Micro-Contact Modeling of MEMS Switch

A Dissertation Presented

by

Hassan Eid

to

The Department of Mechanical and Industrial Engineering

in partial fulfillment of the requirements
for the degree of

Doctor of Philosophy

in the field of
Mechanical Engineering

Advisors:
George Adams, MIE Department
Nick McGruer, ECE Department

Northeastern University
Boston, MA, 2012
Acknowledgements

I am deeply grateful to the following individuals for their generous help and support throughout the course of my graduate study, without which this thesis would not have been possible. I would first like to express my sincere gratitude and indebtedness to my advisors, Professor George G. Adams and Professor Nick E. McGruer, for their continued guidance, support, mentorship and encouragement throughout this work. There are no words to truly express my gratitude to you. Your lessons will always be an invaluable asset throughout my life.

I am grateful to all the faculty and staff of the Department of Mechanical and Industrial Engineering at Northeastern University. I would like to thank Mary Traboulsy and Noah Japhet especially for all of your help.

I’ve also been fortunate to have a great group of friends and colleagues at Northeastern University and would like to thank them all, though I cannot name everyone here. I would like to express my gratitude to my research group; I have learned so much from all of you. I would like to thank my friends for your contributions, which are highly appreciated and made this thesis possible. I would like to give a special thanks to Kariem Elebiary and Amr Abdelrasoul.

Finally, I would like to dedicate this work to my family. Without your unending kindness, support and love, I never would have made it through this process or any of the tough times in my life. Mere words are not enough to express how grateful I am for you. Thank you all so much.
Abstract

A three-prong methodology was rigorously carried out in order to gain a thorough (fundamental) understanding in the field of MEMS switch contact tip mechanics. The first prong focused on quantifying the effect of adhesion of layered media. This was achieved by developing a finite element model of a layered hemisphere contacting a rigid flat. In this analysis elastic-plastic material properties were used for each of the materials comprising the layered hemisphere. The inclusion of the effect of adhesion, which was accomplished with the Lennard-Jones potential, required a special procedure. This configuration is of general theoretical interest in the understanding of adhesion. It has also been suggested as a possible design for a microswitch contact because, with an appropriate choice of metals, it has the potential to achieve low adhesion, low contact resistance, and high durability. The effect of the layer thickness on the adhesive contact was investigated. In particular the influences of layer thickness on the pull-off force, maximum contact radius, and contact resistance were determined. The results are presented as load vs. interference and contact radius vs. interference for loading and unloading from different values of the maximum interference.

The second prong of the method emphasized investigating the effect of nanoscale asperities by developing a combined molecular dynamics and finite element model simulation of contact and adhesion between a rough sphere and a flat surface. This model uses the results of molecular dynamics (MD) simulations, obtained by other collaborators using an embedded atom potential, of a nanoscale Ru-Ru asperity contact. A continuum finite element model of an elastic–plastic microscale Ru-Ru contact bump is then created. In this model, the surface roughness is represented by a system of nanoscale asperities,
each of which is represented by a nonlinear hysteretic force vs. distance relationship. The nonlinear hysteretic character of these relations is determined from curve-fits of the MD results. Load vs. interference and contact area vs. interference are determined using this two-scale model for loading and unloading. Comparisons with a single-scale continuum model show that the effect of the nanoscale asperities is to reduce both the adhesion and the real area of contact. The choice of Ru as the material for this work is due to its relevance in microswitches.

Unlike the two numerical aforementioned prongs, the last prong evaluated contact materials by testing, supported by modeling. The testing used an improved SPM (Scanning Probe Microscope)–based contact tester, constructed and used for cyclic testing of various metal contacts. Collaborators introduced the tester which is especially designed for metal-contact MEMS switch applications, and is capable of simultaneous measurements of contact force and resistance. It was found that a dissimilar contact pair of Au-Ru with O₂ plasma cleaning can provide low contact adhesion and low resistance as compared with Au, Ru, and Ir contact pairs. Layered structures with a thin layer of Ru on top of Au were also modeled and tested. Ru layers between 50 and 100 nm were effective in reducing adhesion and contact resistance provided the contact force is greater than 300 µN.
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Chapter 1: Introduction
1.1 MEMS and RF MEMS switch devices

Microelectromechanical systems (MEMS) are small mechanical devices that are built onto semiconductor chips and are measured in micrometers or less. In MEMS the electronics are adopted from existing state-of-the-art integrated circuit (IC) fabrication technologies. The micromechanical components are fabricated using silicon wafers or deposited structural layers to form the mechanical material and MEMS devices. The MEMS technology and the Radio Frequency (RF) circuitry fabrication lead to relatively new RF MEMS switches.

RF MEMS switches are micromachined devices interacting with electrical signals up to the radio frequency range. These switches can be either direct contact, which are called ohmic switches, or capacitive switches where high-frequency signals can be directed along different signal paths using conductors that are separated by an insulating dielectric layer. RF MEMS is believed to have a large market potential since the high volume consumer market of personal communication devices already exists and literally cries out for new technologies expanding its possibilities. Technology reliability, and the risk of taking a completely new type of component into a high volume product in a very competitive market, have inhibited the transition from research labs to commercial production lines. High-end applications such as automated measurement and test equipment, automotive safety and communication systems, and military and space applications are believed to be the initial application fields of MEMS switch components.

Figure 1 shows a typical diagram of a microelectromechanical switch as in RF MEMS. The flat surface is coated with metal as well as the microbump. When a voltage is applied between the beam and the substrate, the beam is attracted downward to the
substrate due to the electrostatic force causing metal-to-metal contact, which turns on the switch. Similarly when the voltage is removed the beam will be pulled away from the substrate using the stored energy during bending to cause the switch to pull-off the drain.

**Figure 1.** Diagram of a microelectromechanical switch (Adapted from Rebeiz, Gabriel M. RF MEMS: Theory, Design, and Technology)

Electrical metal-to-metal contacts in RF MEMS switches have failure mechanisms which include adhesion, stiction, melting, resistance increase due to contaminate film layers, and reshaping of contacts due to plastic deformation, material transfer and creep behavior, all of which lead to premature switch failure. The failure mechanisms due to organic deposits and contamination around the contact area can be less severe with a clean packaging environment. Surface films occur after microfabrication processes can cause excessive increase in contact resistance leading to stuck-open switch failure where it becomes unusable. Stiction due to adhesion occurs when the surface interaction energy at the contact surfaces is greater than the restoring forces needed to put the switch in the open position. The stuck-closed position will cause a failure in an RF MEMS switch.
1.2 Related work

Cold switching contact failures can be caused from many sources such as contamination on the surface or contact wear-out, causing an increase in resistance. When the restoring force of the cantilever is less than the pull-off force, stiction will occur causing permanent closure of the switch. Thus fundamental understanding is required of the mechanisms and detailed models of contact with adhesion between surfaces. Classical contact mechanics theories can play an important role in the contact studies even in the case of RF MEMS where the contact problem is at the submicron scale.

Hertz contact theory (1882) [1] was the first theory to calculate contact area between two smooth interacting elastic bodies. Hertz assumed a continuous pressure distribution for elastic contact between two surfaces in the absence of adhesion. Johnson, Kendall and Roberts [2] introduced the JKR contact theory with adhesion using an energy approach which balances elastic energy, potential energy, and surface energy. The Derjaguin, Muller and Toporov [3] DMT model followed the JKR model. The DMT model assumes that molecular force interaction exists outside the contact zone. This cohesive zone, which is the area region just outside the contact area zone, was extremely small in the JKR model. The DMT model assumes the cohesive zone will not change the Hertzian contact profile. Tabor [4] anticipated that the DMT and JKR models were two opposite ends of the solution range of elastic spherical contact with adhesion. The JKR and DMT theories each give results which should be general since they are independent of the elastic modulus. Tabor suggested that the JKR and DMT were extreme limiting cases and introduced the Tabor parameter $\mu = \left( \frac{R \Delta y^2}{E r^2 Z_0} \right)^{1/3}$ as a transition parameter between DMT and JKR models. In the Tabor parameter formula, $R=[R_1^{-1} + R_2^{-1}]^{-1}$ is the
composite radius of the sphere, $E^*$ is the effective Young’s modulus given by

$$\left[\left(1-v_1^2\right)E_1^{-1} + \left(1-v_2^2\right)E_2^{-1}\right]^{-1},$$

in which $E$ is Young’s modulus and $v$ is the Poisson ratio, $\Delta \gamma$ is the adhesion energy, and $Z_o$ is the atomic equilibrium separation between surfaces.

Tabor introduced the adhesion parameter to distinguish the transition between the JKR and DMT models and suggested the conditions under which interactions within and outside the contact zone needed to be accounted for. Tabor’s theory was then supported by Muller et al. [5] numerically using a Lennard-Jones potential and demonstrated a continuous DMT to JKR transition as the Tabor adhesion parameter increases. When $\mu > 3$ the JKR model is applicable while the DMT model is applicable when $\mu < 0.1$. Maugis [6] used the Dugdale assumption to offer an analytical solution to the contact problem with interactions inside and outside the contact zone and represented the transition from the DMT to JKR behaviors using his own Maugis parameter (similar to the Tabor parameter) as a continuous spectrum. When the contact problem with adhesion goes into irreversible elastic-plastic deformation, numerical simulation techniques can be used to describe the solution (e.g. [7]).

In MEMS, surface roughness and asperity behavior are important factors that affect contact behavior at the submicron scale. It is essential to understand the influence of the asperities behavior in the contact devices, especially because of the large surface to volume ratios which occur in MEMS.

The Greenwood and Williamson (GW) [8] theory on contact mechanics proposed a multi-asperity contact model based on Hertz theory. In the case of elastic-plastic deformation, Chang, Etison, and Bogy (CEB) [9] introduced their elastic-plastic asperity model, based on volume conservation of the asperity plastic deformation, for analyzing the contact of rough surface. The CEB multi-asperity model was extended in [10] to
include adhesion based on the DMT adhesion model. In [11] Kogut and Etsion (KE) developed an elastic-plastic asperity model with adhesion based on finite element analysis (FEA) similar to their elastic-plastic KE model without adhesion [12]. They used the KE model along with the GW procedure [8] to present an elastic–plastic model for the contact of rough surfaces without adhesion using method of [10].

1.3 Thesis organization

The focus of this thesis is twofold. First to add more knowledge to the field of contact mechanics with adhesion. Second to study stiction failure mechanisms of contact type MEMS switches with metal-to-metal contacts using modeling and simulations with finite element modeling (FEM). Chapter 2 presents contact and adhesion of an elastic-plastic layered microsphere model as a good potential configuration for electrical microcontact tip design giving larger contact area and lower adhesion. In Chapter 3 a multi-scale model of contact and adhesion for a rough sphere is presented. The model incorporates the contact mechanics effect of nanoasperities with adhesion (obtained from the molecular dynamics simulations developed by other collaborators) and the overall continuum elastic-plastic deformation of the sphere. Chapter 4 introduces an improved SPM-based contact tester for study of microcontacts leveraging real scale contact modeling simulations and lessons learned from the previous chapters to develop electrical simulations of the contact (constrictive) resistance. Chapter 5 is over all conclusions and Chapter 6 is a description of future work such as including more physics in the contact simulation modeling for achieving better understanding of the electrical contact phenomena in MEMS switch.
1.4 References


Chapter 2: A Model of Contact with Adhesion of a Layered Elastic-Plastic Microsphere with a Rigid Flat Surface
2.1 Abstract

A finite element model of a layered hemisphere contacting a rigid flat, which includes the effect of adhesion, is developed. In this analysis elastic-plastic material properties were used for each of the materials comprising the layered hemisphere. The inclusion of the effect of adhesion, which was accomplished with the Lennard-Jones potential, required a special procedure. This configuration is of general theoretical interest in the understanding of adhesion. It has also been suggested as a possible design for a microswitch contact because, with an appropriate choice of metals, it has the potential to achieve low adhesion, low contact resistance, and high durability. The effect of the layer thickness on the adhesive contact was investigated. In particular the influences of layer thickness on the pull-off force, maximum contact radius, and contact resistance were determined. The results are presented as load vs. interference and contact radius vs. interference for loading and unloading from different values of the maximum interference.

2.2 Introduction

The contact mechanics of layered surfaces is an important research area in the development of many microscale devices. The layer coating is generally applied on the surface in contact in order to achieve a different mechanical behavior than that of the uncoated substrate. Furthermore adhesion strongly affects the contact of layered components with other surfaces especially in micro-fabricated components such as MEMS devices.

Interest in MEMS switches has recently increased due to their advantages over solid state switches in many electronic devices. MEMS switches demonstrate reduced
insertion loss and excellent isolation compared with standard solid state switching devices. However MEMS switches face reliability problems which affect their operating life. One primary failure mode is “stuck-closed” in which the adhesion force between the metallic tip and the metal electrode exceeds the restoring force of the actuator. Many other MEMS devices can experience contact sticking due to adhesion between the contacting surfaces, which is a similar phenomenon to that which occurs in MEMS switches. Because of the scaling effect at the microscale, the influence of the surface adhesion forces becomes relatively greater compared with other forces. Adhered contact failures are among the most significant problems facing MEMS switch reliability. Thus an important objective is to enhance the performance of microswitches by achieving a better understanding of the mechanics of metal contacts.

Hertz presented the first theoretical analysis of the contact of two locally spherical elastic solids. After Hertz, significant research has been devoted to the study of the contact between solid bodies. Elastic-plastic contact deformation occurs when the contact loads exceeds a critical value, producing a region of plastic flow which is initially surrounded by an elastic region. Numerical solution of the elastic-plastic contact problem has become the most achievable way to understand this contact phenomenon. A finite element method (FEM) based model for elastic-plastic contact of an asperity with a rigid flat surface was developed by Kogut and Etsion [1]. That model provides dimensionless expressions for the contact load and contact area for a range of contact interference. Jackson and Green [2] developed a similar model based on the FEM and concluded that the ratio of the Young’s modulus (\(E\)) to the yield stress (\(\sigma_y\)) has an important effect on the contact behavior at large interferences. Along with these previous models, many other studies used the FEM to study elastic-plastic contacts.
For adhesive elastic contact analyses, Johnson et al. (JKR) [3] and Derjaguin et al. (DMT) [4] solved the adhesive contact problem between two elastic spheres. The pull-off force was determined to be $1.5\pi\Delta\gamma R$ and $2\pi\Delta\gamma R$ for the JKR and DMT models respectively. The work of adhesion $\Delta\gamma$, is represented by $\Delta\gamma = \gamma_1 + \gamma_2 - \gamma_{12}$, where $\gamma_1$ and $\gamma_2$ are the surface energies and $\gamma_{12}$ is the interfacial energy which vanishes if the two materials are identical. The effective radius $R$ is defined as $R = R_1 R_2 / (R_1 + R_2)$, where $R_1$ and $R_2$ are the radii of curvature for each sphere.

Tabor [5] introduced a dimensionless parameter $\Gamma = \left( R \Delta\gamma^2 / E^2 Z_0^3 \right)^{1/3}$, where $Z_0$ is the interatomic equilibrium spacing of two half-planes based on the Lennard-Jones potential. The composite Young’s modulus is given by $E = \left[ (1 - \nu_1^2) / E_1 + (1 - \nu_2^2) / E_2 \right]^{-1}$, where $E_1$, $E_2$, $\nu_1$ and $\nu_2$ are the Young’s moduli and the Poisson’s ratios for the two contacting bodies. Muller et al. [6] numerically solved the elastic adhesive contact problem and used the Tabor parameter to show that JKR and DMT models represent two opposite extremes of adhesion spectrum. Maugis [7] introduced an approximate analytical solution for adhesive elastic contact which spanned the range from the JKR (large Tabor number) to the DMT (small Tabor number) theories. Maugis offered a JKR-to-DMT transitional parameter $\lambda$ using the Dugdale adhesive stress assumption, which assumes a constant adhesive stress $\sigma_0$ in an annular region outside of the contact. The adhesive stress falls to zero when the gap distance is greater than a critical value $h_0$. Thus the work of adhesion in the Maugis model is $\sigma_0 h_0$. If the uniform Dugdale adhesive stress ($\sigma_0$) and Maugis work of adhesion ($\Delta\gamma$) are chosen to match the maximum adhesive stress and work of adhesion of the Lennard-Jones potential, then $h_0 = 0.97Z_0$ and consequently $\lambda = 1.16 \Gamma$, i.e. $\sigma_0 = 1.03(\Delta\gamma/Z_0)$. 

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Adhesion can have a very important role in the elastic-plastic deformation of microcontacts even when no external load is applied. Maugis and Pollock [8] developed a simplified analytic model for analyzing that configuration. More recently adhesive elastic-plastic contacts have been more accurately studied numerically. Kogut and Etsion [9] used the FEM and the DMT [4] approximation to study the elastic-plastic adhesive contact between a sphere and rigid plane. In [10] this method is used by Kadin et al. to analyze the corresponding unloading problem.

Adhesive elastic-plastic microcontacts were recently studied by Du et al. [11, 12] using the FEM and the Lennard-Jones (LJ) potential to model the surface interaction. The surface deformations in the gap between the surfaces are influenced by the surface interaction LJ stress. Results are presented for up to a maximum approach equal to thirty times the critical interference (i.e. the interference at which yielding would initiate in the absence of adhesion). Using the FEM they demonstrated that both ductile and brittle separation modes were possible, depending primarily on the ratio of the theoretical strength in adhesion compared to the yield strength. Qualitatively similar phenomena were observed in molecular dynamic simulations in nanoscale contacts [13] and in experimental investigations [14].

Contact problems involving layered materials have become important in modern day engineered devices where coatings are widely used. Extensive reviews of the modeling of elastic and elastic-plastic contacts of layered solids without adhesion are presented in the review articles by Bhushan [15] and Adams and Nosonovksy [16]. For adhesive elastic-layered medium, Sridhar et al. [17] used the JKR assumptions to model the mechanics of adhesive layered medium. Using the FEM Sridhar et al. [18] extended the methodology of [17] to study effect of Poisson’s ratio on adhesive contact of layered
media and provided the results in empirical formulations. Sergici et al. [19] performed an analytical investigation of the contact and adhesion mechanics between a layered medium and spherical indenter in which adhesion is included using a Maugis type of formulation.

The aim of this investigation is to study the contact problem of an elastic-plastic layered hemisphere, with adhesion, in contact with a rigid flat surface. This configuration has yet to be reported in the literature. The current study is of general theoretical interest and may also provide a means to improve the contact tip of MEMS switch designs by reducing the occurrence of the stuck-closed failure mode without sacrificing electrical functionality.

### 2.3 Model Formulation

The focus of this research is on the adhesive mechanical contact behavior of a layered hemisphere with a rigid flat surface. The specific configuration is comprised of a gold (Au) hemisphere coated with a thin ruthenium (Ru) layer. It is expected that this material combination will lead to a large contact area (due to the softness of the underlying Au) along with a small adhesion force (due to the moderate adhesion energy and high hardness of the Ru). The combination of the large contact area and underlying high conductivity gold hemisphere is expected to give low electrical contact resistance. Thus this material pair is a potential candidate to achieve low adhesion and excellent electrical characteristics for use in MEMS switches. The tip is modeled as a layered hemisphere with radius R using the FEM (Figure 1). A rigid flat surface was pressed against the layered hemisphere causing the layered hemisphere to deform in an elastic-plastic manner.
Based on the FEM, an elastic-plastic model of the layered microhemisphere is developed based on the adhesive contact model introduced in [11], which utilizes the multi-purpose finite element commercial package code ANSYS®. Symmetry allows the contact structure to be modeled using axisymmetric elements and boundary conditions. The finite element mesh is an arrangement of 7850 axisymmetric elements as shown in Figure 2. The radius of the hemisphere is $R = 4\mu m$ with axisymmetric boundary conditions on the left side. Outside of the contact region the curved side is stress-free except for the adhesive stress which is discussed later in this section and is treated

Figure 1. Contact with adhesion between a layered hemisphere and rigid flat.
separately. The bottom of the hemisphere is fixed in the vertical direction but free to move radially.

![Figure 2. Axisymmetric FEM mesh of a layered micro-hemisphere.](image)

The effect of the adhesion stress on the deformation is accounted for by its dependence on the interatomic separation $Z$. The attractive and repulsive stresses are determined by using the local separation and determining the stress between two corresponding parallel surfaces from the Lennard-Jones potential, i.e. the Derjaguin approximation. This procedure leads to the surface interaction stress $\sigma(Z)$ given by

$$\sigma(Z) = \frac{8}{3} \frac{\Delta \gamma}{z_0} \left[ \left( \frac{z_0}{Z} \right)^3 - \left( \frac{z_0}{Z} \right)^9 \right]$$

(1)
where $Z$ is the local separation between the two surfaces and $Z_0$ is the equilibrium spacing, i.e. the spacing where the stress between two half-spaces vanishes.

The application of these adhesive stresses requires the use of the programming feature of ANSYS®. Furthermore this nonlinear dependence of the stress on the separation requires some special steps in order to obtain a converged solution. The essence of the problem is that the peak Lennard-Jones stress between two half-planes occurs at a separation distance which is 20% greater than the equilibrium spacing, i.e. the stress goes from zero to a maximum over a separation distance of less than an Angstrom. In order to capture this extremely sharp peak, without using an extraordinarily large number of grid points, the special interpolation technique developed by Du et al. [11] is used.

### 2.4 Results and Discussions

Results are presented as applied force vs. contact displacement and contact radius vs. contact displacement for two different layer thicknesses. The contact radius is important because in a MEMS microswitch the constrictive resistance is directly related to the contact radius. The greater the contact radius, the lower is the resistance. However, because of the layered material structure the contact resistance is not inversely proportional to the contact radius as it is for the contact of homogeneous materials.

The material properties of the Au and the Ru are assumed to be elastic-plastic, each with 2% linear isotropic hardening of the elastic modulus. The Young’s moduli ($E$), Poisson’s ratios ($\nu$), yield stresses are, respectively, 410 GPa, 0.3, and 3.42 GPa for Ru, and 80 GPa, 0.42 and 0.67 GPa for Au. The adhesion stresses were based on the adhesion energy of the Ru as $\Delta \gamma = 1 \text{ J/m}^2$ with an intersurface equilibrium spacing $Z_0 =$
0.169 nm given in [11]. This value was obtained by employing the method proposed by Yu and Polycarpou [20].

Two Ru layer thicknesses of 100 nm and 50 nm were modeled. Figures 3 and 4 (100 nm Ru thickness) and Figures 5 and 6 (50 nm Ru thickness) show the applied load vs. contact displacement and the contact radius vs. contact displacement, all for loading and unloading from maximum loadings of 270 $\mu$N and 500 $\mu$N. Note that there is a common loading curve for both maximum loadings. However unloading shows considerable hysteresis which is due to a combination of plasticity and adhesion. Furthermore the pull-off force is greater for the higher maximum loading force. This behavior differs from the elastic adhesion problem where the pull-off force is independent of the maximum loading. For an elastic-plastic contact the greater the load the greater is the plastically deformed radius of curvature. Thus even though the unloading is mainly elastic, the pull-off force increases with the maximum loading force. This behavior was also found by Mesarovic and Johnson [21] for a homogeneous hemisphere and an approximate analytic expression for that case was presented.
Figure 3. Force vs. contact displacement for 100 nm Ru on Au.

Figure 4. Contact radius vs. contact displacement for 100 nm Ru on Au.
Figure 5. Force vs. contact displacement for 50 nm Ru on Au.

Figure 6. Contact radius vs. contact displacement for 50 nm Ru on Au.
Comparing Figures 5 and 6 with Figures 3 and 4 it is seen that for the same maximum loading the thinner layer gives a larger contact area which is expected to result in a lower contact resistance. However the pull-off force due to adhesion increases due to the increased contact area for a thinner Ru layer. Thus a suitable design space of acceptable adhesion and low contact resistance can be found for a particular application.

**Table 1.** Pull-off force, maximum contact radius, and contact resistance.

<table>
<thead>
<tr>
<th></th>
<th>$P_{\text{Max}} = 270$ (μN)</th>
<th></th>
<th>$P_{\text{Max}} = 500$ (μN)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$P_{\text{adh}}$ (μN)</td>
<td>$a_{\text{Max}}$ (μm)</td>
<td>$R_e$ (Ω)</td>
</tr>
<tr>
<td>Pure Ru</td>
<td>30.3</td>
<td>0.157</td>
<td>0.219</td>
</tr>
<tr>
<td>100 nm Ru</td>
<td>36.6</td>
<td>0.210</td>
<td>0.140</td>
</tr>
<tr>
<td>50 nm Ru</td>
<td>58.5</td>
<td>0.250</td>
<td>0.102</td>
</tr>
<tr>
<td>Pure Au</td>
<td>138</td>
<td>0.273</td>
<td>0.031</td>
</tr>
</tbody>
</table>
Table 2. Resistivity for different thicknesses.

<table>
<thead>
<tr>
<th>Thickness</th>
<th>Resistivity (μΩ-cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure Ru</td>
<td>14.82</td>
</tr>
<tr>
<td>100 nm</td>
<td>21.34</td>
</tr>
<tr>
<td>50 nm</td>
<td>25.89</td>
</tr>
<tr>
<td>Pure Au</td>
<td>3.60</td>
</tr>
</tbody>
</table>

Detailed comparisons of the adhesion pull-off force and the maximum contact radius between the Ru-on-Au layered microsphere and the pure Ru or Au are shown in Table 1. Both pure Ru and pure Au have been investigated as material candidates in MEMS switch fabrication. Electrical simulations of the contact resistance ($R_c$) were performed using ANSYS® and these results are also presented in Table 1. The resistivity of thin films is known to depend on the film thickness, with thinner films possessing higher resistivities. Shown in Table 2 are the measured resistivities, for different thickness films, which were used in the simulation. It is noted that the higher resistivity which is characteristic of a thinner layer lessens the benefit of using a thin layer. Pure Au gives low contact resistance, high adhesion, and an expected poor durability whereas pure Ru gives high contact resistance, low adhesion, and an expected good durability. The results signify the advantages and disadvantages of the suggested layered switch-tip.

The simulations which were carried out in this investigation show that neither pure Ru nor pure Au contact tip will give the most desirable electromechanical behavior. The pure Au contact tip is soft and gives a large contact area, i.e. a low contact resistance. However the tradeoffs are an unwanted large pull-off force in additional to the surface
contact damage caused by ductile separation [20] due to the combination of low hardness and high adhesion energy. On the other hand pure Ru has the advantage of high hardness and low adhesion which tends to promote brittle separation, helping to protect the contact surface operation life. However the expected low contact area for pure Ru, as well as its higher resistivity, increase the contact resistance. As explained above, a layered Ru-on-Au contact tip shows promise to combine the desirable properties of both materials and achieve a large contact area and a low pull-off force. The Ru layer can make a durable low adhesion brittle separation while the underlying high conductivity and soft Au will help lower the contact resistance by creating a large contact area.

The value of the work of adhesion varies considerably with surface conditions such as the presence of contaminants and roughness. In Figures 7 and 8 are the results for loading and unloading for 50 nm of Ru on Au and for different values of the work of adhesion. It is observed that the loading curves are all similar, with a smaller contact force and a larger contact radius corresponding to the same contact displacement as the work of adhesion increases. On unloading the differences are far more pronounced. The pull-off force (Figure 7) varies significantly with the work of adhesion. Furthermore the displacement at which separation occurs decreases as the work of adhesion increases, indicating a competition between plastic compressive plastic deformation incurred during loading and tensile plastic deformation on unloading, i.e. a transition from brittle to ductile separation.
Figure 7. Applied force vs. contact displacement for 50 nm Ru on Au with different values of the work of adhesion.

Figure 8. Contact radius vs. contact displacement for 50 nm Ru on Au with different values of the work of adhesion.
2.5 Conclusions

Mechanical and electrical finite element contact models of an elastic-plastic layered hemisphere with a rigid flat surface in the presence of adhesion were developed. The mechanical simulations show that the adhesion force and contact radius are each greatest for high forces and thin layers. The electrical simulations use thickness-dependent measured values for the resistivities. Thinner layers give lower resistance due to the larger contact area and increased conduction through the underlying Au. A suitable design space of low adhesion and low contact resistance can be guided by these results.
2.6 References


Chapter 3: A Combined Molecular Dynamics and Finite Element Analysis of Contact and Adhesion of a Rough Sphere and a Flat Surface
3.1 Abstract

A combined molecular dynamics [31] and finite element model and simulation of contact and adhesion between a rough sphere and a flat surface has been developed. This model uses the results of molecular dynamics (MD) simulations, obtained by collaborators using an embedded atom potential, of a nanoscale Ru-Ru asperity contact. A continuum finite element model of an elastic–plastic microscale Ru-Ru contact bump is then created. In this model, the surface roughness is represented by a system of nanoscale asperities, each of which is represented by a nonlinear hysteretic force vs. distance relationship. The nonlinear hysteretic character of these relations is determined from curve-fits of the MD results. Load vs. interference and contact area vs. interference are determined using this two-scale model for loading and unloading. Comparisons with a single-scale continuum model show that the effect of the nanoscale asperities is to reduce both the adhesion and the real area of contact. The choice of Ru as the material for this work is due to its relevance in microswitches.

3.2 Introduction

Contact mechanics problems have enormous importance in microelectromechanical systems (MEMS) design and development. The roughness of solid surfaces tends to be random, and no perfectly smooth surface exists due to the finite atomic size. Thus, real contact occurs at the asperity peaks. For macroscale contacts, the real contact area is very small compared with the apparent contact area. However, at the microscale, the ratio of the real to the apparent contact area is expected to be considerably greater. Furthermore, adhesion at the microscale is particularly important because the surface area–to-volume
ratio increases as the scale diminishes. As a consequence, a common problem encountered in MEMS is stiction, in which two surfaces fail to separate due to the force of adhesion.

The JKR (Johnson, et al. [1]) and DMT (Derjaguin, et al. [2]) models are widely used for predicting the adhesive force of elastic contacts. For an elastic sphere with radius $R$ contacting a flat surface, the JKR and DMT models determine the force of adhesion as $1.5\pi R \Delta \gamma$ and $2\pi R \Delta \gamma$, respectively, where $\Delta \gamma$ is the work of adhesion. In the JKR theory, the stress state of the elastic sphere and substrate includes infinite tensile stress along the boundary of the circular contact between the sphere and substrate. These large stresses lead to the formation of a neck and a corresponding finite contact area at any finite load. The DMT theory assumes that the contact profile is similar to that in the Hertz contact theory. The adhesion is weak and is assumed to act outside the contact zone, resulting in an overall contact load that is greater than the applied load.

Muller, et al. [3] used the Tabor [4] parameter to show that the JKR and DMT models represent two opposite extremes of the adhesion contact spectrum, from a compliant solid with large surface energy (JKR) to stiff solids with small contact radius and low surface energy (DMT). An analytical model that makes a continuous transition between the JKR and DMT limits was developed by Maugis [5] using the assumption of a constant adhesive stress in the region where the gap between the contacting sphere and flat surface is less than a critical value (i.e., the Dugdale approximation borrowed from plasticity).

A multi-asperity contact model was first introduced by Abbott and Firestone [6] assuming perfectly plastic deformation. Greenwood and Williamson [7] presented a pioneering asperity-based approach (GW model) in which the rough surface is modeled
by randomly distributed elastic asperities, each of which follows the laws of Hertz contact. They found that the real contact area was nearly proportional to the applied load over a several orders of magnitude variation of the load. Greenwood and Tripp [8] showed that the contact between two rough surfaces is equivalent to a single elastic rough surface pressed against a rigid flat. Numerous other elastic multi-asperity models exist. Recently, Jackson and Green [9] used several measured surface profiles to compare various asperity models with a deterministic calculation. Chang, et al. [10] extended the GW model to include a transition to perfectly plastic deformation. More recently, a numerical model of the elastic–plastic contact of rough surfaces was presented by Wang, et al. [11]. Hardness is known to be scale dependent; this effect was incorporated into a multi-asperity contact model by Jackson [12].

The elastic–plastic deformation of a single asperity can be analyzed more accurately via finite element method (FEM) simulations rather than with analytical models. Kogut and Etsion [13], [14] studied single microcontact asperities without and with adhesion using FEM. In Kogut and Etsion [14], the effect of adhesion was included using the DMT assumptions. The results of Kogut and Etsion [13] were incorporated into a multi-asperity model by Kogut and Etsion [15]. Jackson and Green [16] showed that the deformation of a hemisphere against a rigid flat corresponds to a lower nominal contact pressure (hardness) in the fully plastic region rather than a rigid sphere indenting a deformable half-space. This geometry effect on hardness is associated with the smaller constraint on lateral displacement of the hemisphere compared with the half-space.

Du, et al. [17], [18] recently used FEM to investigate single asperity contact deformation with adhesion by developing an elastic–plastic adhesion model for microcontacts that includes the effect of adhesion on deformation. They demonstrated
that both ductile and brittle separation modes were possible, depending primarily on the ratio of the theoretical strength in adhesion compared with the yield strength. Similar observations were found from molecular dynamics (MD) simulations. Kadin, et al. investigated adhesion problems using kinematic hardening for loading and unloading (Kadin, et al. [19]) and cyclic loading (Kadin, et al. [20]).

Archard [21] modeled a rough elastic spherical contact with spherical protuberances distributed over the surface of the sphere as a model of asperities. His model was hierarchical in that it included several levels of protuberances upon protuberances. More recently, Jackson [22] extended this approach to include elastic–plastic deformation. Greenwood and Tripp [23] studied the elastic contact of a rough sphere using the GW statistical distribution of asperity heights in which each asperity is modeled as a Hertz contact. Hughes and White [24] presented analytical approximations for the elastic contact of a rough sphere that are in good agreement with Greenwood and Tripp’s [23] results. In the elastic–plastic analysis of Li, et al. [25], the contact of a rough sphere with a flat surface was investigated to determine the relative contributions of bulk and asperity deformations. Contacts of both rough elastic flats and spheres pressed against a smooth surface with adhesion were investigated by Fuller and Tabor [26]. Their results showed that the effect of adhesion decreases with increasing roughness because, during separation, the compressed taller asperities help to separate the shorter adhering asperities.

Recently, extensive research has been devoted to developing multiscale modeling approaches for connecting atomistic with macroscopic continuum models in contact problems. Such approaches allow nanoscale phenomena to be captured using MD while maintaining the capability of modeling larger volumes using finite elements. Among
these approaches are the domain decomposition methods of Belytschko and Xiao [27] and the hybrid simulation method of Luan, et al. [28] and Luan and Robbins [29]. In Belytschko and Xiao [27], two different energy-based coupling methods, namely, the overlapping domain decomposition and the edge-to-edge decomposition, were compared. In the hybrid simulation method of Luan, et al. [28] and Luan and Robbins [29], the MD model was directly coupled to the nonlinear material elastic continuum model through an overlap region. These methods removed the restriction of refining the continuum mesh down to the atomic separation spacing and did not require correlation between atoms and continuum nodes in the transition region.

The roughness at the contact interface of aMEMS switch consists of nano-asperities on top of a microsphere. The scale of these nano-asperities is too small to capture the important features within a continuum framework. Conversely, MD simulations of the entire rough microsphere would be unrealistic because of the large number of atoms that must be included in such a simulation, as well as the large number of time steps needed to reproduce experimental time scales.

In this article, we present a two-scale model of a rough microcontact. A continuum finite element model, which includes elastic and plastic deformation, is combined with curve-fits to MD simulation data that represent nanocontacts. The MD data are modeled by replacing nanocontacts with hysteretic nonlinear force vs. distance elements that are intended to reproduce the nanoasperity behavior of the rough frictionless microcontacts. This method has some similarity to a cohesive zone model. In those models, a stress vs. separation law is specified continuously along an initially intact interface to model the decohesion/formation of the surfaces.
The present calculations are designed to represent ruthenium contacts, because Ru is under active consideration for next-generation contacts in MEMS switches. The roughness of an Ru contact can vary significantly among contacts, depending on the details of the fabrication process. Thus, this current study is not trying to mimic the roughness of a particular switch but rather is presenting a framework for this two-scale contact analysis. A continuation of this work could be its extension to a three-scale model with two levels of continuum deformation and one level of molecular dynamics. Such an analysis is beyond the scope of this work. Results of this two-scale model show the variation of contact area and force (including the pull-off force) in a model that includes nano-asperities. Finally, we compare these results to those from a smooth sphere model.

3.3 Two-Scale Model

Figure 1 shows the atomistic configuration for a typical MD cell used to simulate the contact formation and separation of a single Ru nano-asperity and an Ru flat (de Oliveira, *et al.* [30]). Molecular dynamics simulations of the contact of individual Ru nano-asperities and a flat Ru substrate were originally performed by Fortini, *et al.* [31]. An interatomic potential for Ru was developed that yields a stable hcp lattice with reasonable lattice and elastic constants. This potential was based upon the embedded atom method (EAM) approach developed by Cai and Ye [32] that provides a reasonable description of both bulk and surface phenomena. During loading, the asperity was significantly deformed under compression. Unloading was accompanied by plastic stretching of the asperity and in some cases material transfer.
The MD simulation of the nano-asperity contact was conducted by simulating two substrates of roughly 18 close-packed planes facing one another, corresponding to the (0001) planes of the Ru hcp lattice. On the lower substrate, the nano-asperity was prepared starting from a rectangular box of 2,891 atoms of $3.248 \times 3.750 \times 2.786$ nm ($x$, $y$, $z$). It was then annealed at a high temperature close to melting, so its corners were smoothed out. The height of the asperity did not change and remained 2.786 nm. MD simulations were employed to bring the atomically flat surface and the single asperity together in order to model nanoscale contact formation. The lower substrate with the nano-asperity was fixed, whereas the upper substrate was displaced with a constant
velocity of 7 m/s toward the nano-asperity with a time step of 0.0025 ps. This speed of 7 m/s is close to the range of speeds for operation of a microswitch (e.g., 2.4 m/s in McCarthy, et al. [33]) and is well below any material wave speed.

A degree of variability is always present when different asperity realizations are used; that is, asperities with different sizes, orientations, and different thermal starting conditions. A proper averaging would require extensive simulation work. Nonetheless, as demonstrated by de Oliveira, et al. [30], different asperity realizations share the same type of plastic behavior. Furthermore, simulations have been conducted corresponding to the (1122) planes and show very similar results to those conducted for the (0001) planes.

Based on these atomistic simulations, we determined the force vs. approach (Figure 2) and the contact area vs. approach characteristics of this adhesive contact and contact separation. The approach is the downward displacement of the top of the upper substrate with respect to the bottom of the lower substrate. The approach is zero when the undeformed surfaces barely touch; that is, when the rigid surface is separated from the top of the sphere by a distance equal to the undeformed asperity height. Because of the relative size difference between the contact bump and the substrate region, almost all of the deformation in the atomistic simulations occurs in the asperity (Figure 1). Furthermore, in the continuum model the maximum relative displacement between a surface node and a node at a depth of 5.25 nm is only 0.074 nm. Note that the asperity quickly becomes plastic, whereas most of the substrate region is predominately elastic. The contact area in the simulations is the area of the smallest cross section of the neck. The atoms diffusing on the flat surface do not contribute to it.
Figure 2. Contact force vs. contact approach (displacement curves) from MD simulations of a Ru-Ru nanocontact for work of adhesion 6 J/m² for different values of the maximum contact approach [31].

The curve-fits to these MD simulation data (Figure 3) allow us to represent each nano-asperity contact with a nonlinear hysteretic force vs. distance relation. The base of the asperity is fixed in the MD simulation, but the asperity is attached to a deformable continuum model in this two-scale model. Thus, the approach in MD becomes the distance in the force vs. distance relation of the two-scale model. It is noted that the term nonlinear hysteretic spring could be used as a general representation of a force vs. deformation relation. However, such a description could be misleading, because it
implies that the spring deformation is always the same as the approach. These two quantities are only the same when the asperity is in contact with the rigid surface.

Figure 3. Polynomial curve-fits to the MD simulation data for single nano-contact simulation data for loading (blue curve) and unloading for a work of adhesion 6 J/m². The black, purple and red curves correspond to different values of the maximum contact approach.

Fourth- and fifth-order polynomials were used to fit the loading and unloading curves, respectively. Though some of the details of the interactions are, no doubt, lost in the curve-fit approximations, this error should not be critical because in a real system this fine-scale information is averaged over many asperities. The only instance in which it may be an issue is at very low force during the loading phase when few asperities have
come into contact. During unloading, separation occurs at a relatively large contact area and so any loss of detail would be averaged over many asperity contacts.

Single asperity contact simulations show significant hysteresis in the loading/unloading curves as a result of nanoscale plasticity and adhesion. It is noted that in bulk materials plasticity is primarily a consequence of dislocation motion. However, nanoscale plasticity is associated more with dislocation nucleation than with migration and hence it is often referred to as a dislocation starvation process.

Though the loading portions of the Ru-Ru nano-asperity contact force vs. approach are essentially the same, the unloading behavior shows greater variability (i.e., both statistically and depending on the maximum load applied). Due to the computational cost of conducting MD simulations to generate unloading curves, for a given loading range with many different maximum loadings, an interpolation scheme is used when the desired unloading conditions lie between two existing unloading curves. Linear interpolations between the contact forces are used to achieve a range of the unloading curves. The maximum tensile force per asperity is different for each asperity because its value depends on the maximum load exerted on that asperity.

A three-dimensional, continuum, quasi-static finite element model of a microscale Ru contact bump was created within ABAQUS (Simulia, Inc., Providence, RI). The implicit static solver and unconditionally stable implicit methods were used. The material model of this $R = 1$ μm radius hemisphere is considered to be elastic–plastic (we employ a von Mises yield criterion and no strain hardening) with a Young’s modulus of $E = 410$ GPa and a Poisson’s ratio $ν = 0.3$. The yield stress value of 3.42 GPa is taken based on the hardness from a nano-indentation test at a shallow depth (Lee, et al. [34]). It is interesting to note that the Tabor [4] parameter [$Γ = (RΔγ^2/E_0^2Z_0^3)^{1/3}$] based on the
continuum radius is about 5.3, which is well within the JKR region, and for the nanoasperity is approximately 0.76, which is in the DMT regime. These values of $\Gamma$ are based on the ideal Ru-Ru work of adhesion of $6 \text{ J/m}^2$, the composite elastic modulus [$E_C = E/2(1-\nu^2)$], and the atomic separation distance ($Z_0 = 0.169 \text{ nm}$) of two Ru-Ru half-spaces (Du, et al. [17]).

In this model, the effect of roughness on adhesion is represented by a system of identical nonlinear hysteretic force-distance elements, each of which simulates the behavior of a single nanoscale asperity as shown in Figure 4a. The maximum nominal contact radius is about 96 nm, which corresponds to a slope of 0.096 in the undeformed geometry. After deformation, the top surface is almost flat near the edge so that the slopes are even smaller. Thus, the surfaces are approximately parallel in the region in which the adhesive stresses are important. The distribution of the asperities (force-distance elements) is shown in Figure 4b. A general-purpose 10-node tetrahedral element (C3D10) is used to mesh the continuum microsphere. The forces are applied to the integration points of the finite elements. Thus, the finite element mesh size on the surface is such that the area associated with the finite element integration points (at which the load is applied) is approximately equal to the asperity base area ($\sim 12.2 \text{ nm}^2$). In this manner, the loads are applied to the continuum model over an area equal to that of the asperity base.
Figure 4. A meshed, microscale hemisphere where each spring representing a nanoasperity from a) a side view schematically showing only seven springs and b) a top view showing the actual distribution of about 300 springs.
The nonlinear hysteretic force–distance relations, which represent the asperities, are implemented with ABAQUS user subroutines. The asperity interaction is through the continuum FEM mesh. In the loading phase, the bottom of the sphere is moved upward toward the fixed flat, smooth, rigid surface in small increments, causing one asperity after another to come into contact. Although the displacement increment is typically 0.1 nm, it can be as low as 0.01 nm in order to capture the details of asperities making contact. The tensile force that exists at negative values of nano-asperity deformation can cause the nano-asperity and the substrate to deform, resulting in contact. In this study, no more than 200 asperities on the top of the hemisphere came into contact in the cases investigated. After the maximum approach is achieved, the system is unloaded. The compressive load in each force–distance element is reduced progressively, eventually becoming tensile. The nano-asperity will eventually pull off (debond) from the flat surface.

The asperities are placed over a large enough region (50% greater than the maximum nominal contact region) so that only that portion of the sphere that includes the asperities is close to contacting the flat surface. Thus, interactions on the rest of the sphere need not be included. The density of the asperities is high enough that in the nominal contact region only asperities touch. Recall that the asperities are on a deformable sphere so that points between asperities move downward due to the combined action of all the asperity forces. As a consequence, contact in the region between asperities does not occur.

The asperity density ($\eta$) is known to be scale dependent. Furthermore, McCool [35] showed that for a randomly rough surface, the product $\eta\sigma R$ should be approximately 0.019 if the asperity summits are of roughly equal height, where $\sigma$ is the standard
deviation of surface heights. The asperity density ($\eta = 7,900/\mu m^2$), standard deviation of surface heights ($\sigma = 0.79$ nm), and asperity radius ($R = 3$ nm) correspond to that value.

### 3.4 Results

The loading/unloading behavior for this two-scale model of an Ru-Ru contact is presented in this section, in which we present contact load and contact area versus contact approach. However, before we present those results, we first show contours of the von Mises stress on a section containing the axis of the hemisphere partly through the depth of the continuum model under progressively greater loads (Figs. 5a–5c). The multi-nano-asperity (rough) hemisphere is pressed against the rigid surface beyond the point where the elastic–plastic hemisphere experiences plastic deformation and the bodies are then pulled apart. Most of the plastic deformation occurs in the nano-asperities, but microscale continuum yielding initiates at the boundary between the nano-asperity and the microsphere. Such irreversible plastic deformation associated with the high stresses beneath the nanoscale surface asperities may explain the surface damage observed on the contact tip of a switch even under low force.
Figure 5. Von Mises stress distribution under progressively increasing loading with a contact approach in a) of 1.5 nm, in b) of 2 nm, and c) 2.3 nm.
For the smooth hemispherical contact case without adhesion, the maximum von Mises stress occurs below the surface at a depth of 48% of the contact radius. Adhesion does not significantly affect the location of the maximum von Mises stress. In the present simulations, we observe that there is a region of locally maximum von Mises stress at a depth slightly less than one half of the nominal contact radius as the stresses due to each of the asperity contacts combine.

We performed nano-asperity MD simulations for three different values of the work of adhesion; that is, for $\Delta \gamma = 1$, 3, and 6 J/m$^2$. The 6 J/m$^2$ case is the theoretical work of adhesion (de Boer, et al. [36]), and the work of adhesion due to contamination and oxidization will be taken as 1 J/m$^2$. The 3 J/m$^2$ case is an estimate representing a clean metal contact. Figure 6 shows the contact force and contact area as functions of the contact approach for loading and unloading with $\Delta \gamma = 1$ J/m$^2$. The loading curve in Figure 6a starts at a slightly negative approach with barely perceptible negative (tensile) force values. This behavior is due to the attractive force between the nano-asperities and the opposing surface, causing the sphere to deform and the asperities to stretch and, if sufficient, to come into contact. Contacts with a negative force will continue to made for other asperities during loading. The loading curve, after the initial approach, goes into compression. During loading, the bulk hemisphere will be mainly under compression, whereas the surface experiences both tensile and compressive stress.
Figure 6. (a) Contact force and (b) contact area vs. contact approach for the low work of $\Delta \gamma = 1 \text{ J/m}^2$. 

\[ \text{Contact Force (\text{\textmu}N)} \]
\[ \text{Contact Approach (nm)} \]

\[ \text{Contact Area (\text{\mu m}^2)} \]
\[ \text{Contact Approach (nm)} \]
The unloading curve starts at the point where the chosen maximum loading force is reached. Unloading the system to separation consists of many small, nano-asperity pull-off events that are coupled to the larger (micro) scale deformation. The large-scale phenomena consist mainly of hysteresis due to the continuum, irreversible plastic deformation that occurred during loading and is not recovered on unloading. The small-scale unloading consists of phenomenon opposite that which occurred during the loading phase; that is, the nano-asperities stretch plastically during loading (some are in tension during unloading, whereas others are still in compression). As the tensile load increases, some nano-asperities begin to pull off (go out of contact). During displacement-controlled unloading when some asperities pull off there is a concomitant redistribution of the force (less compressive or more tensile) to other asperities. This phenomenon is due to the coupling between asperities through the continuum model; as one asperity goes out of contact, some of the load is transferred to the other asperities if the system is to be maintained with the same value of the approach. The unloading curve indicates a net pull-off force (maximum negative force during unloading) that represents the action of an individual asperity pull-off coupled through the bulk deformation of the hemisphere. We note that in the present simulations, the contact approach is the independent variable rather than the contact force. Nonetheless the results from this displacement-controlled simulation can readily be reinterpreted as force controlled.

The real contact area (composed of the sum of the individual asperity contact areas) vs. the approach is presented in Figure 6b for a work of adhesion 1 J/m². By curve-fits to the MD results for contact area vs. contact approach, the contact area for each individual asperity can be found from the contact approach. The contact area is an important quantity because it controls the electrical contact resistance and also provides
insight into the pulloff force phenomenon. As expected, the contact area increases during loading and decreases during unloading. However, for a given contact approach, the contact area on unloading is greater than on loading during most of the unloading phase of the loading/separation calculation (equivalently, the difference in area between loading and unloading in the contact area vs. contact approach plot is positive). This observation is consistent with the experimental investigation of Ovcharenko, et al. [37] and the theoretical work of Zait, et al. [38] without adhesion. By comparing Figs. 6a and 6b, we see that pull-off occurs at a finite contact area that is a significant fraction of the maximum contact area. In fact, in a force-controlled separation experiment, the contact area during unloading is always greater than on loading for the same value of the approach. This behavior is due to a combination of the plastic deformation that occurred at the maximum loading and the effect of adhesion, which produces additional hysteresis.

In the case of a perfectly clean Ru-Ru metal contact, the energy or work of adhesion is 6 J/m² (de Boer, et al. [36]). An intermediate value of 3 J/m², between the typical and ideal work of adhesion, is now considered. Figure 7 shows that the 3 J/m² case results are qualitatively similar to those for 1 J/m². The loading phases are virtually the same in these two cases, whereas the unloading curves differ significantly. The pull-off forces are approximately double that of the lower work of adhesion case of 1 J/m². The total contact area experiences a slower decrease during the unloading phase and gives a larger contact area on unloading for the 3 J/m² case due to the combination of bulk plastic deformation and nano-asperity hysteresis associated with adhesion. In fact, for all values of the contact approach prior to pull-off, the contact area is greater during unloading than during loading.
**Figure 7.** (a) Contact force and (b) contact area vs. contact approach for the intermediate work of adhesion case, $\Delta \gamma = 3 \text{ J/m}^2$.
Results based on the ideal work of adhesion of 6 J/m$^2$ are presented in Figure 8. Again, the influence of adhesion during loading is small. The system pull-off force (Figure 8a) is more than three times greater than for the work of adhesion of 3 J/m$^2$. However, under displacement control, the contact area during unloading vanishes at a negative value of the approach for all three of the maximum loadings as illustrated in Figure 8b. Due to the highly attractive force caused by the ideal work of adhesion coupled to plastic deformation in the microsphere, contact separation occurs at a lower value of the contact approach. Under displacement control, the separation occurs for negative values of the approach. It is interesting to compare the pull-off force for a single nanoasperity with the global pull-off force. Each depends on the maximum loading. In the cases considered, the nano-asperity pulloff force is no greater than 400 nN (Figure 3), whereas the global pull-off force is no larger than 18 μN (Figure 8a). Thus, for the maximum loading case with the ideal work of adhesion, the global pull-off force is about 45 times as great as for a single nanoasperity.
Figure 8. (a) Contact force and (b) contact area vs. contact approach for the high work of adhesion case, $\Delta \gamma = 6 \, J/m^2$
3.5 Discussion

The contact approach contains a portion due to asperity deformation and another due to the deformation of the hemisphere.

The proportion is different at different locations on the hemisphere and at different stages of loading/unloading. Generally, the asperity deformation dominates in the initial stages of loading, but the deformation inside the sphere gets progressively larger as the load increases. Nonetheless, even for the maximum loads considered here the asperity deformation is about 65% of the total deformation.

No doubt the results are sensitive to large changes in the asperity size, but that investigation is beyond the scope of this work. Nonetheless, the MD simulations in de Oliveira, et al. [30] included a case with 7,000 atoms in the asperity, which is almost two and a half times as many as used here and corresponds to a 34% increase in the linear dimensions such as radius. This increased size led to an approximately 25% increase in the maximum load.

An interesting continuation of this study would be to investigate multiple load–unload cycles. Such an investigation would require MD results for subsequent loading and unloading, which could then be incorporated into the two-scale model. A purely continuum model of load–unload cycling with adhesion and plasticity (Kadin, et al. [20]) shows differences after the first cycle.

The two-scale model presented here could be extended to a three-scale model by including asperities with intermediate values of the radius of curvature. Such asperities would be large enough for continuum representations to be valid. Such a model would have similarities to the “protrubences on protrubences” investigation by Archard [21] that used a continuum approach without plasticity or adhesion.
The results are insensitive to the exact location of the asperities but are expected to depend on the asperity density. As the asperity density increases, the rough surface model begins to resemble a smooth surface with adhesion represented by a cohesive law model. However, differences would still exist due to the difference between nanoscale and bulk plasticity.

The main effect of surface roughness is to decrease the adhesion force and the real contact area between contacting bodies. For completeness, adhesive contact of a smooth hemisphere with the same radius of curvature as the two-scale rough hemisphere will be examined. Comparison between the smooth adhesive elastic–plastic contact model and the rough MD/FEM elastic–plastic contact model with adhesion will be carried out. The smooth adhesive elastic–plastic model is more appropriate for comparison than the elastic smooth model with adhesion (Johnson, et al. [1]; Derjaguin, et al. [2]) or the rough elastic contact model without adhesion (Greenwood and Tripp [23]). Using the finite element software ANSYS (ANSYS Inc., Cannonsburg, PA) and the Lennard-Jones adhesion model developed by Du, et al. [17], the smooth elastic–plastic hemisphere is modeled for $\Delta \gamma = 1 \text{ J/m}^2$. The adhesion pull-off force and the contact areas are higher than the rough hemisphere due to the effect of roughness on diminishing the adhesion force.

The typical work of adhesion case $\Delta \gamma = 1 \text{ J/m}^2$ is presented in Figure 9. The contact approach is defined as the downward displacement of the top surface with respect to the bottom of the hemisphere and it is zero when the undeformed surfaces barely touch. Though the results are qualitatively similar to the rough sphere, the axisymmetric smooth surface model does show significant quantitative differences during both loading and unloading. During loading, the smooth sphere required more than twice the applied
force to achieve the same maximum contact approach. Similarly, for the same contact approach, the contact area is much larger for the smooth sphere model. These trends are directly attributable to roughness. Furthermore, unloading, either from the same maximum contact approach or from the same maximum loading, results in a much greater pull-off force. This trend is to be expected due to the reduced effect of adhesion caused by roughness.
Figure 9. (a) Contact force and (b) contact area vs. contact approach for the low work of adhesion case, $\Delta \gamma = 1 \text{ J/m}^2$, for a smooth hemisphere.
3.6 Conclusions

A three-dimensional combined molecular dynamics and finite element model of the contact of a rough microsphere with a flat surface was developed. Curve-fits from the molecular dynamics simulations were used in order to model each nano-asperity as a nonlinear hysteretic force–distance element. The bulk of the microsphere was modeled as an elastic–plastic body using finite elements. The nano-asperities were placed on the surface of a continuum finite element model to describe the nanoscale surface roughness on the microsphere. The results are presented for the contact force and contact area, each as functions of the contact approach. Three values of the work of adhesion were studied: a typical experimental value of 1 J/m$^2$, an ideal value of 6 J/m$^2$, and an intermediate value of 3 J/m$^2$. Results are compared with the smooth continuum sphere model. These models show significant quantitative differences, in which nanoscale roughness significantly reduces the effect of adhesion and reduces the real area of contact.

The combined MD and finite element model can be extended to account for multiple loading–unloading events when more loading–unloading MD simulations are available. Such a simulation could reveal trends seen during experimental lifetime cyclic testing of switches.
3.7 References


Chapter 4: An Improved SPM-Based Contact Tester

for the Study of Microcontacts
4.1 Abstract

An improved SPM (Scanning Probe Microscope)-based contact tester has been designed, constructed and used for cyclic testing of various metal contacts. It must be noted that the test set-up, apparatus design and testing that will be explained in this chapter is the outcome of the contributions made by different individual working with our research group [1]. The tester is designed for contact materials evaluation, especially for metal-contact MEMS switch applications, and is capable of simultaneous measurements of contact force and resistance. The tester uses a specially designed silicon force sensor with an integrated contact bump and a mating silicon pillar in order to simulate switch operation. The sensor and the pillar are coated with contact materials, allowing a wide range of contact metals and metal pairs to be evaluated. The testing takes place within a custom-built test chamber in which both a plasma and UV-ozone can be introduced for contact cleaning and surface modification.

It was found that a dissimilar contact pair of Au-Ru with O\textsubscript{2} plasma cleaning can provide low contact adhesion and low resistance as compared with Au, Ru, and Ir contact pairs. Layered structures with a thin layer of Ru on top of Au were also modeled and tested. Ru layers between 50 and 100 nm were effective in reducing adhesion and contact resistance provided the contact force is greater than 300 \(\mu\text{N}\).

4.2 Introduction

Microswitches have many advantages over larger mechanical switches (such as reed relays) and smaller solid state diode switches. Microswitches are much smaller in size and switch faster than existing mechanical relays. These switches also offer improved
performance, such as lower insertion loss, higher isolation, better linearity, and lower power consumption than their solid-state counterparts. Thus MEMS switches have the potential to replace conventional relays and p-i-n diodes in many applications. The potential uses of MEMS switches include RF switching in applications such as cell phones, phase shifters and smart antennas [2], as well as reed relay replacement in Automatic Test Equipment (ATE) and industrial and medical instrumentation. However, for many of these applications to be realized lifetimes of tens of billions of cycles or more are required [3]. Thus reliability over the lifetime of a switch has become the major obstacle to commercialization of these switches [4].

For ohmic-type MEMS switches, an ideal contact should have a low contact resistance, low contact adhesion, and high durability. Tradeoffs are often made for real switch applications. The two common failure modes in microswitches are “stuck-open” and “stuck-closed”. In a stuck-open failure the contact resistance gradually increases during cycling until becoming so large that the switch is no longer usable. In contrast during a stuck-closed failure the resistance gradually decreases during cycling. Unfortunately this reduction in resistance is accompanied by an increase in adhesion which can become so great that the actuator is unable to supply the restoring force needed to separate the contacts.

Thus contact material selection is a critical step in the design of RF MEMS metal-contact switches. The selection of contact materials affects switch performance and reliability. Performance and reliability are in turn directly affected by adhesion, resistance, and power handling, all of which are influenced by the contact force, thin film preparation, contact surface treatment, and operational ambient in addition to the choice
of contact materials. It can, however, be extremely time-consuming to evaluate a wide range of materials if these tests are performed in MEMS switches.

To evaluate a wide range of contact materials, and to have better control on microcontact characterization, specially designed contact test vehicles or test methodologies are often used. For instance, in [5], a methodology using a commercial nanoindentor coupled with electrical measurements on test vehicles was used to evaluate soft (Au/Au), harder (Ru/Ru) and mixed materials (Au/Ru) contact configurations. An atomic force microscope (AFM) based test facility is used to evaluate Au Ni alloys [6], with hot and cold switching [7]. An AFM with a conductive tipless cantilever was used in [8, 9] to study field emission and material transfer during making of electrical contact in a MEMS switch with Au, Ru and Pt. Contact surface treatment and ambient conditions can be expected to have an important effect on micro contact characterizations since most RF MEMS ohmic failure modes are surface-related. In [10] and [11], electrical contact resistance measurements and switch lifetimes were reported for RF micro-mechanical switches with Au/Au and Au/Ru contacts, situated within an ultrahigh vacuum system equipped with in situ oxygen plasma cleaning. The effect of low temperatures (5.6 K and 77 K) showed a decrease in resistance of gold contacts as compared to 293 K [12].

In this chapter we report on a new SPM-based contact tester that has been designed, constructed and used for the study of contact materials for MEMS switches. It is very important to mention that the test set-up, apparatus design and testing that will be explained in this chapter is the outcome of the contributions made by different individual working with our research group [1]. I would like to acknowledge by the latter sentence their efforts and team work that made this valuable investigation happen.
The original concept of using JEOL SPM for performing micro-contact tests was used by Chen et al [13]. Dr. Guo modified the force sensor and designed it to have the fixed-fixed beam. Dr. Chen altered the pillar design to make it trapezoidal. The experiments on cleaning methods and contact-resistance measurements that are explained in this chapter were performed Mr. Joshi and Dr. Chen [1].

The tester facilitates the examination of a wide variety of contact materials and allows the direct measurement of contact adhesion, contact force, and contact resistance. The setup consists of a custom built bridge-type force sensor with an integrated contact bump and a planar mating surface (a flat top pillar) to simulate contact operation in a microswitch. After coating various contact materials on both the bridge force sensor and the mating surface, contact tests of various materials and materials combinations were performed.

It is noted that an earlier version of this tester used a cantilever rather than a bridge as a force sensor. By using a cantilever structure as a force sensor, sliding effects were encountered during the contact tests. Also, the measured resistance in this previous setup included the sheet resistance components of the metal films on the cantilever and testing pads. Nonetheless it was successfully used to study several contact metals and metal alloys [13], contact failure mechanisms [14], and the rate-dependent pull-off force of micro-contacts [15].

Compared to the previous version of the test station, the new system has been improved in three ways: 1) more accurate force measurement; 2) better resistance measurement; and 3) the capability for both plasma and UV-ozone treatments. The improvements in the new tester help us to obtain high quality resistance and force data. In this chapter, we demonstrate the capabilities of the contact test system; we report on
the effects of plasma and of UV-ozone cleaning, and on the use of a layered contact, consisting of a soft metal, gold (Au), coated with a thin layer of a hard metal, ruthenium (Ru).

4.3 Contact Tester System

The chamber setup of our SPM-based contact tester is shown in Figure 1. The system consists of three parts: 1) the SPM module which is used for both force measurement and control; 2) the custom-built vacuum test chamber which provides a controlled environment for the contact test and allows the introduction of a plasma and/or UV-ozone cleaning to the contact area; and 3) the MKS-AX7670 remote plasma source used to clean the contacts with plasmas containing Ar and O₂.

Figure 1. A photograph of the SPM-based contact tester with the vacuum chamber and plasma source.
In contrast to the previously used force sensors which were constructed of cantilever beams [13], [15], the newly designed force sensor consists of a fixed-fixed beam structure, with the contact bump located in the middle of the beam (Figure 2a). The deflection of the bump, and hence the applied contact force, is determined by shining the laser beam of the SPM on one of the two optical paddles located on either side of the contact tip (Figure 2b). The use of a fixed-fixed beam structure significantly reduces the sliding effect during the contact tests. Also, the fixed-fixed beam can provide more rotation at the optical lever paddle for a given bump deflection as compared to a cantilever structure of the same length. This increased angular rotation improves the sensitivity of the force measurement. The relationship between the angular rotation of the optical paddle and the applied force was determined using a structural finite element analysis.

Table 1 shows a comparison of the old and new force sensors. In summary, the newly designed sensors provide better resistance and force measurements along with minimal sliding.

Table 1. Comparison between old and new force sensors.

<table>
<thead>
<tr>
<th>Force Sensor</th>
<th>New</th>
<th>Old</th>
</tr>
</thead>
<tbody>
<tr>
<td>Structure</td>
<td>Fixed-Fixed</td>
<td>Cantilever</td>
</tr>
<tr>
<td>Dimension (µm)</td>
<td>120x20x4.5</td>
<td>180x50x30</td>
</tr>
<tr>
<td>Stiffness (N/m)</td>
<td>2500</td>
<td>15000</td>
</tr>
<tr>
<td>Force Resolution (µN)</td>
<td>1</td>
<td>12.5</td>
</tr>
<tr>
<td>Contact Sliding</td>
<td>Minimum</td>
<td>Yes</td>
</tr>
<tr>
<td>Measured Resistance (Ω) (Au-Au at 250µN)</td>
<td>0.15</td>
<td>0.85</td>
</tr>
</tbody>
</table>
Figure 2. (a) An SEM image of a force sensor with the fixed-fixed beam structure. The optical lever paddles are necessary to deflect the laser beam in the SPM; (b) the deflection of the laser beam is monitored by an optical level system.

### 4.4 Contact Testing and Cleaning Experiments

The tester has the capabilities of contact resistance vs. force characterization, contact cycling testing and for plasma and UV-Ozone treatments, thereby providing a platform for contact cleaning and surface modification studies. In this investigation we show the results of three treatments – O$_2$ plasma, Ar plasma, and UV-Ozone on the contact resistance of Ru-Ru contacts [1].

The UV light can directly break the contaminant molecule bonds. At the same time, the UV light can be absorbed by O$_2$ which creates atomic oxygen and ozone [16]. Oxygen radicals and ozone can accelerate the removal of organic layers on the metal surfaces.
An in-situ plasma test of a Au-Au contact which was cycled within the chamber at 1Hz, with a loading force of 100 µN was performed to get the pull-off force and resistance vs. time results. The O₂ plasma rapidly caused the pull-off force to decrease below the detectable level, while the contact resistance increased gradually during the period when the O₂ plasma was turned on. The drop of adhesion for the Au-Au contact, as well as the increase of the resistance during the O₂ plasma treatment, could be due to the formation of layers of Au₂O₃ layer on the contact surfaces [17]. Thus the O₂ plasma treatment also increased the resistance of Au-Au contacts.

4.5 Resistance vs. Force

After measurements of resistance and contact force, the data can be compared for different contact materials. The focus is on the low force region (< 1000 µN) which is of greatest interest for most MEMS switch applications.

As shown in Figure 3, the Au-Au contact yielded the lowest contact resistance. This result is due to the low resistivity and low hardness (forming a large contact area) of Au thin films. Hard metal contact pairs with a higher resistivity, such as Ru-Ru and Ir-Ir, have higher contact resistance compared to Au-Au. Dissimilar metal contact pairs which combine Au with a hard metal, i.e. Au-Ru and Au-Ir, have intermediate values of contact resistance.
In this section, we report on the modeling and testing of a layered contact, consisting of a soft metal (Au), coated with a thin layer of a hard metal (Ru). The idea is that by using such a layered configuration, it may be possible to take advantage of the low hardness of Au to achieve a large contact area, and the high hardness of Ru to enhance the durability. Furthermore after the current passes through the thin Ru layer, conduction can occur through the low resistivity Au. Finite element modeling and simulations (Figure 4a) of the Au/Ru layered structures were performed in both the mechanical and electrical domains. Elastic–perfectly plastic material properties were used for the modeling with
Young’s moduli of 410 GPa for Ru and 82 GPa for Au. The onset of the plastic yielding stress is taken as 3.24 GPa and 0.8 GPa for Ru and Au, respectively, with a Poisson’s ratio of 0.3 for each metal. The pillar height is 24.8 μm. The mechanical modeling, which did not include adhesion, predicted how the contact area varies with the applied force (Figure 4b). Electrical modeling, using these predicted contact areas and the measured thickness-dependent resistivity (Table 2), was used to estimate the contact resistances which are included in Figure 5. The electrical model did not include the effect of native conductive RuOx layers which likely form.

The results show that layered structures should have larger contact areas and lower contact resistance than Ru–Ru contacts. This contact design configuration is supported by a recent study [19] for layered contact with adhesion. The tested contact pairs which consisted of Au–Au and layered Au–Ru contacting layered Au–Ru are listed in Figure 5. Seven samples of each contact pair were measured; the maximum, minimum and median values of the seven measurements are plotted in Figure 5 along with the simulation results. The simulated values can now be compared to the measured resistances at contact forces of 100, 200, 300 and 500 μN. According to the simulations, the thinner the coating, the larger the contact area, and in turn, the lower the contact resistance. However, this tendency is not so clear in the low force measurements. These experimental results show that the contact resistance is indeed lower at contact forces of 500 μN. However, at 100 μN, the contact resistance is higher than for Ru–Ru contacts. Only when the contact force is larger than 300 μN is a lower resistance observed in the contacts with the thinner ruthenium coatings. This result is believed to be due to the contaminate films on the Ru which can only be broken through with sufficient force. As the Ru layer thickness increases, the discrepancy between theory and testing decreases.
This behavior is likely to be in part due to the resistivity of thin films which is known to increase as the film thickness decreases (Table 2). Adhesion for Au–Au contacts was comparable to the contact force, while adhesion for the other contacts was less than 10 μN.

**Figure 4.** (a) ANSYS model for the layered structures, the thickness of Ru coating is 10nm, 50nm, 100nm and 300nm. (b) Contact area estimated based on the simulations.
Figure 5. Maximum, minimum and median value of the measured resistances, and the resistances estimated by ANSYS simulations. The contacts labeled here are: Au-to-Au contacts, and layered-to-Ru/Au layered contacts, with a thickness of Ru layer of 10 nm, 50 nm, 100 nm and 300 nm respectively.
Table 2. Ruthenium resistivity vs. thickness.

<table>
<thead>
<tr>
<th>Thickness (nm)</th>
<th>Resistivity (µΩ·cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>26.6</td>
</tr>
<tr>
<td>50</td>
<td>23.0</td>
</tr>
<tr>
<td>100</td>
<td>20.5</td>
</tr>
<tr>
<td>300</td>
<td>17.9</td>
</tr>
</tbody>
</table>

In addition, the stability of contact resistance under different currents was studied. Figure 6 shows the changes of the resistances after applying DC currents at contact forces of 100 μN and 500 μN. This data suggests that the stability of the resistances for the layered structures is strongly related to the contact force. Large drops of the resistance with current were observed for the layered structures at 100 μN, and less at 500 μN. The stability of the resistances is also affected by the thickness of the layer. The resistances are less stable for the contacts with thinner coatings. In general, the decrease of resistance under large current indicates either the existence of surface films or contact softening. It is found that at 500 μN the contacts with a 100 nm layer of coating showed a stable contact resistance up to 500 mA.
Figure 6. Ratio of the resistance to the initial resistance as a function of current at contact forces.
4.7 Conclusions

An improved SPM-based contact tester has been designed, constructed and used for cyclic testing of various metal contacts. The tester is capable of high resolution simultaneous measurements of contact force and resistance. It was found that a dissimilar contact pair of Au-Ru with O₂ plasma cleaning can provide low contact adhesion and low resistance as compared with Au, Ru, and Ir contact pairs. Layered structures with a thin layer of Ru on top of Au were also modeled and tested. Ru layers between 50 and 100 nm are effective in reducing adhesion and contact resistance, provided the contact force is greater than 300 μN. A contact force greater than 300 μN is recommended for achieving a low resistance. A thickness more than 50 nm is suggested for resistance stability under currents stress.
4.8 References


Chapter 5: Conclusions
5.1 Conclusions

The three-prong approach incorporates quantifying adhesion effect in layered contacts, investigating the impact of nanoscale asperities as well as evaluation of contact materials by testing. Mechanical and electrical finite element contact models were developed for an elastic-plastic layered hemisphere (Ru on Au) with a rigid flat surface in the presence of adhesion. The effect of adhesion is applied as a surface pressure based on the Lenneard-Jones potential. The mechanical simulations show that the adhesion force and contact radius are each greatest for high forces and thin layers, and electrical simulations use thickness-dependent measured values for the resistivities. Thinner layers give lower resistance due to the larger contact area and increased conduction through the underlying Au. A suitable design space of low adhesion and low contact resistance can be guided by these results.

A three-dimensional combined molecular dynamics and finite element model of the contact between a rough microsphere and a flat surface was also developed. Curve-fits from the molecular dynamics simulations were used in order to model each nano-asperity as a nonlinear hysteretic force-distance element. The bulk of the microsphere was modeled as an elastic-plastic body using finite elements. The nano-asperities were placed on the surface of a continuum finite element model to describe the nanoscale surface roughness on the microsphere. The results are presented for the contact force and contact area, each as functions of the contact approach. Three values of the work of adhesion were studied: a typical experimental value of 1 J/m^2, an ideal value of 6 J/m^2, and an intermediate value of 3 J/m^2. Results are compared with the smooth continuum
sphere model. These models show quantitative differences in which nanoscale roughness significantly reduces both the effect of adhesion and reduces the real area of contact.

An improved SPM-based contact tester has been designed, constructed and used for cyclic testing of various metal contacts by other members of our group. Modeling and testing of a layered contact, consisting of a soft metal (Au), coated with a thin layer of a hard metal (Ru) are developed. Layered configuration can take advantage of the low hardness of Au to achieve a large contact area, and the high hardness of Ru to enhance the durability. Elastic–perfectly plastic finite element modeling and simulations of the (Au on Ru) layered structures were performed in both the mechanical and electrical domains. The results show that layered (Ru on Au) structures should have larger contact areas and lower contact resistance than Ru-Ru contacts. Ru layers between 50 and 100 nm are effective in reducing adhesion and contact resistance, provided the contact force is greater than 300 μN. A contact force greater than 300 μN is recommended for achieving a low resistance. A thickness more than 50 nm is suggested for resistance stability under currents stress.

The knowledge obtained in this work has resulted in publications and technical presentations [1-7] as well as the understanding of microcontacts with adhesion, which is a fundamental step towards the design of the contact of a micromechanical switch helping to resolve the reliability problem of microswitches.
5.2 References


Chapter 6: Future Work
6.1 Future Work

Studying hot switching, defined as changing the state of a switch while an electrical signal is applied, is an essential step in order to improve MEMS switch life-cycle time. In the case of ohmic switches, as the switch closes, the electric field is increased, and even at very low power levels hot switching damage can occur which can degrade the switch contacts. This phenomenon needs to be better understood.

Due to low contact forces achievable by MEMS structures, a soft metal is needed in order to obtain low contact resistance. It has been shown that a layered Au/Ru contact configuration can be used as a substitute for a pure Au contact tip. The finite element model of the layered contact could be extended to include the electrothermal effect coupled to the mechanics of the contact. The roles of thickness-dependent resistivity and conduction through the Ru-Au interface also needs to be better understood.

Since a MEMS micro-contact is always rough, studying the multi-nano-asperity contact effect on mechanics below a micro-contact is key to achieving a better understanding of MEMS contact phenomena. The MD-FEA model with the advantage of high-speed processing computers could include different sizes of nano-asperities, resulting in a wider range of contact force and area combinations. The combined MD and finite element model could be extended to account for multiple loading-unloading events when more loading-unloading MD simulations are available. These types of simulation could predict trends seen during experimental lifetime cyclic testing of switches.