}$; following plastic loading - $a < \frac{3K\Delta\gamma}{2\pi H^2}$.

**Brittle ($F_m$) mode:** following elasto-plastic loading - $\frac{6K\Delta\gamma}{\pi(H + p_n)^2} < a < \frac{3K\Delta\gamma}{2\pi H^2}$; not possible after plastic loading.
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**Brittle (\(F_b\)) mode:** following elasto-plastic loading - 
\[ a > \frac{3K\Delta\gamma}{2\pi\mu_m^3} \]; following plastic loading - 
\[ a > \frac{3K\Delta\gamma}{2\pi H^2} \].

Figure 0.16 is the schematic of the three models of adherence. In general, ductile separation is more likely to occur at small loads, and in solids with high Young’s modulus, low hardness and high adhesion energy. But depending on the combination of all the parameters, the separation modes may experience all three modes from \(F_d\) - \(F_m\) - \(F_b\) in order with the increase of loading, or skip \(F_d\) or \(F_m\) modes. Large enough loading should always give brittle \(F_b\) mode. The detail analysis of ductile and brittle separations and its finite element verification are presented in the following chapters.

Figure 0.16 Schematic of the three modes of adherence – ductile separation \(F_d\) and two types of brittle separation \(F_m\) and \(F_b\).
2.6 Applications to real microswitches

The applications of the above theories are made to real microswitches. Ruthenium and gold are the candidate materials. The material properties for the calculations are listed in Table 2.2. The radius of curvature of the contact bump is assumed to be 4 \( \mu m \), the Young’s modulus for ruthenium and gold are 450 \( GPa \) and 91 \( GPa \), respectively. Ruthenium is relatively hard material with a hardness of 15 \( GPa \). The hardness for gold ranges from 0.2 to 2 \( GPa \), corresponding approximately to the measured range of hardness from the macro to nano scales. The work of adhesion of ruthenium is not well characterized but we assume a small value of 0.2 \( J/m^2 \) as a lower bound estimate and 2 \( J/m^2 \) as an upper bound. The work of adhesion of clean gold (2 \( J/m^2 \) is within the normal range for gold [Jiang 2004]) is used here.

Figure 0.17 is the contact radius-force curve for each case during loading using the SAM model and the MP model. We can see for large applied force, the effect of hardness dominates the deformation of contact. Softer material tends to have greater contact radius. However different adhesion energy does not affect the deformation too much. We even can not see the difference between two ruthenium contacts with different adhesion energy. It is worth mentioning that in Figure 0.17 the maximum contact radius is up to 3.5 \( \mu m \) for soft gold which is comparable to the radius of the bump \( R \). The theories used are typically for smaller deformation with \( a << R \), so the results at large deformation may not be accurate.
Table 2.2 Material Properties for Gold (Au) and Ruthenium (Ru)

<table>
<thead>
<tr>
<th>Material</th>
<th>$R$ (µm)</th>
<th>$E$ (GPa)</th>
<th>$H$ (GPa)</th>
<th>$\nu$</th>
<th>$\Delta\gamma$</th>
<th>$Z_0$</th>
<th>$\mu = \left(\frac{R\Delta\gamma^2}{E^2 Z_0}\right)^{1/3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soft Au</td>
<td>4</td>
<td>91</td>
<td>0.2</td>
<td>0.32</td>
<td>2</td>
<td>0.184</td>
<td>6.77</td>
</tr>
<tr>
<td>Hard Au</td>
<td>4</td>
<td>91</td>
<td>2</td>
<td>0.32</td>
<td>2</td>
<td>0.184</td>
<td>6.77</td>
</tr>
<tr>
<td>High $\Delta\gamma$ Au</td>
<td>4</td>
<td>450</td>
<td>15</td>
<td>0.32</td>
<td>2</td>
<td>0.4</td>
<td>1.07</td>
</tr>
<tr>
<td>Low $\Delta\gamma$ Au</td>
<td>4</td>
<td>450</td>
<td>15</td>
<td>0.32</td>
<td>0.2</td>
<td>0.4</td>
<td>0.23</td>
</tr>
</tbody>
</table>

Figure 2.17. Plot of contact radius as a function of applied force for different material properties using the SAM model and the MP model.
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Figure 0.18 shows the area of Figure 0.17 at the beginning of the contact. The Tabor parameters for these four materials are 6.77, 6.77, 1.07, and 0.23, respectively. So the first three materials have jump into contact as predicted by Maugis. Due to the effect of adhesion, the first contact may occur at negative (tensile) force. In addition, since gold is relatively soft, its contact is been elasto-plastic at the first contact. Although the trend of these curves are fairly clear, more points will appear later.

The adherence force as a function of the maximum loading force is shown in Figure 0.19. From Figure 0.19 we can see that the adherence force is a constant for elastic loading, but it depends on the maximum loading force for plastic loading. The y-axis is plotted as semi-log for comparison. Higher hardness leads to less plastic yielding during loading and smaller adherence force during unloading. Higher work of adhesion also
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Asperity contact models with adhesion increases the adherence force. In the four curves of Figure 0.19, only the softer gold experiences ductile separation.

Figure 0.19. Adherence force as a function of the maximum loading force for gold and ruthenium.
Chapter 3

Finite element models for adhering microcontacts

It was seen from the previous chapter that many simplifying assumptions were needed in order to obtain a solution, therefore it is very difficult for analytical analyses to accurately predict complicated phenomena during unloading such as the combined effects of plasticity and adhesion. It is both more accurate and straightforward to solve such problems using numerical methods. For example Kogut and Etsion (KE) built a finite element model (FEM) with ANSYS® to study elastic-plastic contact without [Kogut 2002] and with [Kogut 2003] adhesion. The results allowed simple curve-fit equations for the relations among force, displacement and contact area. Subsequent work by Jackson and Green [Jackson 2005] without adhesion using more nodes agreed well with [Kogut 2002] and allowed for greater displacements. Because the FEM analysis of [Kogut 2003] neglects the effect of adhesion on deformation and stress, it is only applicable for
conditions in the DMT region. By modifying the KE model, we built a more general model which includes the effect of adhesion on the deformation and stress, and is therefore applicable to a wide range of material properties. The results demonstrate that during small loading this model agrees with [Kogut 2003] in the DMT region, but has a large discrepancy with [Kogut 2003] in the JKR region. Since this work is a modification of the KE model, let me introduce the KE model first.

### 3.1 Finite elements analysis model from Kogut & Etsion

Many good numerical results on microcontacts have been obtained by Kogut and Etsion such as in [Kogut 2002]. Figure 3.1 is their finite element model. It consists of 1920 six-node triangular axisymmetrical elements (Plane2), comprising a total of 3987 nodes. The 3-D system was represented by a 2-D model since it is axisymmetric. The top horizontal line represents the rigid flat surface and the bottom quarter circle represents the deformable hemisphere. Boundary conditions are the horizontal straight line on the bottom of the sphere is constrained in the y-direction only and the vertical line on the left side is constrained in x-direction only. The sphere is divided into four different mesh density zones where zones I, II, and III are within 0.01R, 0.05R, and 0.1R distances, respectively, from the sphere tip; zone IV is outside the 0.1R distance. Each of the four zones contains the same number of elements hence, zone I had the finest mesh and each zone has a gradually coarser mesh at increasing distance from the sphere tip.

The sphere surface consists of contact elements (Conta172) that match the size of the elements in zones I to IV. The material of the sphere was assumed to have elastic
linear hardening characterized by a tangent modulus $E_T$. The tangent modulus represents the slope of the stress-strain curve in the plastic region. Its value is influenced by the grain size and the Young’s modulus $E$. A value of 2% of the Young’s modulus was chosen here for simulation because 2% is within the range of values often observed [Galambos 1998] and is consistent with achieving convergence. The rigid flat was modeled by a single, non-flexible element (Targe169). The von Misés yielding criterion was used to detect local transition from elastic to plastic deformation. This meshing was found to be a good combination of computation time and convergence. First it was compared with Hertz’ elastic theory for $\delta_f / \delta_c < 1$, and the models agreed within a 5% error. Another check was made at deep penetration up to $\delta_f / \delta_c = 150$ by increasing the number of elements and ensuring convergence of the results within a pre-selected small
tolerance. Several published papers using this model ([Etsion 2005], [Kogut 2002]) have proven to be in good agreement with others’ work [Jackson 2005].

In [Jackson 2005], Jackson and Green (JG) also performed finite elements simulation with ANSYS®. The JG model is shown in Figure 3.2 which consists of 11,101 elements which are much more than what KE model used. The JG model not only set up very fine mesh density, also monitored the difference of contact force and contact area between each iteration with different mesh density to make sure the results got convergence within 1% difference. Another difference is instead of only constraining y-direction on the bottom line of the sphere by KE model, they also constrained the x-direction, because they thought about two reasons: (1) The asperities are actually

Figure 3.2 Finite element model of Jackson and Green which consist of 11,101 elements.
Chapter 3 Finite element models for adhering microcontacts

connected to a much larger bulk material at the base and will be significantly restrained there, and (2) since the high stress region occurs near the contact, the boundary condition at the base of the hemisphere will not greatly effect the solution. The change in results between the said boundary conditions and one in which the nodes along axis $x$ are allowed to translate radially have shown only marginal difference (less than 3% difference in area, and less than 1% in load.)

The JG model compared the results with the KE model and found the KE model is similar to theirs on the relation of contact force, contact radius, and interference, although the KE model starts to overestimate the contact force from about $\delta_f/\delta_c=50$. Instead of terminating at $\delta_f/\delta_c=110$ in the KE model, the JG model continues to deform the sphere up to $\delta_f/\delta_c=500$ at which the contact geometry changes dramatically, such as $a/R$ (contact radius over radius curvature of the sphere) close to one. They find that the fully plastic mean pressure, or hardness $H$, actually varies with the deformed contact geometry, which in turn is dependent upon the material properties (e.g. yield strength $\sigma_Y$). $\sigma_Y/H = 2.8$ as $a/R$ approaches zero instead of a factor of three as commonly approximated. Since we do not need to consider so highly deformed case as in the JG model, the meshing method of the KE model is used and modified for our research.

There are two ways to simulate the contact problem. The first applies a force to the rigid body and then computes the resulting displacement which is in accordance with the fixed force case in Maugis’ transition model mentioned in the previous chapter. The second applies a displacement and then computes the resulting contact force which is the fixed grip case in Maugis’ model. In both methods, the displacement, stress, and strain in
the elastic body can be determined. In both the KE model and the JG model, the latter
method was used and it is also used in my model.

The main results of KE model are shown in Table 3.1(a) & (b). \( F_s \) is the adhesion
force. The critical interference in Table 3.1 for initial yielding is given by [Chang 1987]
in Eq. (2.26). Two things need to be mentioned here. One is because the KE model
ignored the effect of adhesion, the simulation started from zero interference and the
critical interference is the same with the case without adhesion. Actually with adhesion
the first contact should occur before zero interference and initial yielding should occur
before critical interference in Eq. (2.26). The other one is the result of \( F_s \sim \delta_f \) in Table
3.1(b) seems to exclude the very small interference for \( \delta_f < 0.1 \delta_e \) at
\( 0.005 \leq Z_a / \delta_e \leq 0.5 \), see when substituting \( \delta_f = 0 \) in the corresponding expression we
get adhesion force equal to zero, which is not true.

Table 3.1(a) Empirical results of \( F \sim \delta_f \) and \( a_f \sim \delta_f \) by KE model

<table>
<thead>
<tr>
<th>Contact</th>
<th>( \delta_f / \delta_e )</th>
<th>( F \sim \delta_f )</th>
<th>( a_f \sim \delta_f )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic</td>
<td>Hertz Theory</td>
<td>( F / F_e = 1.03(\frac{\delta_f}{\delta_e})^{1.425} )</td>
<td>( \frac{a_f}{a_e} = 0.93(\frac{\delta_f}{\delta_e})^{1.136} )</td>
</tr>
<tr>
<td>Elasto-plastic or fully plastic</td>
<td>( 1 \leq \delta_f / \delta_e \leq 6 )</td>
<td>( F / F_e = 1.40(\frac{\delta_f}{\delta_e})^{1.263} )</td>
<td>( \frac{a_f}{a_e} = 0.94(\frac{\delta_f}{\delta_e})^{1.146} )</td>
</tr>
<tr>
<td></td>
<td>( 6 \leq \delta_f / \delta_e \leq 110 )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 3.1 (b) Empirical results of $F_s \sim \delta_f$ by KE model

<table>
<thead>
<tr>
<th>Contact</th>
<th>$Z_o / \delta_c$</th>
<th>$\delta_f / \delta_c$</th>
<th>$F_s \sim \delta_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic</td>
<td>0.005 ≤ $Z_o / \delta_c$ ≤ 0.5</td>
<td>N/A</td>
<td>$\frac{F_s}{F_{s0}} = 0.979 \left( \frac{Z_o}{w_c} \right)^{0.29} \left( \frac{\delta_f}{w_c} \right)^{0.298}$</td>
</tr>
<tr>
<td></td>
<td>0.5 ≤ $Z_o / \delta_c$ ≤ 100</td>
<td>N/A</td>
<td>$\frac{F_s}{F_{s0}} = 1.001 + \frac{0.192 \delta_f / \delta_c}{Z_o / \delta_c}$</td>
</tr>
<tr>
<td>Elasto-plastic or fully</td>
<td>0.005 ≤ $Z_o / \delta_c$ ≤ 0.5</td>
<td>1 ≤ $\delta_f / \delta_c$ ≤ 6</td>
<td>$\frac{F_s}{F_{s0}} = 0.792 \left( \frac{Z_o}{w_c} \right)^{0.321} \left( \frac{\delta_f}{w_c} \right)^{0.556}$</td>
</tr>
<tr>
<td>plastic</td>
<td>6 ≤ $\delta_f / \delta_c$ ≤ 110</td>
<td>6 ≤ $\delta_f / \delta_c$ ≤ 110</td>
<td>$\frac{F_s}{F_{s0}} = 1.193 \left( \frac{Z_o}{w_c} \right)^{0.332} \left( \frac{\delta_f}{w_c} \right)^{0.093}$</td>
</tr>
<tr>
<td></td>
<td>0.5 ≤ $Z_o / \delta_c$ ≤ 100</td>
<td>1 ≤ $\delta_f / \delta_c$ ≤ 6</td>
<td>$\frac{F_s}{F_{s0}} = 0.961 + \frac{0.157 Z_o / \delta_c}{Z_o / \delta_c} + \frac{0.261 \ln(\delta_f / \delta_c)}{Z_o / \delta_c}$</td>
</tr>
<tr>
<td></td>
<td>6 ≤ $\delta_f / \delta_c$ ≤ 110</td>
<td>6 ≤ $\delta_f / \delta_c$ ≤ 110</td>
<td>$\frac{F_s}{F_{s0}} = 1.756 - (0.516 - \frac{0.303 Z_o / \delta_c}{Z_o / \delta_c}) \ln(\delta_f / \delta_c) + 0.052(\ln(\delta_f / \delta_c))^2$</td>
</tr>
</tbody>
</table>

3.2 Finite element model for microcontacts in this thesis

When the KE model was used for analyzing the effect of the adhesion, it made the assumption that the adhesion does not affect the deformation profile of contact. So the adhesion effect is not really included during simulation. Post-processing to determine the adhesion force is obtained by taking the deformed surface geometry of the bump after the
simulation is done for the integration of the Lennard-Jones’ stress in Eq. (2.4). For the elastic loading case, since there exists an analytical expression for geometry, the integration is not from the numerical results.

Therefore this model should be applicable for the DMT model. It can not be accurate when the Tabor parameter $\mu$ is bigger ($\mu > 3$) and the contact tends to follow the JKR approximation. These criteria for each model to be valid have been derived by many analytical and numerical works (Maugis 1992, Greenwood 1997). It is necessary to build a general model considering the adhesion effect on the geometry. For simplicity, but still not losing generality a deformable sphere in contact with a rigid flat is considered. The analysis of the above case can be extended to the case of a rigid sphere on a deformable flat or both deformable although the elastic and plastic boundary conditions are slightly different.

Figure 3.3 shows the mesh for the finite element adhesive contact model using ANSYS®. It consists of no more than 17,331 six-node triangular axisymmetrical elements (Plane2), comprising a total of 31,681 nodes depending on the requirement on the loading levels. Fine elements with a size of $3 \text{ nm}$ are added on the surface of the sphere in order to resolve the effect of adhesion, because for small separations the LJ stresses vary very rapidly with separation.

The top horizontal line represents the rigid flat surface and the quarter circle represents the deformable hemisphere. The boundary conditions are that the horizontal surface on the bottom of the hemisphere is constrained only in the y-direction and the vertical line on the left side is constrained only in the radial direction.
Except for the surface layer, the sphere was divided into 2 different mesh density zones in which the zone closer to the apex has the finer mesh. The sphere surface consists of contact elements (Conta172) that match the size of the elements on the surface. The rigid flat was modeled by a single, non-flexible element (Targe169). The von Misés yield criterion was used to detect the local transition from elastic to plastic deformation.

The displacement or the interference $\delta$ of the top flat surface is controlled in this simulation. It is defined as the vertical distance between the top flat and the summit of the sphere without deformation. Negative interference means the top flat is above the undeformed hemisphere summit. The effect of adhesion on the sphere is fulfilled by...
adding the LJ stresses given by Eq. (2.4), using an iterative procedure, as negative pressures acting on the surface of the sphere. The angle between the normal and vertical directions is small enough to neglect this difference. The goal of this simulation is to find the deformation of the sphere under the combined effects of displacement and attractive stresses at each displacement of the flat.

The flat starts to approach the sphere at a prescribed distance above the sphere, e.g. $\delta = -2\delta_c$. The pressure acting on the surface nodes is obtained by $p_j^i = -\sigma(Z_j)$, where $i$ represents the $i^{th}$ iteration and $j$ represents the node number. The separation $Z$ is adjusted to the atomic level by adding $Z_0$. So the edge of the contact is defined to be at $Z = Z_0$ (actually $Z = 1.01Z_0$ is used to overcome a numerical problem). After each iteration, the y-deformation $u_j^i$ of the sphere changes due to the effect of adhesive stresses. The maximum difference of the present iteration and the last iteration is

$$\varepsilon^i = \max|u_j^i - u_j^{i-1}|.$$  \hfill (3.1)

The iteration is stopped when $\varepsilon^i$ is smaller than a preset tolerance $\varepsilon_0$. The resolution used here is $0.001Z_0$. However because this problem is nonlinear, with the possibility of unstable convergence, the pressure at each iteration requires an adjustment by an under-relaxation factor $C \leq 1$, i.e.

$$p_j^i = p_j^{i-1} + C(p_j^i - p_j^{i-1}).$$  \hfill (3.2)

Accordingly the convergence criterion is modified according to

$$\varepsilon^i < \varepsilon_0 C.$$  \hfill (3.3)

An interpolation method for the LJ stresses is used to help convergence. First a curve-fit of $Z$ over $x$ is obtained over a small range of three consecutive nodes $j-1, j,$ and $j+1$,
Chapter 3 Finite element models for adhering microcontacts

\[ Z = Z(x) = \frac{(x - x_j)(x - x_{j+1})}{(x_{j+1} - x_j)(x_{j+1} - x_{j-1})} Z_{j+1} + \frac{(x - x_{j-1})(x - x_{j+1})}{(x_j - x_{j-1})(x_{j+1} - x_j)} Z_j \]

Then the original pressure of node \( j \) is replaced by an average pressure in

\[ p_j^{\text{average}} = \frac{\int_{x_{j-\Delta x_2}}^{x_{j+\Delta x_2}} p(Z(x))2\pi xdx}{\pi(x_j + \Delta x_2)^2 - (x_j - \Delta x_1)^2} \]

which is the force divided by the finite area around node \( j \), spanned from \( x_j - \Delta x_1 \) to \( x_j + \Delta x_2 \) in the radial direction \([\Delta x_1 = (x_j - x_{j-1})/2, \Delta x_2 = (x_{j+1} - x_j)/2]\). By using this method, the total adhesion force is accurately accounted for. The flowchart of the algorithm for the simulation can be found in Figure 3.5.

Theoretically contact elements are not necessary in this model since the Lennard-Jones’ potential itself governs the interaction. I have tried this way and it worked. The integration of the attractive stress is equal to the adhesion force \( F_a \), and the integration of the compressive force is the contact force \( F \). The difference of those two forces is external applied force \( F_e \). But since the compressive stress increases dramatically when the two bodies are closer shown in Figure 0.1(a), it took a lot of computer time and was hard to get convergence. This issue can be solved by using the contact element in ANSYS®. Contact elements work within the contact area and they generate force as contact force which is equivalent to the integration of the compressive stresses. So we only need to consider the adhesive stresses outside the contact area. The Lennard-Jones curve is Figure 0.1(b). So the vertical distance of the atoms on the surfaces of the two bodies is constrained to be not less than \( Z_0 \).
Chapter 3 Finite element models for adhering microcontacts

Less calculation time is always desired in simulation. It is based on the mesh density and the some input parameters such as penalty stiffness and tolerance. Greater stiffness and smaller tolerance will consume more computer time. In addition the amount

\[
p_i^j = \sigma(Z_j)
\]

\[
\varepsilon_i = \max(|u(y)_j^i - u(y)_j^{i-1}|)
\]

\[
\varepsilon_i < \varepsilon_0 \times C^i?
\]

\[
\delta_m = \delta_{m-1} + \Delta\delta
\]

\[
\delta_0 = -2\delta
\]

\[
\delta_j = \sigma(Z_j)
\]

\[
p_j^i = p_j^i + C(p_j^i - p_j^{i-1})
\]

\[
p_j^i = \int p_j^i dA_j / \int dA_j = Eq. (3.5)
\]

\[
\text{Variable Definition}
\]

\[
\delta – \text{The displacement of the flat surface;}
\]

\[
Z – \text{The vertical separation of the surface of the sphere and the flat;}
\]

\[
p – \text{The normal pressure added on the surface of the sphere;}
\]

\[
u(y) – \text{The displacement of the node on y-direction;}
\]

\[
\varepsilon – \text{The difference of } u(y) \text{ between two continuous iterations;}
\]

\[
m – \text{Number of displacement steps;}
\]

\[
C – \text{Under-relaxation factor;}
\]

\[
M – \text{Pre-assigned maximum steps;}
\]

\[
count – \text{number of}
\]

\[
\text{m} = m + 1
\]

\[
\text{Terminates}
\]

\[
\text{Start}
\]

\[
\text{Count} = 0
\]

\[
\text{Start Simulation}
\]

\[
\text{Post-Processing Data}
\]

\[
\text{Decision}
\]

\[
\text{Flow Direction}
\]

\[
\text{ANSYS Action}
\]

\[
\text{Flowchart Key}
\]

\[
\text{Deleted: 3.4}
\]
of under-relaxation factor $C$ used in Eq. (3.3) can be critical to the calculating time. Too much leads to numerical instabilities, while too little slows down convergence. Similarly, a poorly chosen convergence criteria can lead to either poor results (when too loose) or excessive computational times (when too tight). Generally we hope the simulation for each displacement can be fulfilled within 20 outer iterations. So the programming is chosen to stop after the maximum iteration is reached.

The maximum difference of deflection $\epsilon^i$ at each iteration is studied. If it varies around a much bigger value than resolution, the relaxation factor is too big. If they keep decreasing, but it still takes 20 iterations, that means the factor is too small. After appropriate adjustment is made, the simulation is resumed. If after 20 iterations, the simulation is still not converged, use the same method to adjust the factor till we get solutions. Eventually with more knowledge of this issue, a self-adjusted under relaxation factor is desired in each iteration.

Two successful examples of under relaxation method were given by Greenwood. Both of them were used for elastic case. In 1967, he calculated the pressure distribution of a smooth sphere in contact with a rough flat surface without adhesion for different roughness [Greenwood 1967]. The other one was done in 1997. He presented the comprehensive numerical computations of the contact of a micro hemisphere and a flat with the Lennard-Jones potential for the relationship between applied force, contact
radius and interference at different Tabor parameter $\mu$ [Greenwood 1997]. In this work he mentioned that the factor $C$ is very small for $\mu$ larger than 1 which I also found in my simulation. That is because bigger $\mu$ corresponds to the JKR model, and the sharper edge profile causes more difficulty with convergence. More weight of the previous solution should be involved into the calculation. But a tricky thing is if $C$ is too small, after several iterations, the difference of current and previous pressure times $C$ may be small although the difference itself is still relatively big. $\epsilon^i$ is greatly dependent on the changing amount of pressure. Less change of pressure will apparently cause convergence, which is actually false. The solution to this problem is to multiply $C$ by the resolution $\epsilon_o$ so the new resolution gets tighter with smaller $C$.

### 3.3 Comparisons between analytical and numerical models

With the above method, we performed a series of simulations for Ru and Au with the dimensions and material properties listed in Table 3.2. The adhesion energy (double the surface energy) of perfectly clean metals is reported to be more than 3 $J/m^2$ in [de Boer 1988]. It is chosen to be 1 $J/m^2$ here for both metals in consideration of the imperfect surface covered by impurity films when the testing is not done under the UHV conditions. We hope to determine the most appropriate value for adhesion energy with future simulations and experiments.

Table 3.2 Material properties of Ru and Au for finite element simulations
It is needed to be mentioned that the plasticity of a contact at micron scale should account for a material size effect, that is, the smaller the imposed geometric length scale relative to some material length scale, the stronger the material in its plastic response. This strain gradient theory has been advanced by Fleck [1993] based on the idea that a strain gradient leads to enhanced hardening due to the generation of geometrically necessary dislocations. In contrast, conventional constitutive theories of plasticity possess no material length scale. Predictions based on these theories involve only lengths associated with the geometry of the solid. Although the strain gradient plasticity was not included in this FEM continuum model, relatively large values of the hardness were used to compensate this effect.

The comparisons of results for loading are made between the curve-fits for the KE model and our finite element simulation. The results of the Maugis transition model for the elastic region and the SAM model for the elasto-plastic and fully plastic regions are also included for comparison. In order to compare these two cases with different material properties, all figures are plotted in dimensionless coordinates, i.e. dimensionless interference $\delta_f/\delta_c$, dimensionless external force $F_e/F_c$, and dimensionless contact radius $a_f/a_c$. Figure 3.5 is for small loads and Figure 3.6 is for large loads.

<table>
<thead>
<tr>
<th>Case</th>
<th>$R$ ($\mu$m)</th>
<th>$E$ (GPa)</th>
<th>$\nu$</th>
<th>$\sigma_Y$ (GPa)</th>
<th>$Z_\gamma$ (nm)</th>
<th>$\DeltaY$ ($J/m^2$)</th>
<th>$\delta_c$ (nm)</th>
<th>$E/\sigma_Y$</th>
<th>$S$</th>
<th>$\mu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ru</td>
<td>4</td>
<td>410</td>
<td>0.3</td>
<td>3.42</td>
<td>0.169</td>
<td>1</td>
<td>1.70</td>
<td>120</td>
<td>0.6</td>
<td>1.6</td>
</tr>
<tr>
<td>Au</td>
<td>1</td>
<td>80</td>
<td>0.42</td>
<td>0.67</td>
<td>0.184</td>
<td>1</td>
<td>0.41</td>
<td>120</td>
<td>2.7</td>
<td>2.7</td>
</tr>
</tbody>
</table>
Figure 3.5: Comparisons of our FEA model with the Maugis model and KE model for Ru (left) and Au (right) under small loads. The material properties and geometry are given in Table 3.2. (a) & (b) Dimensionless contact radius vs. dimensionless interference; (c) & (d) Dimensionless force vs. dimensionless interference. The star (*) is the initiation of yielding for this work and the triangle (Δ) is for the KE model.
Figure 3.6 Comparisons of our FEA model with SAM model and KE model for Ru (left) and Au (right) under large loads. The material properties and geometry are given in Table 3.2. (a) & (b) Dimensionless contact radius vs. dimensionless interference; (c) & (d) Dimensionless force vs. dimensionless interference.

First let us discuss the comparisons for small load in Figure 3.5. For Ru, the Tabor parameter of $\mu = 1.6$ is not great enough for the adhesion force to cause a large effect on deformation. The comparison for Ru shows our results agree well with the Maugis model in the elastic region and also for small degrees of plastic deformation. However it does demonstrate a larger contact radius and greater external force under the same interference
than those of KE model, although the difference is not large. This difference is reasonable because the KE model represents DMT behavior which requires a smaller force for a given interference [Kogut 2003]. The star (*) represents the initiation of yielding in our model and the triangle (Δ) is that of the KE model. Our model predicts earlier yielding than does the KE model because we include the effect of adhesion on the stress field.

For Au the Tabor parameter \( \mu = 2.7 \) is large enough to see the characteristics of the JKR region. Again the star indicates the onset of plasticity in our model which is seen to occur for low, and in fact for negative loads. Thus there is a significant difference between the Maugis elastic model and our results for force vs. interference. However the plot of contact radius vs. interference is much closer to the Maugis result. Note that the KE model is not capable of predicting the jump into contact and the initial yielding due to adhesion. The discontinuity shown for the force curve of the KE model is due to the mismatch of the curve-fits of two ranges of the interferences [Kogut 2003].

A comparison for the larger plastic deformation cases in Figure 3.6 shows that the discrepancy between the two numerical models tends to be insignificant because the ratio of the adhesion force to the external force is small for both Ru and Au. However the SAM model for the plastic region shows larger value than the two numerical models. In addition, the dimensionless external force and contact radius of Ru and Au under the same dimensionless interference are almost equal which confirms the conclusion that the loading (expressed in the dimensionless form of [Kogut 2002]) is independent of the material properties [Kogut 2002], even with adhesion and large plastic deformation.

Results for unloading are given in Figure 3.7 for contact radius vs. interference and for external force vs. interference. Four loading-unloading curves are obtained based
on different maximum loading interferences. Although the force vs. interference curves are smooth for Au, the contact radius curves during unloading are rough if the edge of the contact was defined using $Z = 1.01Z_0$ as mentioned earlier [Du 2006]. This behavior is most probably caused by numerical problems. But with $Z = 1.2Z_0$ used to determine the contact radius for Au, the numerical problem is solved (Figure 3.7) without affecting the general shape of the curve.

Figure 3.7 Dimensionless contact radius vs. dimensionless interference for a single load/unload cycle for Ru and Au. The material properties and geometry are given in Table 3.2.
Figure 3.8 Dimensionless force vs. dimensionless interference of a single cycle of load and unload for Ru and Au. The material properties and geometry are given in Table 3.2.

It is clear that the loading curves for Ru and Au are consistent in both Figure 3.7 and Figure 3.8, but the unloading curves show very different characteristics. In Figure 3.7, for Ru, the contact radius decreases smoothly to a small value and then separates, while for Au the contact radius decreases stepwise slowly and then suddenly separates. A jump-out-of-contact is obtained from Au. Let us recall the prediction of the separation contact radius by the SAM model that the ductile separation occurs at a constant value $a_f$, while brittle separation can occur at a smaller value $a_{min}$ than $a_f$. In addition Au has
extended further before separation, in some cases even beyond the original undeformed surface. The unloading force curves in Figure 3.8 show that the dimensionless adherence forces for Au are much larger than for Ru instead of only 15 times greater predicted by the elastic theory. In fact at small interferences the adherence force for Au is even greater than its maximum loading force. These phenomena are characteristic of a ductile separation for Au which may be associated with material transfer during separation of the contact, whereas the separation is brittle for Ru. Another piece of evidence is the formation of a neck during the separation of Au, but none for Ru as shown in Figure 3.9.

Figure 3.9 shows the von Misés stresses immediately before separation. Recall that 2% strain-hardening was used. Thus the red area corresponds to the stresses above the initial yield strength without hardening; it does not represent the plastic deformation zone during unloading.

Figure 3.9. von Misés stresses before separation for Ru (left) and Au (right). Note the formation of a neck in the Au. The material properties and geometry are given in Table 3.2.
In Table 3.3 we compare the adherence force obtained from this work to the predictions by the SAM model $F_{\text{adh}}^{\text{SAM}}$ and by the KE model $F_{\text{adh}}^{\text{KE}}$. Using the separation criteria in [Maugis 1984] for the SAM model which assumes unloading is elastic until a brittle or ductile separation occurs, the separation modes for the SAM for both cases shown in Table 3.2 should be the brittle $F_b$ mode. Our FEA results show the brittle mode for Ru, but the ductile mode for Au. We only find one brittle mode in this work, which occurs with a decreasing contact radius, instead of the two brittle modes in the SAM model.

Table 3.3 Comparisons of the adherence force obtained from this work and the analytical approximation for Ru and Au.

<table>
<thead>
<tr>
<th>Material</th>
<th>Ru ($\mu$N)</th>
<th>Au ($\mu$N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta_f / \delta_c$</td>
<td>2.94 10 20 30</td>
<td>2.58 12.20 24.39 29.99</td>
</tr>
<tr>
<td>This Work $F_{\text{adh}}$</td>
<td>52.2 170.8 239.7 321.5</td>
<td>14.0 41.9 76.3 100.3</td>
</tr>
<tr>
<td>$F_{\text{adh}} / F_{\text{adh}}^{\text{SAM}}$</td>
<td>1.61 3.51 3.84 4.44</td>
<td>0.56 0.56 0.56 0.60</td>
</tr>
<tr>
<td>$F_{\text{adh}} / F_{\text{adh}}^{\text{KE}}$</td>
<td>0.83 1.01 0.75 0.68</td>
<td>2.23 1.10 0.90 0.94</td>
</tr>
</tbody>
</table>

For Ru, the separation mode found in this work is the brittle mode. The SAM model gives $F_{\text{adh}}^{\text{SAM, brittle}} = 1.5\pi \gamma R_{\text{res}}$ where $R_{\text{res}}$ is determined from Eq. (2.38). Since the EKK model works in the DMT type of plastic region, we still use $F_{\text{adh}}^{\text{EKK, brittle}} = 2\pi \gamma R_{\text{res}}$, in which $R_{\text{res}}$ is obtained from the curve-fit of the finite element simulation [Johnson 1985]. Note that $R_{\text{res}}$ in [Johnson 1985] is called the residual radius of curvature at the summit of the deformed and fully unloaded sphere, which is found to be greater at the
summit than at other radial positions. Larger ratios associated with larger loading interferences are found in Table 3.2 which means that the approximation of using Eq. (2.389) for $R_{res}$ is not applicable for large deformation. However the comparisons with the $F_{adh}^{EKK}$ of the KE model show the ratios are close to unity, indicating that the KE model is closer to our model than the SAM model in predicting the adherence force.

Similar comparisons were made for Au. The adherence forces from the SAM model can be expressed as $F_a = \pi a_f^2 H$ by Eq. (2.47) since the separation mode is ductile. The ratios of the adherence forces are almost constant around 0.6 for the SAM model, and around unity for the EKK model (except the first smallest loading interference). The smaller ratio compared to the SAM model may be because the SAM model predicts a larger contact radius as shown in Figure 3.6(b) and the maximum mean pressure during separation is still less than the hardness in this work (e.g. $P_{sep}^m \approx 0.87 H$ for the maximum loading interference $\delta_f = 30 \delta_c$).

It was shown above that the FEM model developed in this thesis was able to identify two distinct separation modes, i.e. brittle and ductile separation. In the next chapter, that model is used to conduct a series of simulations to determine the influence of the loading magnitude and of four non-dimensional parameters (including the maximum load parameter) on the contact and on the separation modes.
Chapter 4

Parameter study of separation modes

In the contact of two solids, plastic deformation leads to permanent changes in the contact topography. It can be initiated by large forces applied to the contacts, by adhesion alone even under zero external force, or by a combination of applied load and adhesion ([Du 2007], [McGuer 2006], [Maugis 1984], [Roy 1980]). The plastic deformation produced by adhesion alters the local separation of the surfaces which in turn affects the adhesion force. Achieving an understanding of the mechanics of contacts, which includes both the effects of adhesion and plasticity, is a complex problem which is still not well understood. However developing such an understanding is especially important due to the rapid development of devices at the micron scale or smaller.

It was shown in the previous chapter that a finite element model was developed to study adhesion of elastic-plastic microcontacts. An interesting result was the identification of two distinct separation modes, i.e. brittle and ductile separation. In this chapter, that model is used to conduct a series of simulations to determine the influence of the loading magnitude and of four non-dimensional parameters (including the
maximum load parameter) on the contact and on the separation modes. First let us review the existing theories.

### 4.1 Related work of ductile separation

The characteristics of ductile separation from our previous investigation in Chapter 3 can be summarized by the following four characteristics. First the contact radius decreases slowly and stepwise before it suddenly separates, typically at a significant fraction of the maximum contact radius. In a brittle separation the contact radius decreases steadily to a small value before separating. Second the hemispherical bump is stretched significantly during separation due to plastic deformation. Third the adherence force for a high degree ductile separation is much larger than for a brittle separation. Note that the transition from brittle to ductile separation actually occurs gradually. The force does not suddenly increase at the transition. Fourth a neck is sometimes formed during the ductile separation, but not for a brittle separation. It is noted that Maugis and Pollock (MP) [Maugis 1984] and Johnson [Johnson 1976] mentioned brittle separation and ductile separation as early as 1976. However, although thirty years have passed, the accurate criteria to distinguish between these two modes of adhesive separation are still not clear.
4.1.1 Mauguis-Pollock (MP) model

The MP model [Maugis 1984] has been described in detail in Chapter 2. Here we review some of the most relevant aspects of that model. The MP model is an approximate analytical treatment of plastic deformation in an adhesive contact. For elastic loading, it is the same as the JKR model. For either elasto-plastic or fully plastic loading, the radius of curvature of the deformable body in the contact region changes. Unloading is assumed to be elastic until separation occurs. If the tensile stress becomes equal to the hardness $H$, a ductile separation is said to occur. However the ductile separation is not itself modeled; it is only the assumed completely elastic unloading prior to the ductile separation which is treated. Another possibility during unloading is either of two different brittle separation modes. The occurrence of each of these three modes depends on the maximum contact radius during loading and the material properties. An interesting and somewhat counter-intuitive result of the MP model is that ductile separation is more likely to occur at low loads, provided that the load is large enough for the initiation of some plastic deformation during loading.

4.1.2 Mesarovic and Johnson (MJ) model

Mesarovic and Johnson (MJ) used a combination of finite elements and an analytical method under the assumption that the contact pressure at the end of loading is uniform [Mesarovic 2000]. The near uniformity of the contact pressure is shown to occur well before the onset of full-plasticity. They defined a non-dimensional parameter given by
Chapter 4 Parameter study of separation modes

\[ S' = \frac{\Delta \gamma}{Z_o p_m} \tag{4.1} \]

From Eq. (4.1) \( S' \) is approximately the theoretical stress (defined as the maximum Lennard-Jones stress between two parallel surfaces) divided by the mean contact pressure at the maximum loading level. Note that because the mean pressure cannot be greater than the hardness; therefore \( S' \) cannot be less than the ratio of the theoretical stress to the hardness.

A second parameter in [Mesarovic 2000] is

\[ \chi = \frac{\pi}{2\pi - 4} \frac{\Delta \gamma E'}{p_o^2 a_f} \tag{4.2} \]

which can be interpreted as the ratio of the adhesive energy to the elastic energy stored in the recovered hemisphere. A decohesion map was presented whereby the parameter space \((\chi, S')\) was divided into the regions where decohesion is governed by different physical processes. In all cases it was assumed that the unloading is elastic up until the point of separation. When \( S' < 1 \), the separation is elastic, while for \( S' > 1 \) yielding during separation is expected to be widespread. For \( S' > 1 \), if \( \chi < 2 \) which corresponds to larger loading contact radius, the separation is elasto-plastic; if \( \chi > 2 \), the plastic zone will extend across the whole area of contact which leads to a fully plastic separation, including the formation of a neck. The condition is similar to the ductile separation Johnson suggested in [Johnson 1976].

Both the MP and MJ models conclude that low hardness and small contact size promote ductile separation. Both models assume that the deformation is purely elastic during unloading to the point of either pull-off or the initiation of a ductile separation; in
neither model is the plastic deformation during ductile separation modeled. The simplifying assumptions made in each model, leave room for further research in this area.

4.1.3 Molecular dynamics (MD) model

Another approach to this adhesion problem is through the use of Molecular Dynamics (MD) simulations. Certainly the intrinsic difference is that the MD simulations are applicable to study the atomic scale, while we are using a continuum model to study contacts at a micro scale.

Early work was done by Landman to observe the formation and elongation of a connective neck upon separation between a nickel tip and a gold surface [Landman 1990]. More recent investigations were made by Song and Srolovitz [Song 2006] for Au nanocontacts, and by Yong et al. for NaCl [Yong 2007]. The investigation in [Yong 2007] was focused on the effect of different asperity sizes. It was found that the transition from brittle to ductile separation occurred at asperity contacts above $4 \times 4$ atoms. Larger contact size behaves as a ductile separation, which is the opposite trend to that in the MP and MJ continuum models. Note that the investigation in [Yong 2007] was for NaCl rather than for a metal, and the asperities were pyramid-shaped as opposed to the curved metallic contacts. It was also mentioned in [Yong 2007] that a second transition, this one from ductile to brittle separation, will occur at scales too large for current MD simulations.
Here we introduce the MD model from Prof. Srolovitz and his students in Princeton University such as in [Song 2006] since the model they are using is very similar to ours. Both are gold-on-gold contact with round curve, except their scale is at nano while ours is micro. But it can be a better comparison for the nano contact study.

One of their recent researches was done on the 3-D model shown in Figure 4.1. The initial asperity containing 1280 atoms was placed on a flat substrate. Its relaxed shape is roughly hemispherical with a radius of approximately 2.5 nm. The entire system contained 13880 atoms. The lower layer of the bottom substrate and the upper layer of the top layer are fixed (except for changes in the unit cell to maintain boundary conditions).

Figure 4.1. Molecular dynamics model. The initial asperity containing 1280 atoms was placed on a flat substrate. Its relaxed shape is roughly hemispherical with a radius of approximately 2.5 nm. The entire system contained 13880 atoms.
Chapter 4 Parameter study of separation modes

conditions that normal stresses in x and y direction is kept at zero). The atomic
interactions are described using a potential of the embedded-atom-method. The equations
of atomic motion are integrated forward in time using a velocity-Verlet algorithm [Swope
1982]. The initial separation between the summit of the asperity and the top is 0.8 nm.
Then the top is moved downward at a rate of 1 m/s for 1.96 nm, then the sign of the
displacement is reversed to separate the two materials. A series of simulations are
performed at different adhesion energy which is fulfilled by adjusting the potential
parameters while keeping other material properties the same. Finally critical adhesion
energy for material transfer was found. It was shown to satisfy a simple analytical
relation based on a capillary equilibrium argument.

Figure 4.2 is the morphologies after separation with adhesion energy varying from
0.388 J/m² to 1.37 J/m². With smaller adhesion energy up to 0.53 J/m², the asperity was
flattened which is simply due to large plastic deformation during loading. With the
increase of adhesion energy, the effect of adhesion is strong enough to cause a permanent
stretch of the asperity. From adhesion energy equal to 0.88 J/m², the material transfer first
appeared from the asperity to the top. From the shape we can imagine the neck must be
formed during unloading process. The amount of material transfer is greater with the
increase of adhesion energy. With continuous increase of adhesion energy, the top
surface is also permanently deformed and some atoms from top side can also be found on
the bottom. So the value of adhesion energy does affect the unloading significantly, and
its effect starts to be visible from 0.61 J/m².

The force-displacement curve is shown in Figure 4.4. We can see the loading curve was
not affected by different adhesion too much, but the unloading did. When adhesion
energy is below \(0.61 \text{ J/m}^2\), there is a sharp transition during loading which represents a sudden decohesion event (similar to brittle fracture) rather than a necking followed by ductile fracture event at larger adhesion energy. These results agree with the unloading morphologies demonstrated in Figure 4.2. Under brittle separation, JKR model is still valid to predict the adherence force with multiplied by a constant factor. So the adherence force is still proportional to the adhesion energy. While under ductile separation, it is not the case although the trend is still monotonic. That is because the stress in the neck reaches its maximum which prevents the increase of the adherence force.

So totally we have seen three separation modes in order of increasing adhesion energy – elastic unloading, plastic interface unloading, and plastic non-interface unloading. Although there are two sub modes into plastic non-interface separation – one-way material transfer and two-way material transfer, here I do not distinguish them. His results give us a complete image of the effect of adhesion under a certain loading. But more results such as the contact under different loading are expected.
Figure 4.2 (a) $\Gamma = 1366 \text{ mJ/m}^2$; (b) $\Gamma = 1157.94 \text{ mJ/m}^2$; (c) $\Gamma = 998.82 \text{ mJ/m}^2$; (d) $\Gamma = 881.81 \text{ mJ/m}^2$; (e) $\Gamma = 735.00 \text{ mJ/m}^2$; (f) $\Gamma = 694.23 \text{ mJ/m}^2$; (g) $\Gamma = 610.90 \text{ mJ/m}^2$; (h) $\Gamma = 532.63 \text{ mJ/m}^2$; (i) $\Gamma = 388.43 \text{ mJ/m}^2$. 

Deleted: 4.2
Figure 4.3 Force-displacement curves at different adhesion energy.
4.1.4 Rice fracture mechanics model

Rice also made a significant related contribution by predicting the conditions for separation modes of cracks in fracture mechanics ([Rice 1974], [Rice 1992]). Fracture is commonly categorized as being either ductile or brittle depending on the amount of energy absorption. Brittle fracture only requires a little energy to separate atoms and expose new surfaces along the fracture path, so the separation is elastic or little plastic, such as glass, polystyrene, and some of the cast iron. For crack propagation in brittle way, Griffith in 1920 defined a quantity called the elastic-energy-release rate, \( G \) and it should always be balanced by the energy-create rate of the new surface, or adhesion energy \( \Delta \gamma \). The equilibrium condition for propagation a crack tip is,

\[
G = \Delta \gamma, \tag{4.3}
\]

Conversely, ductile fracture requires not only the energy just mentioned but more additional energy to deform plastically the material ahead of fracture, so the separation is plastic, such as many metals. Griffith condition is not applicable since plastic dissipation is involved into the propagation. Irwin and Orowan proposed to include a plastic term \( \Gamma_p \) in the energy equilibrium condition, and Eq. (4.3) is modified as,

\[
G = \Delta \gamma + \Gamma_p, \tag{4.4}
\]

\( \Gamma_p \) is a function of \( \Delta \gamma \) and its calculation is not trivial.

Rice made a great contribution to predict the conditions for each mode to happen. He described the brittle vs. ductile response as the competition between Griffith cleavage and plastic shear (dislocation nucleation) at a crack tip. As shown in Figure 4.4, a slip plane is assumed to intersect with interface at the front of the crack tip. The cleave energy release rate \( G_{\text{cleave}} \) is determined by the surface energy \( \gamma_s \), and the dislocation energy
dissipation rate $G_{\text{disl}}$ is determined by an unstable stack energy $\gamma_{\text{us}}$ and a dimensional constant $\alpha$,

$$G_{\text{disl}} = \alpha \gamma_{\text{us}},$$  \hspace{1cm} (4.5)

where $\alpha$ depends on the loading mode at the crack tip, the slip plane angle and Burgers vector direction of the active slip system. The fracture mode is going to follow the smaller one of these two rates. So when $G_{\text{cleave}} < G_{\text{disl}}$, the crack moves along the cleave path and the fracture is brittle; and $G_{\text{cleave}} > G_{\text{disl}}$, the tip front moves along the slip plane with atomic level plasticity, it is ductile fracture.

Further he derived the requirement for ductile fracture to occur under single vertical opening mode is

$$\frac{\gamma_{\text{us}}}{\gamma_{\text{us}}} > 9.1(fcc) \quad \text{or} \quad 6.3(bcc),$$  \hspace{1cm} (4.6)

When crack has slip on other directions, the ratio is supposed to be reduced.

---

Figure 4.4 Competition between Griffith cleavage and plastic dislocation. When $G_{\text{cleave}} < G_{\text{disl}}$, the crack moves along the cleave path and the fracture is brittle; and $G_{\text{cleave}} > G_{\text{disl}}$, the tip front moves along the slip plane with atomic level plasticity, it is ductile fracture.
Let us take his results for gold as an example. Gold is a kind of fcc metal. $\gamma_s = 1.56 \text{ J/m}^2$ at $T = 0$, $\gamma_{\text{us}(\text{Frenkel})} = 0.14 \text{ J/m}^2$ by Frenkel model, and $\gamma_{\text{us}(\text{EAM})} \approx 0.7 \gamma_{\text{us}(\text{Frenkel})}$ by embedded-atom model, which gives the ratio is 11 or 15.7 for two kinds of calculation. Either of them predicts the separation for clean gold is ductile. When the surface is not clean, the surface energy is supposed to be lower than the ideal number. Based on Eq. (4.6) and the value for $\gamma_{\text{us}}$, we can calculate the critical surface energy for ductile separation is $0.88 \text{ J/m}^2$ and $0.89 \text{ J/m}^2$ for Frenkel model and EAM model, respectively. This is only for vertical propagation mode, when the propagation in other directions is involved, the critical value is going to be smaller. The data for ruthenium is not available in his paper. $\gamma_s$ varies with contamination. Clean metal has the highest surface energy. When its surface is contaminated, the surface energy decreases. So it might be best to find a $(\gamma_s)_{\text{crit}}$ to separate ductile from cleavage modes.

From the previous description of the MD model, ductile separation first appears at the adhesion energy equal to $0.61 \text{ J/m}^2$. The maximum critical surface energy calculated here based on Rice theory is about $0.88 \text{ J/m}^2$. So the critical adhesion energy is $1.76 \text{ J/m}^2$. It is greater than that of the MD.

Comparing Rice theory with Maugis & Pollock theory, we can conclude the following contradictions in Table 4.1, or more accurately speaking some points two theories have not been integrated.

As can be seen from the foregoing discussion, there exists a variety of work devoted to ductile and brittle separation modes and the criteria to predict the conditions under which each separation mode will occur. But there is still a lack of general results to apply to microscale or nanoscale adhesive contacts. Understanding the unloading of a
Table 4.1 Comparison of Rice theory and Maugis & Pollock Theory

<table>
<thead>
<tr>
<th></th>
<th>Rice Theory</th>
<th>Maugis &amp; Pollock Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>Field</td>
<td>Fracture mechanics</td>
<td>Contact mechanics</td>
</tr>
<tr>
<td>Viewpoint</td>
<td>Crack cleavage and plastic dislocation on atomic level</td>
<td>Mean pressure determined by contact force and contact radius on macroscopic level</td>
</tr>
<tr>
<td>Definition</td>
<td>Brittle – cleavage</td>
<td>Brittle – interface separation</td>
</tr>
<tr>
<td></td>
<td>Ductile - dislocation nucleation</td>
<td>Ductile – non-interface separation</td>
</tr>
<tr>
<td>Criteria</td>
<td>$\gamma_s$ vs. $\gamma_{ss}$</td>
<td>mean pressure vs. hardness</td>
</tr>
<tr>
<td>Difficulties</td>
<td>Hard to predict $\gamma_{ss}$</td>
<td>Hard to predict the relation between mean pressure and hardness during unloading</td>
</tr>
<tr>
<td>Difference</td>
<td>Independent on load</td>
<td>Depends on load</td>
</tr>
</tbody>
</table>

contact is very important because the failure mechanisms in, for example, a microswitch can be attributed to too high an adherence force ([McGruer 2006], [Majumder 2001]). In this chapter we use the previously developed finite element model to study adhesion of elastic-plastic microcontacts with the objective of determining the influence of the various parameters on the separation modes of these adhesive contacts.
4.2 Definition of the dimensionless contact parameters

The first dimensionless parameter is defined by

\[ S = \frac{\Delta \gamma}{Z_p H} \]  (4.7)

This parameter \( S \) is the ratio of the theoretical stress due to adhesion to the hardness. It is similar to \( S' \) defined by Eq. (4.1) except that the mean contact pressure is replaced by the hardness. Note that for fully plastic deformation \( p_m = H \) in which case \( S = S' \).

The second parameter is \( E/\sigma_y \) which is the ratio of the Young’s modulus to the yield strength. It was found in [Etsion 2005] that, without adhesion, this parameter does not affect the loading curves which were plotted using dimensionless parameters. However, during unloading, the residual radius of curvature \( R_{res} \) does depend on \( E/\sigma_y \) which further affects the adhesion force. From [Etsion 2005], the adherence force is equal to \( 2\pi \Delta \gamma R_{res} \) for DMT behavior. More discussion of the role of \( R_{res} \) is presented later.

The third parameter is the Tabor parameter defined in Eq. (2.15) for elastic contact. Note that if the unloading is elastic, an effective \( \mu \) increases with the plastic deformation incurred during loading due to the increase of the residual radius of curvature \( R_{res} \). For elastic unloading smaller \( \mu \) and larger \( R \) correspond to a larger adherence force and smaller contact radius upon separation.

The load level is defined by the dimensionless interference as \( \frac{\delta_f}{\delta_c} \) which is used to study the effect of different loading interferences on adhesion during unloading. Note that both the MP and MJ models predict that the occurrence of ductile separation is related to the load level.
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4.3 Results and discussion

4.3.1 The choice of dimensionless variables

The adhesive contact model is described in detail in previous chapter. To study the importance of each of the parameters, four groups of simulations were performed. In each group, one of the parameters was varied while keeping the other three constant. In order to effectively show the characteristics of ductile and brittle separation from these cases with different material properties, appropriate dimensionless variables are chosen, i.e. dimensionless interference \( \delta / \delta_f \), dimensionless contact radius \( a / a_f \) and dimensionless external force \( F_e / F_f \). The quantities \( \delta_f \), \( a_f \) and \( F_f \) are the interference, contact radius and external force respectively at the final maximum interference during loading.

First we analyze the adherence force. The KE model gives a curve-fit to the finite element simulations for \( R_{res} \) as in Eq. (2.42) for the DMT type of adhesion model with plastic deformation. The adherence force is then \( F_{adh}^{KE} = 2 \pi \Delta \gamma R_{res} \). The ratio of the contact force \( F_{KE} \) to the critical contact force \( F_c \) is a function only of \( \delta_f / \delta_e \), given by

\[
\frac{F_{KE}}{F_c} = \begin{cases} 
1.03(\delta_f / \delta_e)^{1.425} & \text{for } 1 \leq \delta_f / \delta_e \leq 6 \\
1.40(\delta_f / \delta_e)^{1.265} & \text{for } 6 \leq \delta_f / \delta_e \leq 110 
\end{cases} 
\] (4.8)

So the adherence force in the dimensionless coordinate predicted by the KE model is

\[
\frac{F_{adh}}{F_f} = \frac{2 \pi \Delta \gamma R_{res}^{KE}}{F_{KE}} = \frac{12(1-\nu^2)^2}{K_H^3 \pi^2} \left[ 1 + 1.275 \left( \frac{E}{\sigma_y} \right)^{0.216} \left( \delta_f / \delta_e - 1 \right) \right] \] or \[ \left[ 1 + 1.4(\delta_f / \delta_e)^{1.425} \right] \] \( S^3 \) (4.9)

which depends only on the four dimensionless parameters (although in the KE model \( S/\mu \) can be interpreted as a single parameter) and Poisson’s ratio (because \( K_H \) depends on \( \nu \)).
Because the KE model does not include the effect of adhesion on deformation, it is incapable of predicting ductile separation. It was found in chapter 3 that the difference of the adherence forces between our model and the KE model are within the range of 10% to 32% for both the Ru (brittle separation) and for the Au cases (ductile separation), except for the smallest loading interference for Au. The maximum external force is also consistent with $F_{KE}$ for large loading because for large loads the adhesion force is small in comparison. Therefore although Eq. (4.9) alone cannot be used to identify the separation modes, it may be appropriate for brittle separation and to provide qualitative insight into the more general unloading problem.

It was also found in Chapter 3 that the value of the interference at which separation occurs is another important indication of ductile separation. If the separation is brittle, then the sphere is not stretched significantly due to adhesion and the residual interference $\delta_{res}$ after unloading is close to the residual interference caused without the effect of adhesion. That value is only dependent on $\delta_f/\delta_c$ and can be obtained using the curve-fit from the EKK model. For example, from the EKK model $\delta_{res}/\delta_f=0.555$ for $\delta_f/\delta_c = 30$, and $\delta_{res}/\delta_f=0.137$ for $\delta_f/\delta_c = 2.94$ which are two typical loading levels we used for the simulations. From the results obtained in Chapter 3 $\delta_{res}/\delta_f$ is equal to 0.5867 and 0.0655 respectively for brittle separation of Ru, and 0.1674 and -2.2558 for ductile separation of Au. In the following work, the amount of the stretch is the main criterion to identify the two separation modes. It needs to be mentioned that the definition of ductile separation by the MP and MJ models is that there is a sudden transition from elastic unloading to fully plastic separation. In neither model is the plastic separation itself included in the model. In our work the unloading is allowed to be elastic and/or plastic as
dictated by the results of the simulation. Ductile separation is defined as occurring when considerable stretch occurs during unloading.

### 4.3.2 Equivalent set of units

Many simulations with different combination of material properties and dimensions are needed to study the effect of the four dimensionless parameters. It is impractical and inefficient to rebuild each model with a different hemisphere size and remesh it accordingly. Fortunately we can use any consistent system of units. For example in MEMS, it is convenient to set up problems in \( \mu \text{m-kg-s} \) units instead of the standard m-kg-s units. To make use of the existing two models with preset radii of 4 and 1, conversion factors in Table 4.2 are used to convert \( \mu \text{m-kg-s} \) units to a new set of units. Specifically, when length is multiplied by a factor of \( 1/b \), pressure is multiplied by \( b \), and force by \( 1/b \) accordingly. Since the parameters \( S, E/\sigma_Y, \mu, \chi \) are dimensionless, they are constant under this conversion. For example, if we use the model with radius of 4 and want \( S=1, \ E/\sigma_Y=120, \ \mu=1.6 \), we can get the corresponding values for \( E=75419, \ \Delta \gamma=1, \ \sigma_Y=628.5, \ \text{and} \ Z_0=0.0005219 \) input into ANSYS® by using the Eqs. (2.15) and (4.7). The units for those numbers are new units listed on the fifth column of Table 4.2. Those numbers are not necessarily unique. In reality \( Z_0 \) is a constant number, which is 0.169 \( \text{nm} \) for Ru and 0.184 \( \text{nm} \) for Au as mentioned in Chapter 2. Based on this limitation, factor \( b \) can be decided, and so for the values of \( R, E, \sigma_Y \) under \( \mu \text{m-kg-s} \) units. The validity of the above conversion of units is tested by Case 1 and 2 listed in Table 4.3 with consistent curves shown in Figure 4.5. Case 3 is designed to have equal \( S, E/\sigma_Y, \mu, \text{and} \ \delta_f/\delta_c \) to those.
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of Case 2. The overlapping curves show that the four key parameters are the most important factors to affect the contact with adhesion.

With the above unit conversion method, we can design simulations more flexibly based on our needs. For easy understanding, the numbers listed in the following tables have been converted to the real material properties and dimensions instead of the entered data in ANSYS®.

Table 4.2 Mechanical conversion factors for µMKS to New Units used in ANSYS®

<table>
<thead>
<tr>
<th>Mechanical Parameter</th>
<th>µMKS Unit</th>
<th>Dimension</th>
<th>Multiply by This Number</th>
<th>To Obtain New Unit</th>
<th>Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>µm</td>
<td>µm</td>
<td>1/b</td>
<td>b*µm</td>
<td>b*µm</td>
</tr>
<tr>
<td>Pressure</td>
<td>MPa</td>
<td>kg/(µm)(s)²</td>
<td>b</td>
<td>(1/b)*MPa</td>
<td>kg/(b*µm)(s)²</td>
</tr>
<tr>
<td>Force</td>
<td>µN</td>
<td>(kg)(µm)(s)²</td>
<td>1/b</td>
<td>b*µN</td>
<td>(kg)(b*µm)(s)²</td>
</tr>
</tbody>
</table>

Table 4.3 Material properties (entered in ANSYS®) to test the validity of unit conversion

<table>
<thead>
<tr>
<th>Case</th>
<th>R</th>
<th>E</th>
<th>ν</th>
<th>σγ</th>
<th>Z_0</th>
<th>Aγ</th>
<th>S</th>
<th>E/σγ</th>
<th>μ</th>
<th>δ_f/δ_c</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>410</td>
<td>0.3</td>
<td>3.42</td>
<td>0.169</td>
<td>1</td>
<td>0.6</td>
<td>120</td>
<td>1.60</td>
<td>30</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>410*4</td>
<td>0.3</td>
<td>3.42*4</td>
<td>0.169/4</td>
<td>1</td>
<td>0.6</td>
<td>120</td>
<td>1.60</td>
<td>30</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>80</td>
<td>0.42</td>
<td>0.67</td>
<td>0.0345</td>
<td>0.04</td>
<td>0.6</td>
<td>120</td>
<td>1.60</td>
<td>30</td>
</tr>
</tbody>
</table>
Figure 4.5 Dimensionless contact radius vs. dimensionless interference (Fig. 4.5a) and dimensionless external force vs. dimensionless interference (Fig. 4.5b) for a single cycle. The material properties and geometry are given in Table 4.3 ($S = 1.2$, $E/\sigma_Y = 120$, $\mu = 1.60$, $\delta_f/\delta_c = 30$).
4.3.3 Influence of $S$ on the separation modes

The material properties and dimensions listed in Table 4.4 were chosen to study the influence of the parameter $S$ on the separation modes. Two maximum loading levels ($\delta_f/\delta_c=30$ and $\delta_f/\delta_c=2.94$) were chosen while keeping the other two parameters constant ($E/\sigma_Y=120, \mu=1.60$).

Table 4.4 Material properties for the study of the impact of parameter $S$ ($S$ varies from 0.6 to 2.9, $E/\sigma_Y=120, \mu=1.60, \delta_f/\delta_c=30$)

<table>
<thead>
<tr>
<th>Case</th>
<th>$R$ ($\mu$m)</th>
<th>$E$ (GPa)</th>
<th>$\nu$</th>
<th>$\sigma_Y$ (GPa)</th>
<th>$Z_0$ (nm)</th>
<th>$\Delta\gamma$ (J/m$^2$)</th>
<th>$\delta_c$ (nm)</th>
<th>$S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>410</td>
<td>0.3</td>
<td>3.42</td>
<td>0.169</td>
<td>1</td>
<td>1.48</td>
<td>0.6</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>233</td>
<td>0.3</td>
<td>1.94</td>
<td>0.169</td>
<td>1</td>
<td>0.47</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>1.5</td>
<td>54.7</td>
<td>0.42</td>
<td>0.46</td>
<td>0.184</td>
<td>0.28</td>
<td>0.52</td>
<td>1.2</td>
</tr>
<tr>
<td>6</td>
<td>0.2</td>
<td>418</td>
<td>0.42</td>
<td>3.5</td>
<td>0.169</td>
<td>4.8</td>
<td>0.07</td>
<td>2.9</td>
</tr>
</tbody>
</table>

All the simulations experience a single cycle of loading and unloading. For the load level of $\delta_f/\delta_c=30$ it can be seen in Figure 4.6(a) that the loading curves for contact radius vs. interference show little variation with $S$, except for a combination of large $S$ and small loading in which a significant jump-into-contact occurs. However the unloading curves show a significant dependence on $S$. The stars (*) mark the contact radii immediately before separation. A gradual change of separation modes from brittle to ductile can be seen with the increase of $S$. The unloading curves for $S \leq 1.2$ are relatively smooth while for large $S$ the contact radii decrease stepwise during unloading. The curve for $S=1.2$ represents the approximate transition between these two cases. Another
Figure 4.6, Dimensionless contact radius vs. dimensionless interference (Fig. 4.6a) and dimensionless external force vs. dimensionless interference (Fig. 4.6b) for a single load/unload cycle. The material properties and geometry are given in Table 4.4 ($S$ varies from 0.6 to 2.9, $E/\sigma_Y = 120$, $\mu = 1.60$, $\delta_f/\delta_c = 30$).
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phenomenon characterized by $S > 1.2$ is that the hemispherical bump is stretched considerably due to plastic deformation during separation. The dimensionless interference upon separation for $S = 2.9$ is equal to 0.2 which is significantly less than the 0.555 value calculated earlier from the EKK model.

Figure 4.6(b) gives the dimensionless external force vs. interference. The negative peak represents the adherence force needed to separate the bump from the flat surface. Its magnitude generally increases with an increase of $S$ as shown in Eq. (4.9). By taking the ratios of the adherence forces obtained from our simulations with those calculated from Eq. (4.9), the ratios 0.96, 0.73, 0.84, and 0.16 are obtained respectively for cases 1 and case 4-6. We can see that the results are close for the first three cases with $S \leq 1.2$, but a large difference is obtained for case 6. Let us recall that $R_{res}$ in Eq. (4.9) is the residual radius of curvature at the summit of the fully unloaded sphere without adhesion which is flattened more at its apex than elsewhere [Etsion 2005]. The large discrepancy obtained for case 6 further demonstrates that the residual radius of curvature in our simulation is significantly changed due to large $S$. The separation mode has changed to ductile and therefore Eq. (4.9) is no longer applicable. Ductile separation causes the sphere to stretch during unloading, thereby reducing its radius of curvature. Hence the adherence force is also reduced.

The transition from brittle separation to ductile separation for $\delta_f / \delta_c = 30$ is at $S = 1.2$. That this ratio of the peak adhesive stress to the hardness needs to be greater than unity is due in part to the greater non-uniformity in the stress field during unloading than during loading. It is also because 2% strain hardening is used for the simulation and thus the effective hardness is greater during unloading.
Another group of simulations are performed for small loading $\delta_f/\delta_c=2.94$ for the cases in Table 4.4. The results are shown in Figure 4.7 which are very similar to those of the above large loading case in that the magnitude of the adherence force increases with an increase of $S$ and the transition between the separation modes occurs at about $S = 1.0$, which is a smaller than for large loading. At $S = 1.2$ the ductile behavior is much more obvious than for large loading. Again it is emphasized that the transition between brittle and ductile separation is gradual. That lower loading should correspond to a lower $S$ for the brittle-to-ductile transition is no doubt due to the reduced strain hardening during loading.

It is mentioned earlier in this paper that the onset of ductile separation for Au obtained by MD simulations [Song 2006] is at an adhesion energy equal to 0.61 $J/m^2$. To compare that model with ours, we take typical values of $Z_0=0.184nm$ and $H=2GPa$ for Au in Eq. (4.7). Note that the radius of curvature $R$ does not affect $S$ in Eq. (4.7). The FEM model gives the criterion of $\Delta\gamma > 0.44 J/m^2$ for ductile separation showing reasonable agreement with the MD results. Differences are no doubt primarily due to applying the continuum concept of hardness to the atomic scale as well as the different ratio of the length scale governing the adhesion force to the geometric dimensions of the hemisphere.
Figure 4.7, Dimensionless contact radius vs. dimensionless interference (Fig. 4.7a) and dimensionless external force vs. dimensionless interference (Fig. 4.7b) for a single load/unload cycle. The material properties and geometry are given in Table 4.4 ($S$ varies from 0.6 to 2.9, $E/\sigma_Y = 120$, $\mu = 1.60$, $\delta_f/\delta_c = 2.94$).
4.3.4 Influence of $E/\sigma_Y$ on the separation modes

Based on the above results, $S = 1.2$ is chosen as the brittle-ductile transition for $\delta_f / \delta_c = 30$ in order to study the influence of $E/\sigma_Y$. This parameter was varied from 120 to 500. The value for $\mu$ was kept at 1.60 and the other material properties are summarized in Table 4.5. It can be seen from both Figure 4.8(a) and Figure 4.8(b) that the loading curves coincide very closely, and the unloading curves show only a small difference. Hence the parameter $E/\sigma_Y$ does not affect the separation modes nearly as much as does $S$. In addition, a large change of its value only causes a small change of $F_{adh}/F_f$ as predicted in Eq. (4.9).

Table 4.5 Material properties for the study of the impact of parameter $E/\sigma_Y$ ($E/\sigma_Y$ varies from 120 to 500, $S = 1.2$, $\mu = 1.60$, $\delta_f / \delta_c = 30$)

<table>
<thead>
<tr>
<th>Case</th>
<th>$R$ ($\mu$m)</th>
<th>$E$ (GPa)</th>
<th>$\nu$</th>
<th>$\sigma_Y$ (GPa)</th>
<th>$Z_0$ (nm)</th>
<th>$\Delta \gamma$ (J/m²)</th>
<th>$\delta_c$ (nm)</th>
<th>$E/\sigma_Y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1.5</td>
<td>54.7</td>
<td>0.42</td>
<td>0.46</td>
<td>0.184</td>
<td>0.28</td>
<td>0.52</td>
<td>120</td>
</tr>
<tr>
<td>7</td>
<td>4</td>
<td>410</td>
<td>0.3</td>
<td>1.79</td>
<td>0.169</td>
<td>1</td>
<td>0.41</td>
<td>229</td>
</tr>
<tr>
<td>8</td>
<td>20.9</td>
<td>85.9</td>
<td>0.3</td>
<td>0.17</td>
<td>0.184</td>
<td>0.1</td>
<td>0.44</td>
<td>500</td>
</tr>
</tbody>
</table>
Figure 4.8, Dimensionless contact radius vs. dimensionless interference (Fig. 4.8a) and dimensionless external force vs. dimensionless interference (Fig. 4.8b) for a single load/unload cycle. The material properties and geometry are given in Table 4.5 ($E/\sigma_Y$ varies from 120 to 500, $S = 1.2$, $\mu = 1.60$, $\delta_f/\delta_c = 30$).
4.3.5 Influence of $\mu$ on the separation modes

Table 4.6 Material properties for the study of the impact of parameter $\mu$ ($\mu$ varies from 1.60 to 3.50, $S = 1.2$, $E/\sigma_Y = 120$, $\delta_f / \delta_c = 30$) gives the material properties for studying the effect of $\mu$ and Figure 4.9 are the results. Similarly to $E/\sigma_Y$, the parameter $\mu$ does not affect the separation mode significantly, but it does change $F_{adh}/F_f$ substantially. From the combination of the KE model and the EKK model the adherence force is inversely proportional to $\mu^3$ as shown in Eq. (4.9). The trend in this work is very close to this dependency if the separation is brittle. Note that in an elastic contact, greater adherence force also corresponds to smaller $\mu$, but the dependence is weak.

Table 4.6 Material properties for the study of the impact of parameter $\mu$ ($\mu$ varies from 1.60 to 3.50, $S = 1.2$, $E/\sigma_Y = 120$, $\delta_f / \delta_c = 30$)

<table>
<thead>
<tr>
<th>Case</th>
<th>$R$ ($\mu$m)</th>
<th>$E$ (GPa)</th>
<th>$\nu$</th>
<th>$\sigma_Y$ (GPa)</th>
<th>$Z_0$ (nm)</th>
<th>$\Delta \gamma$ (J/m$^2$)</th>
<th>$\delta_c$ (nm)</th>
<th>$\mu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1.5</td>
<td>54.7</td>
<td>0.42</td>
<td>0.46</td>
<td>0.184</td>
<td>0.28</td>
<td>0.52</td>
<td>1.60</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>54.7</td>
<td>0.42</td>
<td>0.46</td>
<td>0.184</td>
<td>0.28</td>
<td>2.17</td>
<td>2.57</td>
</tr>
<tr>
<td>10</td>
<td>15</td>
<td>54.7</td>
<td>0.42</td>
<td>0.46</td>
<td>0.184</td>
<td>0.28</td>
<td>5.46</td>
<td>3.50</td>
</tr>
</tbody>
</table>
Figure 4.9, Dimensionless contact radius vs. dimensionless interference (Fig. 4.8a) and dimensionless external force vs. dimensionless interference (Fig. 4.8b) for a single
load/unload cycle. The material properties and geometry are given in Table 4.6 (μ varies from 1.60 to 3.50, \( S = 1.2, E/\sigma_Y = 120, \delta_f/\delta_c = 30 \)).

### 4.3.6 Influence of \( \delta_f/\delta_c \) on the separation modes

The above simulations have shown that under the same large loading (\( \delta_f/\delta_c = 30 \), so that the contact during maximum loading is almost fully plastic) the parameter \( S \) has the greatest effect on the separation mode, while \( E/\sigma_Y \) and \( \mu \) change the adherence force to a lesser degree. To study the influence of different loading levels, simulations at different load levels are performed with the four groups of material properties respectively listed in Table 4.7 which cover several combinations of \( S, E/\sigma_Y, \) and \( \mu \). The results are plotted in Figure 4.10 - Figure 4.13. In Figure 4.10, the profiles of the curves are very similar and the separation is brittle under different loading levels with \( S = 0.6 \). For \( S = 1.2 \) the separations in both Figure 4.11 and Figure 4.12 are in the transition mode for \( \delta_f/\delta_c = 30 \), but in the ductile mode for \( \delta_f/\delta_c = 2.94 \). This behavior means that when \( S \) meets the criteria for ductile separation, \( \delta_f/\delta_c \) is another critical factor for the occurrence of ductile separation. Lower \( \delta_f/\delta_c \) tends to cause ductile separation. This behavior, although

**Table 4.7 Material properties for the study of the impact of parameter \( \delta_f/\delta_c \) (\( \delta_f/\delta_c \) varies from 2.58 to 30)**

<table>
<thead>
<tr>
<th>Case</th>
<th>( S )</th>
<th>( E/\sigma_Y )</th>
<th>( \mu )</th>
<th>( \delta_f/\delta_c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.6</td>
<td>120</td>
<td>1.60</td>
<td>2.94</td>
</tr>
<tr>
<td>5</td>
<td>1.2</td>
<td>120</td>
<td>1.60</td>
<td>2.94</td>
</tr>
<tr>
<td>8</td>
<td>1.2</td>
<td>500</td>
<td>1.60</td>
<td>2.94</td>
</tr>
<tr>
<td>11</td>
<td>2.9</td>
<td>120</td>
<td>2.57</td>
<td>2.58</td>
</tr>
</tbody>
</table>
Case | $R$ (µm) | $E$ (GPa) | $\nu$ | $\sigma_y$ (GPa) | $Z_0$ (nm) | $\Delta \gamma$ (J/m²) | $\delta_c$ (nm) | $S$ | $E/\sigma_y$ | $\mu$
---|---|---|---|---|---|---|---|---|---|---
11 | 1 | 80 | 0.42 | 0.67 | 0.184 | 1 | 0.36 | 2.9 | 120 | 2.57

**Diagram a):**
- Legend: $\delta / \delta_c = 2.94$, $\delta / \delta_c = 10$, $\delta / \delta_c = 20$, $\delta / \delta_c = 30$
- Loading and Unloading paths

**Diagram b):**
- Legend: $\delta / \delta_c = 2.94$, $\delta / \delta_c = 10$, $\delta / \delta_c = 20$, $\delta / \delta_c = 30$
- Loading and Unloading paths
Figure 4.10. Dimensionless contact radius vs. dimensionless interference (Fig. 4.10a) and dimensionless external force vs. dimensionless interference (Fig. 4.10b) for a single load/unload cycle. The material properties and geometry are given as Case 1 of Table 4.7.
Figure 4.11. Dimensionless contact radius vs. dimensionless interference (Fig. 4.11a) and dimensionless external force vs. dimensionless interference (Fig. 4.11b) for a single load/unload cycle. The material properties and geometry are given as Case 5 of Table 4.7.
Figure 4.12. Dimensionless contact radius vs. dimensionless interference (Fig. 4.12a) and dimensionless external force vs. dimensionless interference (Fig. 4.12b) for a single load/unload cycle. The material properties and geometry are given as Case 8 of Table 4.7.
Figure 4.13. Dimensionless contact radius vs. dimensionless interference (Fig. 4.13a) and dimensionless external force vs. dimensionless interference (Fig. 4.13b) for a single load/unload cycle. The material properties and geometry are given as Case 11 of Table 4.7.

counter-intuitive, is qualitatively similar to the MP and MJ models. For Case 11 in Table 4.7 (S=2.7), Figure 4.13 shows that all the unloading curves are ductile for loading up to $\delta_f/\delta_c=30$.

The impact of four parameters i.e. $S$, $E/\sigma_Y$, $\mu$, and the load level $\delta_f/\delta_c$ on the separation modes of adhesive contacts was investigated. The results show that $S$ and $\delta_f/\delta_c$ are the key parameters, while $\mu$ and $E/\sigma_Y$ are less important. Ductile separation occurs when $S>1.2$ for $\delta_f/\delta_c=30$, and the transition value of $S$ is about 1.0 for a lower maximum loading interference (i.e. $\delta_f/\delta_c=2.94$). When $S$ is near the transition, a smaller loading level can more readily cause ductile separation. The definition of ductile separation in this model is the occurrence of considerable stretch during unloading which is often accompanied by the formation of a neck.

The results of this model are qualitatively consistent with two previous models in that smaller loading and greater adhesion energy are more apt to cause ductile separation. However there are quantitative differences with those models. The knowledge obtained in this work for the relations between the contact force, contact radius and interference, and the adherence force, are important for use by designers in a variety of single contact problems.
Chapter 5

Finite element models for adhering nanocontacts

Due to the intrinsic problems of fabrication, the top of the micro sphere is not perfectly smooth. There are a lot of small asperities sitting on it. One method to model these asperities is to assume that they have the same radius of curvature, but different height, and their distribution is Gaussian. Its roughness can be represented by standard deviation $\sigma$. So the macroscopic contact of the flat with the micro bump is the statistic results of many individually small contacts. Depending on the penetration of the flat into the sphere, there are more and more asperities involved in the contact. In the previous chapters, we took the whole microbump as a smooth sphere. That could be true when the loading force is large enough to assume all the asperities are in contact. And for unloading, since different asperities with different height are going to be out of contact at different time, the multi-asperity model is still needed to study this problem. So first it is
necessary to understand the contact information of each nano asperity, then the results may be used to build a multi-asperity model.

For such a small contact, the effect of adhesion should dominate the contact and lead to some novel phenomena, especially for unloading. Analytical models mentioned in Chapter 2 are not accurate even for micro scale contacts, and they are not expected to be used directly. The existing KE model for adhesion is also not applicable because it did not include profile changes due to adhesion. Recall that I mentioned strain gradient plasticity in Chapter 3. For microcontact with contact radius from 0.1 $\mu m$ to 10 $\mu m$, the yield strength of material is much greater than that of the macroscopic material. Although gradient strain plasticity is not included in the FEM microcontact model, we used a higher hardness than that of bulk material to resolve this problem. While for the nanocontact, the plasticity is not completely caused by dislocation. It is recognized that the procedures used in the FEM microcontact should not be suitable for the study of nano contact plasticity. But it is still good to know what the contact looks like, especially it takes much less time to obtain results for nano case because the much smaller size of the contact. Another good and straightforward method to study the nano contact is to use molecular dynamics model as mentioned in Chapter 4. I will compare my results with the molecular dynamics model.

### 5.1 The FEM model for nanocontacts

The FEM model for nanocontacts can be found in Figure 5.1, which is similar to the model used for microcontacts in the previous chapters, except that it uses much less
elements, than those, used for the microcontact over the whole hemisphere. But we still need a relatively fine mesh on the surface because the adhesion effect will dominate the contact here. A fine mesh generally can give good results but consume long computer time, while coarse mesh does the opposite. We want to find a good combination of resolution and time, so a set of simulations for the same material properties were run with different surface mesh densities.

![Finite elements model for the nanocontact.](image)

Figure 5.1. The finite elements model for the nanocontact.

The adhesion energy was picked at 0.5 \( J/m^2 \) because simulations had been performed for different adhesion energies with very rough meshing just for a quick view of how this model will work and very similar results were obtained to those of the
Molecular Dynamics model. An adhesion energy of 0.5 $J/m^2$ is believed to be able to show significant adhesion effects, without convergence problems seen at higher adhesion energies. The material properties for gold are listed in Table 5.1.

Table 5.1 Material Properties for Gold

<table>
<thead>
<tr>
<th>Material</th>
<th>Hardness $H$ (GPa)</th>
<th>Young’s Modulus $E$ (GPa)</th>
<th>Poisson’s Ratio $\nu$</th>
<th>Radius of Curvature $R$ (nm)</th>
<th>Intermolecular Distance $Z_0$ (nm)</th>
<th>Strain Hardening</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gold</td>
<td>3</td>
<td>91</td>
<td>0.32</td>
<td>3</td>
<td>0.184</td>
<td>2%</td>
</tr>
</tbody>
</table>

The force-displacement curve of a cycle of loading and unloading is shown in Figure 5.2 in different mesh densities. The meshing for Mesh 1 to Mesh 4 is denser and denser with 25, 50, 100, 200 elements on the surface, respectively. The meshing on the other two straight lines are the same. So the meshing density is gradual from the surface to the interior. The mesh density does not affect the loading too much, but it does change the unloading profile a lot. We can see Mesh 3 and Mesh 4 gave a good convergence on the unloading curve. But it seems the magnitude of the maximum unloading force is independent of mesh density because although mesh density affects more on the edge of the contact where the Lennard-Jones stress is the strongest. A fine mesh on a relatively small area does not change the total integration of the stresses over the area too much. So
Mesh 3 is assumed as a good mesh. It consists of 5357 nodes and 2753 elements as shown in Figure 5.1. The element size is 0.047 nm on the surface.

Figure 5.1 Force-displacement curve for a cycle of loading and unloading with 4 different mesh densities.

5.2 Some preliminary results

A series of simulations were performed using the material properties listed in Table 5.1 to compare with those of the MD model. The radius of curvature of the round bump is 3 nm, in contact with a rigid flat. Since the simulations were done very early for trial purposes
to see how the method works, the roughest mesh number 1 was used, which may not quantitatively accurate, but should be applicable qualitatively.

The first group of simulations was done with indentation starting at -0.75 nm up to 0 nm and then unloading for adhesion energy varying from 0.4 J/m² to 1.5 J/m² in Figure 5.3. A second group of simulations was for an indentation of 0.5 nm in Figure 5.4. In both plots the dashed lines represent loading path, and the solid lines represent unloading path. The dash lines at the beginning of loading are very straight which is because only two points are simulated. More points should be added to get a better curve. Both plots show the increase of adherence force with the increase of adhesion energy. The closed paths for the simulations with adhesion energies of 0.4 J/m², and 0.6 J/m² represents the accomplishment of a cycle of loading and unloading, while the curve did

![Figure 5.3: Force-displacement curve with indentation at 0 nm.](image-url)
not close at higher adhesion energy which is due to convergence problems encountered. The last point on the unloading curve is the furthest point at which ANSYS® can find a solution. The possible reasons for that and the non-smooth curve during unloading are going to be discussed in the next section.

Figure 5.5(a) & (b) are the equivalent von Misés stress contour under different adhesion energy for maximum interference up to 0 nm and 0.5 nm, respectively. Recall that 2% strain-hardening was used. Thus the red area corresponds to the stresses above the initial yield strength without hardening; it does not represent the plastic deformation zone during unloading. For adhesion energy below 0.6 J/m², the contour is at the point upon
separation, while for the higher adhesion energy, the program failed to converge, so the contour is for the last point with converged results. Generally the bump is stretched more under higher adhesion energy and has more global plastic deformation. The expected neck formation for ductile separation was not observed.

\[ \Delta \gamma = 0.4 \text{ J/m}^2, \delta_i = 0 \text{ nm} \]

\[ \Delta \gamma = 0.6 \text{ J/m}^2, \delta_i = 0 \text{ nm} \]

\[ \Delta \gamma = 0.8 \text{ J/m}^2, \delta_i = 0 \text{ nm} \]

\[ \Delta \gamma = 1.5 \text{ J/m}^2, \delta_i = 0 \text{ nm} \]

Figure 5.5(a) Equivalent Von mises stress contour upon separation under different adhesion energy for maximum interference up to 0 nm.
Figure 5.5(b) Equivalent von Misés stress contour upon separation under different adhesion energy for maximum interference up to 0.5 nm.

With the right meshing in Figure 5.1, the simulation for a cycle of load and unload was done for adhesion energy equal to 0.5 J/m² at different maximum interference in Figure 5.6. All four separations showed a stretched process before separation. But the distance of stretch is not monotonic with the increase of maximum interference. Similar
to the result obtained from the micro scale adhering contact in Chapter 4, the loading level also plays an important role on the separation modes. Figure 5.7 is the plot of the adherence force as a function of maximum interference. The curve shows a linear trend except that the largest maximum interference 1 nm gives a slightly higher adherence force than the linear trend. The comparisons of the adherence force obtained from this work, the Maugis-Pollock (MP) model [Maugis 1984] and the EKK model [Etsion 2005] are listed in Table 5.2. Although none of the above models are expected to describe the plasticity occurring at atomic scale accurately, they can still serve as a starting point for understanding this problem. Depending on the criteria discussed in Chapter 2, the MP model predicted a ductile separation for all the four loading levels. The adherences predicted by this work and the MP model are very close although the MP model gives a bigger value as what we obtained in Au microcontacts in Chapter 3. But the EKK model gives a much higher adherence force, at least 27 times greater than this work. Recall that the EKK model was built without adhesion. It gives a curve-fit to the finite element simulations for the residual radius of curvature at the summit of the deformed and fully unloaded sphere. To make it applicable, the contact should be the DMT type, the adherence force is then \[ F_{\text{adh}}^{\text{EKK}} = 2\pi\Delta\gamma R_{\text{res}}^{\text{EKK}}. \] Critical interference used in obtaining \( R_{\text{res}} \) is equal to 0.0019 nm which is calculated based on the continuum model without adhesion. Its value without considering the discrete dislocation mechanism occurring at nano scale leads to the adherence force obtained by the EKK model such great.
Figure 5.6. Force-displacement curves for a cycle of load and unload for adhesion energy equal to 0.5 J/m$^2$ at different maximum interference.

Figure 5.7. The adherence force as a function of maximum interference.
Table 5.2 Comparisons of the adherence force obtained from this work (Figure 5.6), the Maugis-Pollock analytical model and the EKK model.

<table>
<thead>
<tr>
<th>Interference (nm)</th>
<th>This work</th>
<th>1</th>
<th>0.8</th>
<th>0.5</th>
<th>0.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adherence Force</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(nN)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MP</td>
<td></td>
<td>55</td>
<td>45</td>
<td>29</td>
<td>13</td>
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<tr>
<td>EKK</td>
<td></td>
<td>2392</td>
<td>1915</td>
<td>1199</td>
<td>482</td>
</tr>
</tbody>
</table>

5.3 Existing problems and the solutions to the FEM model

As presented in the previous chapters and in this chapter, a finite element model was developed to study the contact and adhesion of microcontacts and nanocontacts. It is shown to be a valid model for the study of the microcontacts by identifying two separation modes and determining the key parameters for the occurrence of each mode. However, to get accurate and complete results and further used for switch design and verification of experiments, the following existing problems found during simulations, especially for the nanocontact study, still need to be addressed and appropriate solutions found.

With the increase of adhesion energy, there are two kinds of failure encountered in ANSYS®. The first failure is a sudden generation of a sharp corner during unloading as shown in Figure 5.8 which is believed to be unreasonable and caused by how the adhesion is modeled, i.e. the adhesive stresses are added normal to the spherical surface.
Chapter 5 Finite element models for adhering nanocontacts

The other one is the failure to get convergence and ANSYS® gives the error report like “The ESAV file has been detected to be corrupted. The file is incomplete due to termination while the file was being written”. This is probably due to an unreasonable shape change on some elements.

Figure 5.8 and Figure 5.9 are the contour of the principle stresses on the \( x \)-direction. Both of them show maximum stresses on the edge which can only be caused by the \( x \) component of the Lennard-Jones stresses added on the normal direction. It does not bring any problems during loading. But during unloading, due to the big effect of adhesion, the surface of the sphere is stretched up and the edge of the contact is going to be relatively sharp compared with the original round shape which may cause the parallel assumption to be invalid. Continuing to use the same method of determining the force from the Lennard-Jones potential may cause a significant magnitude of lateral force on the surface and cause the results to be unstable. But the difficulty is that ANSYS® does not provide a convenient way to define the direction of the added pressure. By default the pressure can only be added on the normal direction. Otherwise extra surface elements should be used to define an arbitrary direction. It is better not to involve more elements in the simulations.

The easiest way to solve this problem probably is by using an equivalent body force on each node of the surface instead of the pressure. The model in Figure 5.1 is a 2-D axisymmetric model. The force on node \( i \) can be calculated by multiplying Lennard-Jones stresses by the annular finite area \( A \) around that node,

\[
F = p_i A
\]

where
Figure 5.8: The contour of stresses on x-direction during unloading at adhesion energy equal to 1 J/m².

Figure 5.9: The contour of stresses on x-direction during unloading at adhesion energy equal to 0.8 J/m².
\[ A = \pi x(i) \sqrt{\left( x_{i-1} - x_i \right)^2 + \left( y_{i-1} - y_i \right)^2 + \left( x_{i+1} - x_i \right)^2 + \left( y_{i+1} - y_i \right)^2} \]

\( x_i \) and \( y_i \) represent the coordinates of the node \( i \) in \( x \) and \( y \) directions respectively. Note that they are the values after the sphere is deformed. A simple simulation was performed to verify this conversion. It is found the external force simulated from adding pressure on the normal direction is also the same with adding the adhesion force on the normal direction which shows the conversion is effective. However a greater external force was obtained by adding the adhesion force on the vertical direction.

Therefore now the most concern is about whether the Lennard-Jones stresses between two parallel surfaces are applicable for this model with metal contact. The following section is going to give a preliminary discussion.

### 5.4 Sutton-Chen potential - a modification of the LJ potential

The Lennard-Jones (LJ) stresses between two parallel surfaces were used to represent the interaction between the contacting bodies in our previous work. The LJ potential for two parallel surfaces is derived from the LJ 6-12 pair potential by volume integration over the whole body. It is not very accurate for our model for the following three reasons. First it describes long-range van der Waals forces, but the real interaction is metal-to-metal. It does not include the influence of the third neighbor on the pair of atoms – this effect is more important for nanoscale contacts. Therefore it gives a poor description of surface relaxation in metals. Surface relaxation is a small and subtle rearrangement of the surface layers which may nevertheless be significant energetically, and seems to be commonplace for metal surfaces. It involves adjustments in the layer spacings perpendicular to the
surface, there is no change either in the periodicity parallel to the surface or to the symmetry of the surface. In general, the surface stress in the direction of the surface normal determines the relaxation direction except for Al (110) surface. When the surface stress is negative (compressive), the surface relaxation is inward; otherwise, the relaxation is outward. An interesting result is that the surface tension does not always decrease after relaxation. The outward relaxation will induce the increase in surface tension while the inward relaxation induces the decrease in surface tension. For example, the LJ potential predicts the outward relaxation of most Cu surfaces and the negative surface tension, but these predictions are in contradiction to experiment and first-principle calculations [Wolf 1990]. Secondly, the contact is between a flat and a deformed hemisphere which are not parallel over the length scale for which the adhesive forces are significant. Thirdly the direction of the force is not necessarily vertical.

To treat this complicated problem, a more accurate physical description of the phenomena is needed. Some preliminary results based on the Sutton-Chen (SC) potential [Sutton 1990] were recently obtained. The SC potential may be less accurate for modeling particular metals than some of the other potentials, but has several advantages. First it provides a method for analyzing trends in properties in different metals; secondly there are analytic and approximate expressions for various quantities which may be obtained in terms of the potential parameters; thirdly it is particularly suitable for computer modeling as the potential is efficient to evaluate; and finally it is longer ranged than most semi-empirical potentials, a property that may be important for the correct modelling of surface phenomena. If these potentials turn out to describe metals well, then it is likely that they will play the same role for metals as the Lennard-Jones potential has.
played in the description of rare gas and molecular solids and liquids, since they contain
the essential physics and give at least a good qualitative description of various
phenomena displayed by these systems.

The Sutton-Chen potential leads to an accurate description of many properties of
metals and their alloys, such as Au, Rh, Ru, and Ir. It is a good combination of the short
range $N$-body Finnis-Sinclair potentials [Finnis 1984] to obtain a good description of
surface relaxation, and the van der Waals force to give a correct description of the long-
range interactions. The total energy is the sum of the potential between each atom and all
of its neighbors which can be written as

\[ E_T = \sum_i E_i = \epsilon \left[ \sum_i \left( \frac{1}{2} \sum_{j \neq i} V(r_{ij}) - c\sqrt{\rho_i} \right) \right], \quad (5.2) \]

where

\[ V(r) = (l/r)^n, \quad (5.3) \]

\[ \rho_i = \sum_{j \neq i} \left( \frac{l}{r_{ij}} \right)^m. \quad (5.4) \]

where $r_{ij}$ is the separation between atoms $i$ and $j$, $c$ is a positive dimensionless constant, $\epsilon$
is a parameter with the dimensions of energy, $l$ is the crystal lattice constant, and $m$ and $n$
are positive integers. Please note that symbol $a$ is normally used to represent the crystal
lattice constant and it was used in [Sutton 1990] as well. Since $a$ has already been used
for contact radius in this thesis, $l$ was used here. The pair potential, $V$ is purely repulsive
and the $N$-body term is purely cohesive. Although this is truly a many body potential, the
force on each atom can be written as a sum of pairwise contributions,

\[ F_i = \sum_{i \neq j} F_{ij}. \quad (5.5) \]

where
In Eq. (5.5) \( r_{ij} \) is the vector pointing from the atom \( i \) to the atom \( j \). A positive force means an attractive force and a negative force means a repulsive force. We can see that the \( N \)-body cohesive term in Eq. (5.1) includes a \( 1/r^m \) van der Waals tail (it is \( 1/r^6 \) in van der Waals force). However the square root in that term gives rise to \( N \)-body interactions in the sense that the force in Eq. (5.5) exerted by one atom on another depends on the disposition of all neighbors to both atoms concerned. By contrast, a pair potential alone gives rise to a force that depends only on the separation of the two atoms concerned. Therefore the SC potential is good at obtaining a correct description of surface relaxation.

The values for \( c, \varepsilon, m \) and \( n \) that are provided in [Sutton 1990] have been fitted to the experimental cohesive energy and crystal lattice parameter for a variety of fcc metals. The SC potential has been modified to include quantum corrections (e.g. zero-point energy) in comparing properties to experiment, leading to the quantum Sutton-Chen, or Q-SC force field [Kimura]. The Q-SC parameters were optimized to describe the lattice parameter, cohesive energy, bulk modulus, elastic constants, phonon dispersion, vacancy formation energy, and surface energy. The parameters obtained from the SC and the Q-SC force field are listed in Table 5.3 for the ease of use. The values for \( c, \varepsilon, m \) and \( n \) obtained from the Q-SC are going to be used for the following calculations.

Let us take gold as an example to start the study of SC potential. Two identical flat bodies are put in parallel with a separation \( Z \) between the atomic planes. Each of the
bodies contain 20x20x4 unit cells aligned along a <001> direction. The atoms within the bodies are fixed in position.

First we plot the total energy of the single body in terms of the length of the cube to test the validity and SC potential and our programming. In Figure 5.10 the minimum total energy corresponds to length equal to $0.405 \text{ Å}$ which is the same with the real crystal constant.

<table>
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<tr>
<th>Table 5.3 Potential parameters for f.c.c. metals</th>
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Figure 5.10. Total energy (Joules) vs. crystal constant (Angstroms) for <001> direction.

The adhesion energy and equilibrium distance of two bodies can also be numerically obtained by the SC potential. Much work has been done with adhesion energy while little has been devoted to obtaining the equilibrium distance between separate bodies, although it is a very important parameter in the study of contact with adhesion. The adhesion energy $\Delta \gamma$ is defined as the work per unit area needed to separate two bodies from some distance $Z$ to infinity, i.e.

$$\Delta \gamma = \frac{E_f(Z) - E(\infty)}{A}, \quad (5.7)$$

where $A$ is the surface area of one body.

Figure 5.11 is the plot of adhesion energy vs. separation. The equilibrium distance $Z_0$ between two parallel surfaces is the distance at which the adhesion energy reaches its minimum. As mentioned in Chapter 2 often the value of 0.4 nm is used for $Z_0$. Yu and Polycarpou proposed a method to calculate $Z_0$ based on the nearest neighbor distance $r_N$. 

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Chapter 5 Finite element models for adhering nanocontacts

[Yu 2004] leading to a value of $Z_0 = 0.184 \text{ nm}$ for Au. The value of $Z_0$ found by the SC potential is $0.266 \text{ nm}$ for Au which is about 1.45 times greater than the continuum based prediction of [Yu 2004]. The dashed line in Figure 5.11 is the Lennard-Jones potential with the same value of the adhesion energy. Certainly these curves should depend on the arrangement of the atoms. We can see the peak of SC is sharper than that of LJ which can be expected to lead to differences in the adherence force in a nanoscale contact.

![Graph showing adhesion energy at different separations for <001> direction](image)

**Figure 5.11** Adhesion energy at different separations for <001> direction. The equilibrium distance $Z_0$ at the minimum adhesion energy is $0.266 \text{ nm}$.

A similar study was also done for <111> direction. The atoms in the {111} planes are in the most close-packed arrangement possible for spheres. The stacking sequence of {111} planes is $ABCABC$ with equal spacing distance $\sqrt{3}/2 \ l$ ($0.235 \text{ nm}$ for Au) between...
each layer. The arrangement of the atoms is illustrated in Figure 5.12 in two dimensions of \( x-y \) plane. There are 6 layers with total 19440 atoms included in each body. The top layer \( C \) of one body faces the top layer \( A \) of the other body. We define the \( z \)-axis as being along the surface normal pointing out of the metal. The position of each atom is still fixed. Figure 5.13 is the plot of adhesion energy vs. separation. The equilibrium distance \( Z_0 \) at the minimum adhesion energy is 0.227 \( \text{nm} \) which is smaller than for \( <001> \) direction since \( <111> \) direction is more close-packed.

![Figure 5.12](image-url) Arrangement of atoms in \{111\} planes in two dimensions (3240 atoms on one layer, 6 layers in each body).
Figure 5.13. Adhesion energy at different separations for $<111>$ direction. The equilibrium distance $Z_0$ at the minimum adhesion energy is 0.227 nm.

In the previous calculations the atoms are fixed which neglected the energy minimization and surface relaxation. Therefore it is not realistic. If considering only single body of the two bodies, it is found that there exist net forces on the atoms of the top layer which point inward due to surface relaxation. More advanced methods such as Molecular Dynamics are available to investigate and understand the microscopic processes. As a preliminary work about modifying the LJ potential with a more realistic potential for metals in this thesis, the top layer was adjusted to get a zero force on a single atom within the top layer. Due to the limitation of the method that only the position of the top layer is adjusted and all the atoms within the layer move the same distance, the energy minimization can not be satisfied, and neither the zero force for each atom within
the top layer. A certain amount of movement can only lead to offset the force on a single atom.

Considering the symmetric property of the body, the atoms were picked along the symmetric line of \( y \)-axis. Since the force in \( z \)-direction is much greater than the forces in \( x \) and \( y \) directions (at least 8 times greater), the offset is specially considered for \( z \)-direction. The plot in

Figure 5.14 is the curves of force in \( z \)-direction vs. the displacement of the top layer. Positive force means attractive force pointing inward. Decreasing the force corresponds to the displacement moving from the original spacing inward. It is found that the zero force for the first atom of the symmetric line is reached when
Figure 5.14. The net force vs. the displacement of the top layer on the third atom from the edge. The displacement of the top layer inward the surface. The displacement is about 5.2% of the original spacing ($\sqrt{3} l$) while the displacement is about 2.6% of the original spacing for all the atoms except the first one at the edge. Therefore the surface relaxation has the effect of moving atoms inward and the movement is greater for the edge of the atom than the inner atoms. Keeping moving the atoms inward leads to a negative force corresponding to the repulsive region which is consistent with the reality. Therefore a displacement of $0.015 l$ was used to adjust the force on the second atom to be zero and for the following research. The adjustment was done for the surface of each body facing each other. Doing the calculation with the surface adjustment, the equilibrium distance $Z_0$ is 0.2295 nm which is a little greater than that without surface adjustment in Figure 5.13.

In using the LJ potential the interaction force depends only on the local separation of the surfaces. With the SC potential the interaction force depends on both the local separation and angle of inclination between the surfaces. Thus the next step is to determine the force on a certain surface atom when the surfaces are separated by a distance $Z$ and at angle $\theta$. Figure 5.15 is the draft for this purpose.

For the angle ranging from 0 degree to 90 degree, the following results were found from a preliminary study. Due to symmetry, the force in $y$-direction is very small. The force considered here is the total of the force in $x$ and $z$ direction. It changes from repulsive force to attractive force with the increase of the local separation. Although the transition separation from repulsive force to attractive force increases with the increase of the angle of inclination, the direction of the force in $z$-direction is always vertical to the
original surface except for the area around the transition point. The non-vertical problem may be because both the force in $x$ and $z$ direction are turning to be close to 0 and the net force cancellation was only roughly done for the surface force in $z$ direction. The net force acting on the atom brings the instability when the surface force is comparable with the net force. Comparing with the stress distribution of the Lennard-Jones potential, the result is similar to the comparison of the total energy in Figure 5.13. The peak of SC is sharper than that of LJ which can be expected to lead to differences in the adherence force in a nanoscale contact. More work can be done such as getting curve-fitting results for the SC potential at different separations and angles for use in our FEM model.

Figure 5.15: Draft for the study of the interaction force depending on both the local separation and angle of inclination between the surfaces.
Chapter 6

Conclusions and future work

6.1 Finite elements model summary

A finite element model with ANSYS® has been built and simulations have been performed for both microcontacts and nanocontacts. Comparisons have been made between our results and some existing methods. For simplicity, the model is for a deformable hemisphere in contact with a rigid flat. The effect of adhesion is applied on the surface of the sphere as a surface pressure based on the Lennard-Jones potential for two parallel surfaces. The assumption is that the sphere and the flat can be treated as two parallel surfaces when determining the surface pressure. An iteration method with an under-relaxation factor is used to find the corresponding reaction force and deformation profile under a certain penetration with adhesion.
For microcontacts, the comparisons are among this model, theoretical models (i.e. the Maugis transition model for elastic contact, and a simple plastic model), and Kogut and Etsion’s finite element model. In the elastic contact region, this model agrees well with the Maugis transition model for both Ru and Au which tend to be in DMT and JKR region, respectively. But this model only agrees with the KE’s model in the DMT region and shows a big discrepancy in the JKR region since the KE’s model did not consider the change of deformation due to adhesion force. In the plastic region, since the ratio of adhesion force over the applied force is smaller with the increase of applied force, the discrepancy between my model and the KE’s model is smaller. But both of them show the simple theoretical plastic model is not very accurate.

The impact of four parameters i.e. $S$, $E/\sigma_y$, $\mu$, and $\delta_f/\delta_c$ on the separation modes of adhesive contacts was investigated. The results show that $S$ and $\delta_f/\delta_c$ are the key parameters, while $\mu$ and $E/\sigma_y$ are less important. Ductile separation occurs when $S>1.2$ for $\delta_f/\delta_c=30$, and the transition value of $S$ is about 1.0 for a lower maximum loading interference (i.e. $\delta_f/\delta_c=2.94$). When $S$ is near the transition, a smaller loading level can more readily cause ductile separation. The definition of ductile separation in this model is the occurrence of considerable stretch during unloading.

The results of this model are qualitatively consistent with two previous models in that smaller loading and greater adhesion energy are more apt to cause ductile separation. However there are quantitative differences with those models. The knowledge obtained in this work for the dependence of the adherence force on the contact force, contact radius and interference is of general interest in the understanding of adhesion and is also
important for use by designers in a variety of single contact problems such as, for example, the contact in a micromechanical switch.

For the nanocontact, a rough meshing was first used in order to quickly get results and see the validity of the model. The simulations were done for the flat loaded up to 0.5 \text{nm} at different adhesion energies ranging from 0.4 \text{J/m}^2 to 1.5 \text{J/m}^2 to compare with Molecular dynamics (MD) models. Because the working mechanism is different for these two models, exact comparisons on the same plots is not possible. But the trend is very similar. Higher adhesion energy causes ductile separation with adhesion force slowly decreasing until separation and lower adhesion energies result in brittle separation with the pull-off force sharply decreasing at a sudden separation. Later on the force-displacement curve is plotted for different mesh densities to find an appropriate meshing, because we want to get a good trade-off of the computing time and accuracy. With the right meshing, simulations were done for adhesion energy equal to 0.5 \text{J/m}^2 under different interferences. The plot of pull-off force vs. maximum interference is approximately linear.

Modeling metals poses a particular problem as one requires a potential which depends only on the nuclear positions while the bonding is caused by delocalized electrons. Lennard-Jones potential between two parallel surfaces used in this thesis has given very valuable information as a first time step to study the microcontact and nanocontact involved in the reliability problem of microswitches. However to get an accurate result, a more realistic potential for metal is needed. It is more convenient to use a semi-empirical atom potential with many-body terms in it. The Sutton-Chen potential was briefly studied due to several advantages mentioned in Chapter 5. It was found that
the direction of the force between two non-parallel surfaces is almost perpendicular to the other surface and has very little dependency on the inclination angle between two surfaces.

### 6.2 Significance of this work

To the best of our knowledge this is the first time that a finite element model has predicted the effect of adhesion on deformation and on stress with plastic deformation in an adhesive contact. Two separation modes - brittle and ductile separation were identified. Other theoretical models, such as the Maugis-Pollock and the Mesarovic-Johnson models, assume a sudden transition from elastic unloading to an expected fully plastic separation. In our work the unloading is allowed to be elastic and/or plastic as dictated by the results of the simulation. The knowledge obtained in this work for the dependence of the adherence force on the contact force, contact radius and interference is of general interest in the understanding of adhesion and is also important for use by designers in a variety of single contact problems such as, for example, the contact in a micromechanical switch.

### 6.3 Future work

The algorithm of the finite element model has been modified to resolve the numerical problems such as from Eq. (3.1) to (3.5). The next step is to get curve-fitting
results for the Sutton-Chen potential at different separations and angles for use in our FEM model.

With an accurate potential model, more work can be done for nano-scale contact like what has been done for microcontact, such as to understand the effect of adhesion energy, loading force, hardness, and strain hardening. In addition, a curve fitting expression should be given based on the simulation results for the relation of force, displacement, and contact radius. The empirical expression for a single nano asperity contact under different roughness can be integrated into a multi-asperity contact model for microscopic contacts under plastic deformation.

It is very important to have a multi-asperity contact model to analyze the real contact of the MEMS switches. There existing a lot of work on this case. However how realistic it could be is still dependent on the accurate analysis of the discrete nanocontact.

In Appendix B I will briefly introduce some related work to help the next study.
Appendix A

Contact mean pressure between two spheres

A general case is the contact between two spheres with the radius of curvature \( R_1 \) and \( R_2 \) respectively. Their Young’s modulus is \( E_1 \) and \( E_2 \) and the Poisson ratio is \( \nu_1 \) and \( \nu_2 \). The mean pressure \( p_m \) is the contact force \( F \) divided by the contact area \( \pi a_f^2 \) in which \( a_f \) is the contact radius. The mean pressure is a very useful concept in the sense of judging the initial yielding and fully plastic. It is going to be discussed in details for different types of contact condition.

I. purely elastic contact between two spheres

If the contact is purely elastic, the relation between the contact radius and contact force is given by Hertz theory,

\[
a = \left( \frac{FR}{K} \right)^{1/3} = \frac{\pi p_m R}{K}
\]  
(A-1)
In Eq. (B-1) \( \frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2} \), and \(\frac{1}{K} = \frac{3}{4} \left( \frac{1-v_1^2}{E_1} + \frac{1-v_2^2}{E_2} \right)\) in which \( R \) is the effective radius of curvature and \( K \) is the effective modulus of elasticity. If the one of the two spheres is replaced by a flat surface, Eq. (A-1) is still applicable by taking the radius of curvature of the flat as infinite. If one of the two spheres is rigid, its Young’s modulus is infinite and \( K \) is twice than that of both deformable spheres.

II. elasto-plastic contact between two spheres

When the contacting bodies experience sufficient pressure, a plastic zone first appears below the surface and causes some permanent deformation. This state, in which some material is plastic, while the surrounding material is elastic, is called elasto-plastic deformation. The mean pressure of the initial yielding in terms of the yielding strength \( \sigma_y \) can be calculated from the derivation of [Johnson 1985],

\[
p_m = a \sigma_y \begin{cases} 
\alpha = 1.1 & \text{for } \nu = 0.3 \\
\alpha = 1.25 & \text{for } \nu = 0.5 
\end{cases}
\]  

(A-2)

The semi-empirical formula of the mean pressure of the rigid sphere in contact with the flat metallic surface was given in [Studman 1976] and [Studman 1977] for \( \nu = 0.5 \),

\[
p_m = \frac{P}{\pi a f} = \sigma_y \left( 1 + \frac{2}{3} \ln \frac{Ea_f}{3\sigma_y R} \right).
\]  

(A-3)

But it was found in [Maugis 1984] that it mismatches Eq. (A-4) at the onset of plastic deformation. Therefore let us take the format of Eq. (A-5) and rederive the appropriate parameters to match the two ends of the elasto-plastic deformation. The expression of the
mean pressure for the contact of the rigid sphere with the flat surface with unknown parameters $A$, $B$ and $C$ is,

$$p_m = \sigma_y (A + B \ln \frac{Ea_f}{C\sigma_y R})$$  \hspace{1cm} (A-4)$$

At the transition point from elastic contact to elasto-plastic contact, both Eq. (A-1) and Eq. (A-4) are applicable. They are both equal to Eq. (A-2) for any material properties. Therefore the second term should be zero with non-zero $B$ which gives the critical contact radius

$$a_c = C \frac{R\sigma_y}{E},$$ \hspace{1cm} (A-5)$$

and the first term $A=a$.

Substituting Eq. (A-1) into Eq. (A-5) we get

$$C = \frac{\pi a E}{K}$$ \hspace{1cm} (A-6)$$

For the contact between one rigid surface and one deformable surface,

$$C = \frac{3\pi a (1 - v^2)}{4} = \begin{cases} 2.3 & \text{for } v = 0.3 \\ 2.2 & \text{for } v = 0.5 \end{cases}$$ \hspace{1cm} (A-7)$$

$C$ for the contact between two deformable surfaces is twice of that in Eq. (A-7).

Now the only unknown parameter is $B$ which can be obtained by matching Eq. (A-4) with that of the fully plastic deformation. The mean pressure becomes constant $H$ (material hardness) where it is fully plastic contact,

$$p_m = \frac{P}{\pi a^2} = 2.8\sigma_y = H,$$ \hspace{1cm} (A-8)$$

The critical contact radius from elasto-plastic contact and fully plastic contact is
Appendix A

\[ a_p = \frac{60 R \sigma_y}{E}, \]  \hspace{1cm} (A-9)

which was reported in [Maugis 1984] in agreement with experiments. Eq. (A-9) is only for \( v=0.5 \). It is supposed to be little different for other \( v \) values.

Therefore \( B=0.51 \) for \( v=0.5 \) and \( B=0.52 \) for \( v=0.3 \) if assuming Eq. (A-9) is still applicable for \( v=0.3 \). Finally the mean pressure can be expressed as

\[ p_m = \sigma_y (1.1 + 0.52 \ln \frac{E a_f}{2.3 \sigma_y R}), \]  \hspace{1cm} (A-10)

for \( v=0.3 \) and

\[ p_m = \sigma_y (1.25 + 0.51 \ln \frac{E a_f}{2.2 \sigma_y R}), \]  \hspace{1cm} (A-11)

for \( v=0.5 \).

Maugis used \( H/\sigma_y=3 \) in his derivation instead of 2.8 used in Eq. (A-8). Therefore he derived the expression of the mean pressure a slightly different from the above, [Maugis 1984]. For \( v=0.3 \) it is,

\[ p_m = \sigma_y (1.1 + 0.58 \ln \frac{E a_f}{2.3 \sigma_y R}). \]  \hspace{1cm} (A-12)
There existing a lot of work on this case. The first step is to define the physical model of the rough surface. There is considerable evidence that asperities on real surfaces can have any shape and any distribution of heights. However the most used model is to treat the asperities as sphere near their summits with a uniform radius of curvature ([Greenwood 1967], [Majumder 2003], [Sahoo2005]). The heights $Z$ of the asperities follow the normal, Gaussian, distribution about a mean surface,

$$\phi(Z) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{Z^2}{2\sigma^2}\right),$$  \hspace{1cm} (6.1)

$\sigma$ is the standard deviation of the height distribution which can be measured through the technological measures of roughness. In addition a simplified treatment is to consider one side smooth and the other rough. Further consideration is whether the asperities are far apart and there is no interaction between contacting asperities. A lot of work has been done with no interaction between contacting asperities ([Chang 1988], [Roy 1994], [Greenwood 1967]). However
for considering interaction, Sahoo mentioned in his paper [Sahoo 2005], “To the best of the authors’ knowledge, there is no literature available on adhesive contact analysis of rough surfaces that considers interaction of asperities.” Results in [Sahoo 2005] show that asperity interaction influences the loading-unloading behaviour in elastic-plastic adhesive contact of rough surfaces and in general asperity interactions reduce the effect of surface forces.

If no interaction between asperities, the macroscopic effects is just the linear summation of those occurring at each asperity. If the base of the rough surface is flat, the problem is simpler. Considering there are $N$ asperities on the flat. The height of the $i^{th}$ asperity is $Z_i$ from its reference plane. Let the original separation between the reference planes be $d$. if there is no adhesion, only the asperities with their heights greater than $d$ come into contact. However more asperities will be involved into contact if considering adhesion. The vertical deformation (interference) of asperity $i$ is given by

$$\delta_i = Z_i - d$$  \hspace{1cm} (B-1)

The interference is negative if two bodies do not touch without deformation. In case we already known the curve-fits for the relation of external force, contact radius and interference, the total values can be obtained easily. Majumder [2003] found in his theis that with the same value of contact force, smoother surface has more number of contacting asperities which is very reasonable.

A numerical multi-asperity contact model for elastic deformation of a rough sphere has been built by Greenwood and Tripp [Greenwood 1967]. It is found that the Hertzian results are valid at sufficiently high loads, but at lower loads the effective
Appendix B

pressure distribution is much lower and extends much further than for smooth surfaces. The results can be found in Fig. (B-1) and Fig. (B-2).

Figure B-1 At low loads the pressure is much lower than predicted by Hertzian theory and is spread over a much larger area.

Figure B-2 At high loads calculated and Hertzian pressures agree well.
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