Analysis of Contact Forces Using AFM Data of Polycrystalline Silicon Surfaces

Michael J. Starr[1], Hartono Sumali[1], James M. Redmond[1], Erin E. Flater[2], and Robert W. Carpick[2]
[1]Sandia National Laboratories, MS 0847, P.O. Box 5800, Albuquerque, NM 87185
[2]University of Wisconsin – Madison, Engineering Physics, 1500 Engineering Drive, Madison, WI 53706

ABSTRACT

The atomic force microscope (AFM) has evolved to the point of enabling the resolution of sub-nanometer features on a surface. Rather than artificially generated surfaces, high-resolution AFM images of polycrystalline silicon can be used to characterize the contact forces in micro- and nanoscopic devices. In this work, finite element models of characteristic features of the polysilicon surface are developed to explore the evolution of contact forces during a frictional sliding event. In conjunction with these analyses, discrete contact models are developed and applied to a novel MEMS device. This work also illustrates some of the fundamental limitations of Greenwood-Williamson and other homogenized surface models when attempting to characterize the contact and frictional properties encountered in MEMS devices. There is evidence that accurate contact analyses of MEMS devices involving either very light loads or small numbers of contacting asperities can only be performed if spatial information for the contacting surfaces is retained. In investigating that hypothesis, 2D and 3D geometrically based contact simulations are performed to characterize an experimentally observed phenomenon during frictional sliding.

Keywords: contact mechanics, friction, finite element model, discrete contact

INTRODUCTION

This paper discusses the fundamental phenomena that occur when two surfaces are pressed against each other and, later, when those surfaces are slid relative to one another. For decades, researchers have relied on a few extremely well used classical theories [1-3]. However, surface profiling by the atomic force microscope (AFM) in the last several years has revealed new information that brings us closer to understanding the contact phenomena on the nanometer asperity scale [4]. The main driver of this work is the need to explore the contact, adhesion and frictional properties of polysilicon and coated polysilicon, as they pertain to response and longevity of MEMS devices. Technological advances in miniaturization and manufacture of MEMS have outstripped our mechanical knowledge of such systems. Fundamental research on the physics of these systems is therefore essential to further the growth and development of MEMS devices.

Homogenized or statistically based surface models have endured for decades in the literature and were instrumental in leading to an understanding of the relationship between friction and contact area. However, these methods as well as fractal surface representations are not completely satisfactory as the implementation of some of these techniques requires a level of arbitrariness through the selection of certain parameters [5,6]. Of course a certain level of approximation will always exist in calculations because of the dependence on the accuracy of the representation of the surface by the measuring device. Additionally, statistical methods require a statistically significant number of contacts in order to be representative of the true surface, while fractal methods still possess a level of arbitrariness in the parameter selection process. Both of these techniques assume a pre-existing knowledge of the surface and its length scales or distributions.

There is evidence that for surfaces in contact under very light loads, it is the outliers that will dictate performance, in which case homogenized models may not be able to appropriately capture the response or nature of the surface [7,8]. In fact, the correct description of MEMS response characteristics, may require the retention of all the spatial information of two contacting surfaces. To this end, the development of discrete analysis tools, in conjunction with tradition finite element models with adhesion capabilities are essential elements for progress.

CLASSICAL GREENWOOD-WILLIAMSON MODEL VS. DISCRETE ANALYSIS

An extensive literature review of surface contact and friction shows that a model developed by Greenwood and Williamson four decades ago [1] is quite likely *the* classic foundation of surface contact research. That model (henceforth referred to as *GW model*) provides an elegant means of calculating the effective contact area, among other variables, when two surfaces are pressed against each other. Of the surface features, the model involves only statistical features, namely, the distribution of the peak height (*e.g.* Gaussian, exponential, *etc.*), and an average radius of curvature of the asperities. It does not take into account individual asperities. However, the model also shows that the true contact area is very small compared to the

apparent contact area, as is the number of asperities that are in contact. In many MEMS applications, the apparent contact area is already quite small. Therefore, the number of asperities in contact may be so small that it is necessary to treat each asperity "individually". Today, atomic force microscopy (AFM) enables us to retain full spatial information on the surface topography. Based on the measured surface profile it is possible to use Hertz-based solutions to perform discrete calculations of contact forces and contact areas. Thus, we embarked on an investigation of how well the GW model predicts contacts in MEMS surfaces, using actual topography of polycrystalline silicon surfaces.

Greenwood and Williamson showed that a purely elastic model yields a linear relationship between true contact area and applied normal load. In fact, that model shows that only very few contacts are needed to obtain the expected linear relationship between contact area and applied load. However, that is not the entire story. Maintenance of that relationship requires that sufficient numbers of contacts be added as contact force increases and/or plasticity is initiated at sufficient numbers of contacts. As shown in a very finely controlled experiment by Archard [2], the exponential relationship between contact area and normal force can typically exist within a range of values. This is an extremely important observation especially in instances when the number of contacts is expected to be very few and/or the contact force is small in magnitude.

Following the GW model, the relationship between force acting through an asperity and true contact area can be given by the following equation

$$P = KA_r^{\,n} \tag{1}$$

where P is the asperity force, K is a constant obtained from material and geometric parameters in the Hertzian contact formula, and A_r is the real contact area. For a single asperity elastic contact, the exponent will have the value $n = 1.5$ according to Hertz theory. Depending on the nature of the surface, as more and more asperities come into contact the GW model implies that this exponent should trend towards $n = 1$, although as shown by Archard [2], for example, the value of n will depend strongly on the surface conditions and could lie within the envelope $1.0 < n < 1.5$. For example, Archard's experiments with corrugated Perspex specimens gave a value of n of approximately 1.23.

To investigate whether the GW model can predict the contact behavior of real polysilicon surfaces, we calculated the expoential in Equation (1) using a 10μm x 10μm polysilicon surface (1024 x 1024 pixels), with surface roughness of 2.7 nm rms. The surface data was obtained using an atomic force microscope (AFM). A portion of this surface, with the heights exaggerated, is shown in Figure 1.
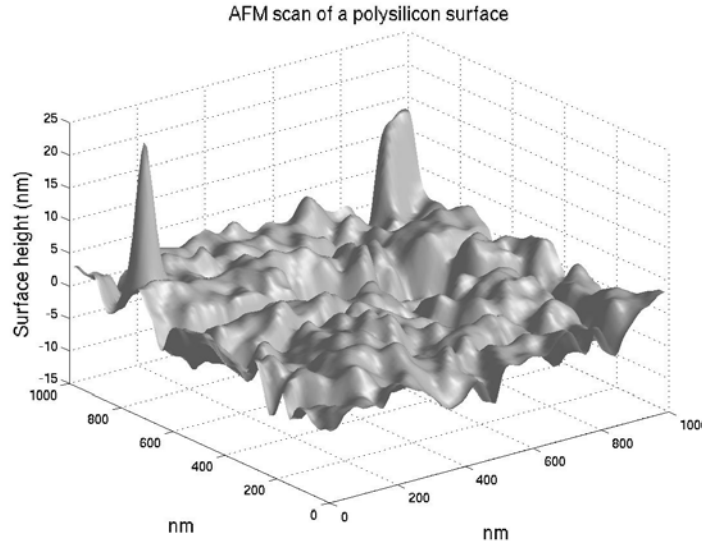

Figure 1: *AFM surface profile for analysis. 1μm x 1μm sample from the full image. Height measure taken with respect to mean surface height.*

Summits were arbitrarily identified as local maxima within a 200 nm x 200 nm box, a size that roughly corresponds to the average grain size of the polysilicon surface analyzed. Computation resulted in the number of summits = 676 and the peak height standard deviation $\sigma_s = 4.5$. Following the GW derivation, we simulated the case where a hypothetical flat, rigid plane was pressed into the polysilicon surface, and calculated the exponent n as a function of the distance w the rigid plane was pressed into the polysilicon. All of the intrinsic assumptions of the GW model were followed for this calculation. However, in contrast to GW derivation, we took each discrete asperity into account as it made contact with the flat surface. Asperities were

identified and the corresponding radii of curvature were calculated by fitting elliptic parabolloids. Using the expressions for force and true contact area as functions of interference distance, the power n can be derived as the following function of the interference distance:

$$n(w) = \frac{3}{2} \frac{\sum_{i=0}^{m}\left[r_i(w-z_i)\right]^{1/2} H(w-z_i) \sum_{i=0}^{m} r_i(w-z_i)H(w-z_i)}{\sum_{i=0}^{m} r_i H(w-z_i) \sum_{i=0}^{m}\left[r_i(w-z_i)^3\right]^{1/2} H(w-z_i)} \qquad (2)$$

where r are the summit radii of curvature, z are the summit distances measured with respect to the initial location of the smooth contacting plane (for convenience these are ordered $z_0 < z_1 < ... < z_m$), $H(\cdot)$ is the Heaviside function, and m is the number of summits on the rough surface. A representative schematic is shown in Figure 2(a).

Figure 2(b) shows the exponent n resulting from the above discrete calculation. The figure also gives a plot of the number of discrete contacts (referenced to the right axis) involved in the calculation as a function of the interference distance. The exponent value, referenced to the left axis, is initially $n = 1.5$, and subsequently at a large enough interference distance enters an envelope around $n = 1$. The initial drop at slightly less than 5 nm interpenetration corresponds to the initiation of contact at the second asperity. Subsequent drops correspond to additional contacts achieving intimate contact with the compressing rigid plane. The plot indicates that only a very small number of contacts involving asperities with different heights (and presumably different radii of curvature) are needed to obtain exponent values near 1.
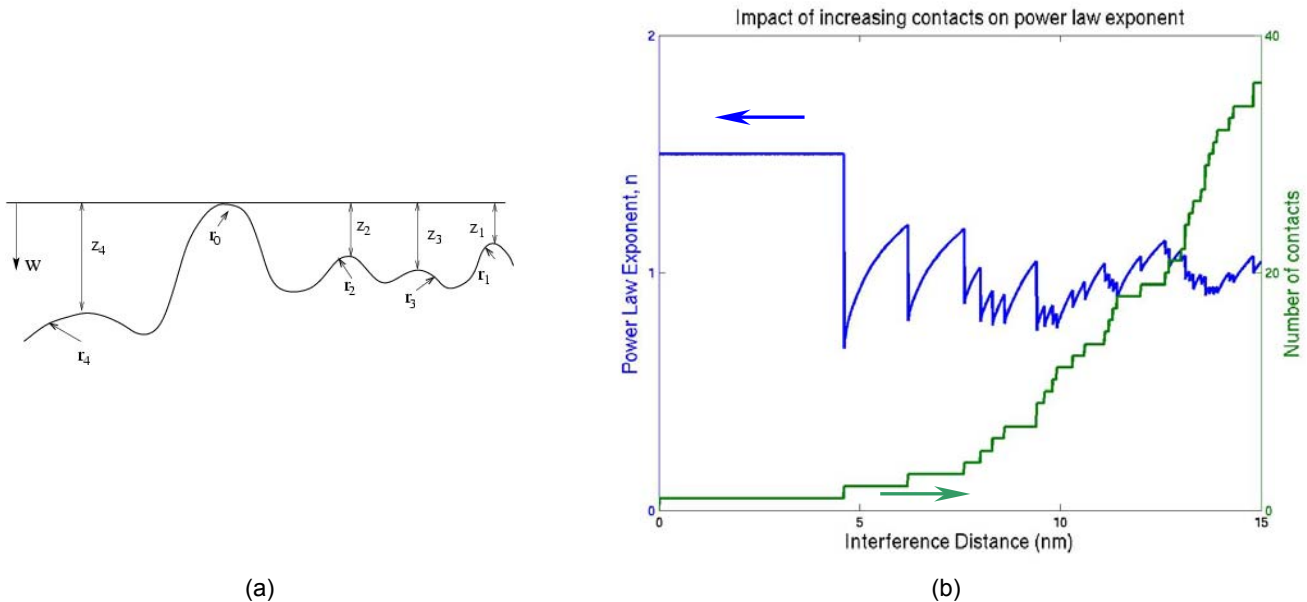

| (a) | (b) |

Figure 2: (a) *Schematic defining parameters of Equation 2.* (b) *Effect of contacting asperities on the contact area exponent.*

An important point needs to be made however: the maintenance of an exponent in the vicinity of $n = 1$ requires the continuous introduction of new contacting asperities at a sufficiently high rate as the surfaces come together. This rate must be high enough that the difference in asperity heights becomes less significant as the total interference distance increases. If that is not the case, then n will be other than 1. Figure 2(b) shows that, when only the first asperity is in contact, the power n is 1.5 as determined by Hertz' law. The figure also shows that the second asperity comes in contact approximately 5 nm after the first asperity. If these were the only two asperities on an otherwise perfectly smooth surface, the contact area exponent would asymptotically approach $n = 1.5$ for increasing interference distance.

Normal distribution assumption and resulting contact area exponent
Part of the Greenwood and Williamson paper (GW) discusses a case where the distribution of asperity heights is assumed to be an exponential function. This exponential distribution yields a constant value of $n = 1$ regardless of interference distance. However, GW suggests, and it is commonly assumed that the distribution of asperity heights is Gaussian. In fact, the Gaussian probability density function resembles an exponential function only at the leading tail; therefore, for sufficiently large interference distances, n should diverge from the constant value obtained from the exponential distribution, and the value $n = 1.5$ should be approached. Figure 3 shows the divergence from $n = 1$ (dashed line) as interference distance w grows.
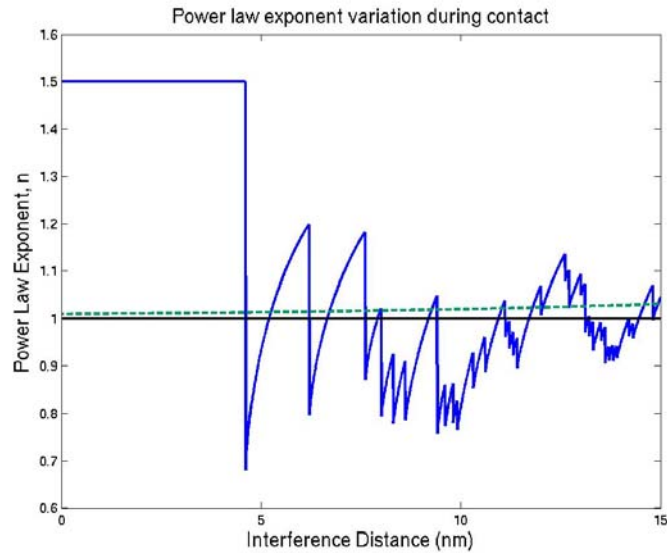
Figure 3: *Comparison of contact area exponents for discrete calculation(solid/jagged), normal distribution(dashed), and exponential distribution(constant).*

To further show whether the experimentally profiled surface could fit the power law in the GW model with Gaussian height distribution, we plot the number of contacts as a function of interference distance again in Figure 4. In Figure 4 we overlay the plot of the number of contacts as a function of interference distance as predicted by the GW model with Gaussian height distribution (smooth curve). The graph shows that the GW model does not accurately predict the number of contacts, where the GW curve is shifted to coincide with the experimental curve at w = 15 nm.
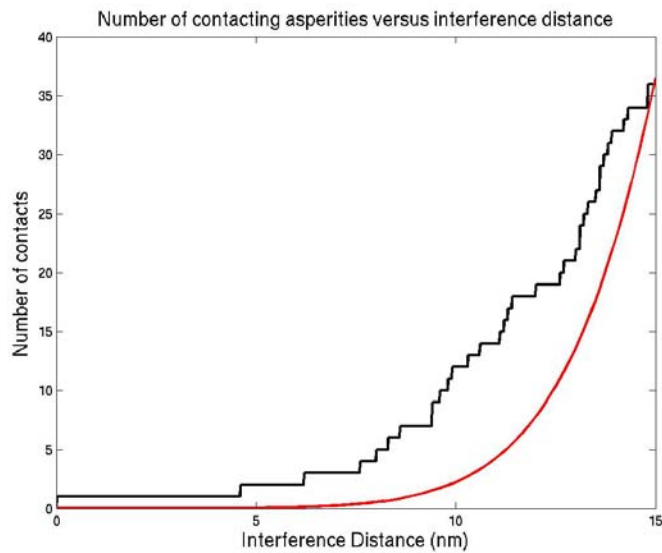

Figure 4: *Comparison of number of contacting asperities for discrete contact model vs. Gaussian approximation. Discrete case(stepped); shifted Gaussian tail to match number of contacts at 15 nm interference (smooth).*

Another well-used classical model was derived by McCool [3] as an extension to the GW model. This method uses the zeroth, second, and fourth spectral moments (m_0;m_2;m_4) of the asperity height distribution. Although not shown here in a graph, simulations using McCool model exhibits the same behavior as the GW model using a normal distribution.

The above calculation demonstrates that it is extremely important to understand the nature and distribution of the *highest* asperities of the surface. In particular, if low loads are applied to contacting surfaces and a tightly packed distribution of tall asperities dominate the contact behavior, the discrete nature of contact cannot be captured by a GW-based model. Moreover,

it should *not* be assumed that increasing the number of contacts will guarantee $n = 1$. The exponent n depends strongly on the nature of the surface.

SIMULATIONS OF SLIDING CONTACT

As described previously, homogenized models may not be suitable for describing multi-asperity contact, hence they would not be suitable for describing sliding contact. Because the operational physics of certain MEMS devices [7,9] is essential to its subsequent performance, discrete and finite element simulations of sliding contact can provide important pieces of information. It has been demonstrated in the literature [10,11] that an atomic force microscope, an ideal singe asperity, observes the proportionality between friction and true contact area for a variety of systems. For surfaces with multiple contacting asperities, the historical difficulty has been calculating the true contact area.

The global complexity of a representative apparent contact area makes it difficult to isolate interacting phenomena. Therefore, we have initially sampled a small coupon of the polysilicon surface over which to run sliding contact simulations. Figure 5 shows a slice from the AFM-profiled polysilicon surface. The length of this slice is 100 nm; the width, 35 nm. Above the bottom slice, a synthesized polysilicon die with a spherical surface is pressed down with a ramping-up pressure until the pressure on its top side reaches 800 MPa. The die is slid across the bottom surface with a prescribed lateral displacement. The prescribed pressure and position are shown in Figure 5(b). Both the die and substrate are assumed isotropic with elastic modulus, $E = 161$ GPa and Poisson's ratio $\nu = 0.23$.
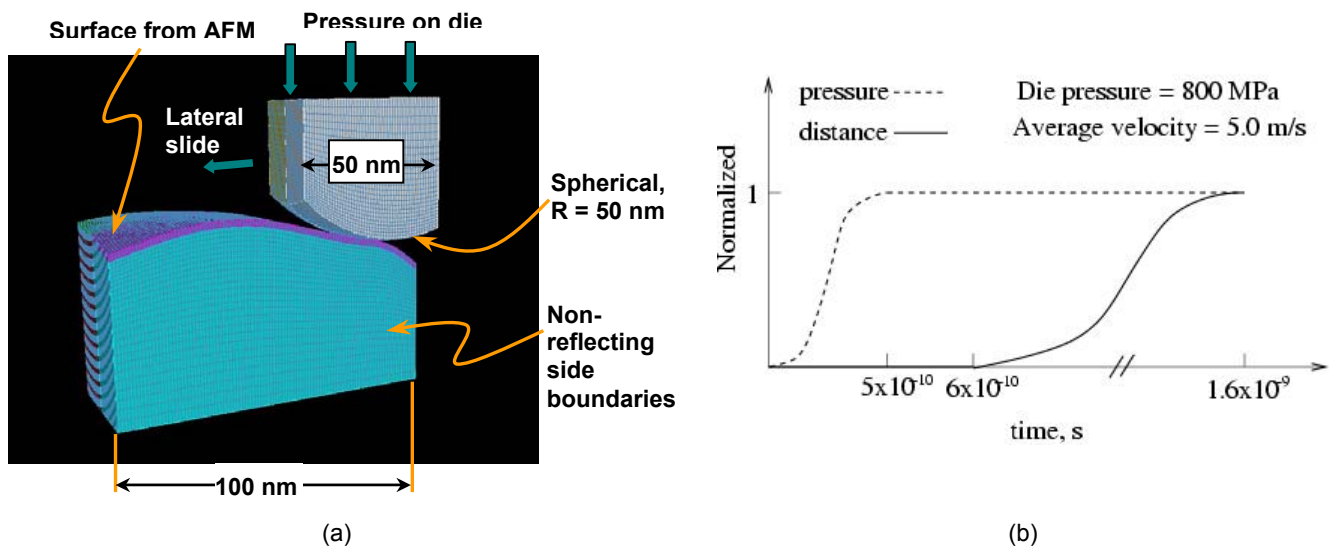

(a)   (b)

Figure 5: *A spherical die slid across a slice of real surface,* (a) *Finite element mesh,* (b) *Prescribed pressure and lateral displacement*.

Sandia's transient dynamics finite element code *Presto* ran the simulation and calculated contact pressures, stresses, strains, displacements, and forces. The simulation used 250,000 8-node hexagonal elements, with the surface elements in the contacting planes having dimension 0.5 nm x 0.5 nm x 0.5 nm. Non-reflecting boundary conditions are applied on the non-contacting surfaces to absorb stress waves.

Surface coating
Single-atomic monolayers (SAM) on the substrate have been used as a lubricating film to reduce the friction between an AFM-tip and the substrate [11]. We have also performed a simulation to explore the effect of a CH_3-thiol SAM on contact properties and friction. The SAM is assumed isotropic with elastic modulus, $E = 8$ GPa and Poisson's ratio $\nu = 0.4$. The effect of the SAM was compared to the case of pure polysilicon in contact. A proposed sliding friction model for such systems is the junction model, in which the frictional force is linearly related to the true contact area through the junction strength, a material constant determined experimentally [10]. Finding the local variation in friction is then captured through finding the local variation in true contact area. Figure 6 shows the results of some preliminary simulations of contact area during sliding, both with and without the SAM. The dashed curve shows the results for polysilicon-on-polysilicon sliding contact. The dotted curve shows an approximate calculation of contact radius of polysilicon-on-polysilicon using Hertzian theory and calculating the local radius of curvature. Despite the use of an average value for local curvature at contact, the Hertzian approximation provides a reasonable estimate of contact radius. The solid curve shows the modification to the contact radius that occurs when a thin compliant SAM is included in the analysis. As expected, the contact area is larger than that for the case of polysilicon-on-polysilicon, although due to the small layer thickness and relative magnitude of the applied force, the contact radius is substantially smaller than what is theoretically predicted for polysilicon on a pure CH_3-thiol SAM substrate.
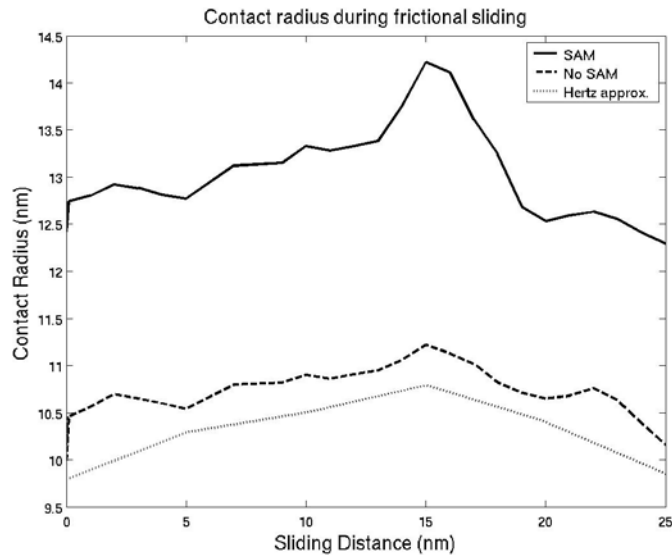
Figure 6: *Contact radius calculations for geometry pictured in Figure 5 for frictional sliding over a polysilicon substrate and a SAM CH₃-thiol coated substrate.*

CONCLUSIONS

Although the analysis described in this paper is limited to small force, nominally elastic contact of polysilicon, it is still of importance because the force levels considered are within the range of those seen during operation of some MEMS devices. Some important conclusions to draw from the analysis are the following:

- The exponential relationship between force and true contact area cannot be found unless discrete contact analysis is performed.
- It is unlikely that any actual polysilicon surface would exhibit a normal distribution, much less one that is exponential.
- The addition of a SAM layer substantially increases contact area, while reducing tangential force.

Discrete analysis, although not elegant, is necessary when certain classes of contact problems, most notably MEMS. Although large-scale finite element analyses of sliding contact problems are expensive computationally, our capabilities of performing simulations with representative contact areas are rapidly improving. In the very near future enhanced computing abilities will allow a more complete treatment of the preceding analysis including the impact of adhesion on the frictional and contact response.

ACKNOWLEDGEMENTS

REFERENCES

[1] Greenwood, J. A. and Williamson, J. B. P., 'The contact of nominally flat rough surfaces', Proc. Roy. Soc., A495, 300-319, 1966.

[2] Archard, J. F., 'Elastic deformation and the laws of friction', Proc. Roy. Soc., A243, 190-205, 1957.

[3] McCool, J. I., 'Comparison of models for the contact of rough surfaces', Wear, 107, 37-60, 1986.

[4] Carpick, R. W. and Salmeron, M., 'Scratching the surface: Fundamental investigations of tribology with atomic force microscopy', Chem. Rev., 97, 1163-1194, 1997.

[5] Greenwood, J. A. and Wu, J. J., 'Surface roughness and contact: An apology', Meccanica, 36, 617-630, 2001.

[6] Majumdar, A. and Bhushan, B., 'Role of fractal geometry in roughness chacterization and contact mechanics of surfaces', J. Trib. (ASME), 112, 205-216, 1991.

[7] Luck, D. L., de Boer, M. P., Ashurst, W. R., and Baker, M. S., 'Evidence for pre-sliding tangential deflections in MEMS friction', in Transducers 2003, 404-407, Boston, 2003.

[8] Fujimoto, T., Kagami, J., Kawaguchi, T., and Hazakawa, T., 'Micro-displacement characteristics under tangential force', Wear, 241, 136, 2000.

[9] de Boer, M. P., Luck, D. L., Ashurst, W. R., Maboudian, Corwin, A. D., Walraven, J. A., and Redmond, J. M., 'High-performance surface-micromachined inchworm actuator', J. MEMS, 13(1), 63-74, 2004.

[10] Carpick, R. W., Enachescu, M., Ogletree, D. F., and Slameron, M., 'Making, breaking, and sliding of nanometer-scale contacts', Mat. Res. Soc. Symp. Proc., 539, 93-103, 1999.

[11] Burns, A. R., Houston, J. E., Carpick, R. W., and Michalske, T. A., 'Molecular level friction as revealed with a novel scanning probe', Langmuir, 15, 2922-2930, 1999.