CONTACT MECHANICS

Student Author

Petros Charalambides is a senior in mechanical engineering at Purdue University. A native of Cyprus, he is studying in the United States with a scholarship granted from the Cyprus Fulbright Commission. He also has been awarded the Kaiser Aluminum and Chemical Company Scholarship and John M. Bruce Memorial Scholarship while at Purdue. In the summer of 2011, Charalambides joined a multidisciplinary project on designing advanced micro-electromechanical systems (MEMS) devices. Upon graduation, he plans to attend graduate school on applied thermodynamics and heat transfer area.

Abstract

Physics-based simulations are playing an increasingly important role in materials and device engineering, providing information that can help engineers understand current technology and optimize designs. We describe a model and simulation tool for the characterization of the interaction between surfaces with nanoscale asperities relevant in nano- and micro-electromechanical systems (N/MEMS) whose operation involves periodic contacts. A mesoscale contact model was developed to characterize the interaction and adhesion between two surfaces in terms of surface topography and fundamental materials properties. The model computed the long-range van der Waals attractive forces and repulsive interactions originating from the contact between solid surface asperities. The tool has been deployed in nanoHUB.org and is available for fully interactive, free online simulations using a web browser.

Charalambides, P. (2012). Contact mechanics: Modeling the interaction between surfaces with nanoscale asperities for MEMS via online simulations in NanoHUB, *Journal of Purdue Undergraduate Research*, 2, 2–7. doi:10.5703/jpur.02.1.01

Mentors

Benjamin P. Haley received his bachelor's degree in physics from Purdue in 1998. At the University of California, Davis, he received a master's degree in engineering applied science in 2001 and his Ph.D. in 2005. Haley joined the NCN@Purdue team in November 2006 and transferred to the HUBzero team in January 2010. He also works as a research scientist with the Center for Predictive Materials Modeling and Simulation at Purdue.

Hojin Kim is a postdoctoral research associate working with Professor Alejandro Strachan in the School of Materials Science and Engineering at Purdue University. His research focuses on the characterization of contact physics involving metal against metal or metal against dielectrics by using multiscale computational techniques such as molecular dynamics (MD) simulation or mesoscale models, and the integration of multiscale modeling and simulations.

Keywords

micro-electromechanical systems, nanoHUB, physics-based simulation, surface interaction, surface adhesion

Alejandro Strachan is an associate professor of materials engineering at Purdue University and the deputy director of the National Nuclear Security Administration's Center for the Prediction of Reliability, Integrity and Survivability of Microsystems. He received a Ph.D. in physics from the University of Buenos Aires, Argentina, in 1999. Strachan's research focuses on the development of predictive atomistic and molecular simulation methodologies to describe materials from first principles, their application to problems of technological importance, and quantification of associated uncertainties.

CONTACT MECHANICS:

Modeling the Interaction Between Surfaces with Nanoscale Asperities for MEMS via Online Simulations in NanoHUB

Petros Charalambides, Mechanical Engineering

INTRODUCTION

Physics-based predictive modeling and simulation of materials and devices is playing an increasingly important role not only in helping understand the performance of current technologies, but in the design and optimization of new ones. Simulations can provide insight and quantitative information to reduce the cost and time involved in the design, optimization, and even certification of new materials or devices. This information can be used to help focus experiments on a small number of promising cases, avoiding trial-and-error-based studies (Kalil & Wadia, 2011).

Traditionally, the barrier to scientific computing has been high—potential users had to find the appropriate code, download it, compile it, and install it. Thus, advanced simulations remained restricted to expert users and developers. The U.S. National Science Foundation-funded nanoHUB.org at Purdue University has radically changed this situation. NanoHUB users can perform fully interactive simulations without the need to download, install, or maintain any software—they just need a web browser. This brings advanced simulations to a large number of people, including students, educators, and researchers. Research-grade simulations, restricted to experts until recently, are now routinely being used in undergraduate classes (Brophy, Magana, & Strachan, in press). We consider easy access to such tools by the scientific and engineering communities as critical for materials modeling to achieve its potential in helping design new materials and devices with improved properties.

Contacting MEMS and NEMS are important for a large number of applications including RF switches (Goldsmith, Yao, Eshelman, & Denniston, 1998), memory (Rebeiz & Muldavin, 2001), and logic applications in electronics (Kam, Lee, Howe, & King, 2005). The performance

of these devices is often dominated by the interaction between surfaces. Stiction, static friction, can often lead to failure as the device is unable to open the contact. Therefore, for these devices one needs to understand the mechanics behind two surfaces that come into contact and what governs adhesion (Giuliano & Clarke, 2006).

This paper first examines nanoscale interactions between two rough surfaces and then shows how the complex mathematics involved have been translated into a NanoHUB simulation tool. The major forces present during the adhesion process are identified and explained. A random surface roughness is generated for the simulation and the online simulation tool is used to obtain the force-displacement curves. Finally, the effects of root-mean-square (RMS) roughness and stiffness on the force-displacement curves is discussed.

Mesoscale Contact Model

The interaction between two rough surfaces is governed by various interactions including long-range, attractive van der Waals interactions (Delrio, de Boer, Knapp, Reedy, Clews, & Dunn, 2005) and short-range repulsion when asperities in the two surfaces come into contact.

Attractive van der Waals forces originate from induced-dipole interactions between atoms. These atomistic interactions can be integrated to describe the interaction between two flat, infinitively large surfaces leading to the expression:

$$F_{vdW}(d) = \sum_{i,j}^{N^2} f_{ij}$$
$$f_{ij} = \begin{cases} \frac{A}{6\pi(h_{ij} + d)^3} & \text{for } (h_{ij} + d) > r_c \\ 0 & \text{for } (h_{ij} + d) \leq r_c \end{cases}$$

Where A is the Hamaker constant, i and j are assigned iteration variables, h is grid height with zero mean, and d is the average separation (Figure 1). The attractive interaction is only important up to the point where the average separation plus the grid height is bigger than the critical radius, r_c . Theoretically, the average separation plus the grid height can go to zero, which would cause an infinite attractive force. Therefore, a “cutoff value” is selected as the minimum value where the attractive force is no longer significant. A value of 0.3 nm is considered for the “cutoff value,” which is an acceptable approximation of the critical radius of an atom.

The short-range repulsive interactions originate from the direct contact between surface asperities. We use a Hertz contact model modified to account for plastic deformation. Each individual contact is described via the interaction of a sphere with curvature equal to the local value of the surface with a flat surface. Approximations made in the Hertz contact model are elastic deformation. The contact area needs to be much smaller than the radius of the sphere, and friction is insignificant.

The total repulsive force is calculated as the sum of the actual contacts (Figure 2). Within the elastic limit the contact force is obtained using characteristic lengths of the sphere and elastic half-space. When the elastic limit is reached, the contact force is then a function of hardness and contact area. The plastic deformation of nanoscale objects is known to exhibit strong size effects (Kim & Strachan, 2011). Typically, hardening is observed with decreasing size. The contact model uses the hardness (H)-contact area ($A_{contact}$) relationship obtained from extensive MD simulations:

$$H(A_i) = H_{macro} + H_{nano} * A_{contact}^{-0.25}$$

Thus, the total repulsive force is obtained by the following formula with each contribution following:

$$F_{cont}(d) = \sum_i^{N_{cont}} g_i$$

$$g_i = \begin{cases} \frac{2}{3} E^* \sqrt{R_i \delta_i^3} & \text{for } \frac{2}{3} E^* \sqrt{R_i \delta_i^3} < H(A_i) \cdot A_i \\ H(A_i) \cdot A_i & \text{otherwise} \end{cases}$$

E^* is called effective elastic constant, R_i is the radius of curvature of each asperity, and δ_i is the local asperity indentation. The adhesion process can be described with respect to the energy well because the overall process is the accumulation of individual atoms forming bonds together. Material properties like Elastic

Figure 1. Schematic representation of surface interactions and model variables.

constant, Hamaker constant, and hardness are utilized to characterize the contacting surface and effectively calculate the attractive and repulsive forces.

Stochastic Description of Rough Surfaces

A random surface roughness can be created by generating a power spectrum using the following formula (Persson, 2006):

$$C(q) = \frac{1}{2\pi^2} \int d^2x \langle h(x)h(0) \rangle e^{-iq \cdot x}.$$

Where $C(q)$ is power spectrum, $h(x)$ is the asperity height at a point on the mesh, and q is a randomly generated wave vector.

The surface generated is considered to be a self-affine fractal. This means that every time we zoom in on the surface, it always looks the same. The power spectrum of a self-affine fractal is found to be:

$$C(q) \sim q^{-2(H+1)}$$

Where H is the Hurst exponent. This value can be between 0 and 1 and is specified by the user.

The asperity height $h(x)$ can be calculated using:

$$h(x) = \sum_q B(q) e^{i[q \cdot x + \varphi(q)]}$$

Where $\varphi(q)$ is a randomly generated vector and

$$B(q) = (2\pi/L)[C(q)]^{1/2}$$

Where L is the length of the grid.

The simulation begins with the generation of a random surface roughness with the required input data from the user. The user specifies RMS roughness and roll-off vector q_0 and Hurst exponent. This fractal exponent expresses the slope of the power spectrum against the

wave vector q on a logarithmic scale. In order for this plot to be meaningful, a smallest possible wave vector q_L and a cutoff wave vector q_I need to be specified. The generated wave vectors have their own magnitude and phase. Moreover, a real space grid needs to be created to define the surface for the simulation. Therefore, the user needs to specify a lower and upper limit to be assigned to real space.

Upon execution of the simulation code, the force-displacement curve corresponding to the surface roughness and materials properties selected is generated. The force displacement curves obtained are due to the addition of the attractive van der Waals forces and repulsive contact forces mentioned earlier.

MESO CONTACT MODEL SIMULATION TOOL IN NANO HUB

We deployed the Mesoscale Contact Model tool via nanoHUB.org using the Rappture toolkit (McLennan, 2005). Rappture stands for “rapid application infrastructure,” and it is an easy way to utilize graphical user interfaces based on different programming languages. Users specify the input parameters by employing four main categories (Figure 3):

- Surface characteristics variables provide information about the surface to be analyzed. RMS roughness is the arithmetic mean of the asperity heights. The Hurst exponent is obtained from the power spectrum of a random surface when plotted on a logarithmic scale. Maximum k corresponds to cutoff wave vector q_I discussed earlier. Rollover k corresponds to roll-off vector q_0 and minimum k corresponds to smallest possible wave vector q_L (Persson, 2006).
- Surface generation: A real space surface grid is generated with the number of grid points and grid size indicated. The number of k points needs to be specified for the reciprocal space to be generated.
- Surface materials properties: The surface properties are the effective Elastic constant, effective Hamaker constant, and hardness of the material, as discussed earlier. These properties are characteristics of the materials used in the simulation.
- The variables required for simulation pertain to initial separation, the step size, and the number of steps that the adhesion process will take place.

RESULTS AND DISCUSSION

We first exemplify the force-displacement relationship for a rough surface with a flat rigid surface for given materials, silicon nitride (Si_3N_4) and titanium (Ti), obtained from the Mesoscale Contact Model tool via

Figure 2. Total force displacement curve as the sum of the attractive and repulsive components.

Figure 3. (a) The “Surface characteristics” tab allows users to specify the properties of the surfaces involved. (b) The “Surface generation” tab tells the simulation code how to generate the model. (c) The “Surface material properties” tab corresponds to material properties for the surface to be generated. (d) The “simulation variables” tab controls the duration of the simulation.

Figure 4. Typical results of the simulation tool. Force distance curve and 3D view of surface generated. Plots in nanoHUB.org are fully interactive.

nanohub.org with RMS roughness, 25 nm, and effective Elastic constant, 160 GPa. Obtained total force curves, sum of attractive and repulsive forces, as a function of displacement are shown in figure 4. The inset figure indicates the created and used random rough surface.

In this study we also testify the effects of RMS roughness and material stiffness on deciding the force curves for given materials. RMS roughness reflects how rough the surfaces are. Thus we can anticipate that rough surface with high RMS roughness comes into contact earlier than one with low RMS roughness. We show the force-displacement curves with two different RMS roughness (100 and 25 nm) in figure 5. The result shows the larger equilibrium distance r_0 with higher RMS roughness shifts the whole curve to right, as we expected. We also indicate that the slope of the repulsive force in figure 5 is higher with RMS roughness 25nm, showing that it takes more force per unit length than RMS roughness 100nm. As the contact area increases, contacting asperities become softer. Since the contacting points are now more soft, less force is required to bring them closer and closer. Decrease in RMS roughness causes an increase to the slope of the curve and therefore it takes more force to push down on a flat plate.

Figure 5. Effect of stiffness on force displacement curves.

Figure 6. Effect of RMS roughness on force displacement curves.

The stiffness of the material indicates the how much the material resists deformation. Often it is a critical material parameter and used for deciding the optimal material for a given application. A material with higher stiffness will require a higher force to deform (Figure 6). The force displacement curve for a higher stiffness material at a given equilibrium position r_0 retains its shape but is more narrow. The slope of the repulsive curve increases with stiffness. As the stiffness increases the whole graph shifts to the left, that is, it takes more force to reach the equilibrium point because the material is now more resistant to deformation.

CONCLUSION

Online simulation is important for reducing experimental costs, saving time, and disseminating scientific knowledge to the general public. The importance of contact mechanics in designing advanced MEMS devices and the effects of computer-based simulation have been discussed. A nanoHUB tool, using the Rappture toolkit, has been developed in order to help people understand the adhesion process between two conducting surfaces by obtaining the force displacement curves. The effects of RMS roughness and stiffness are explained.

ACKNOWLEDGMENTS

This work was supported by the U.S. National Science Foundation through grant EEC-0634750 (Network for Computational Nanotechnology) and the U.S. Department of Energy's National Nuclear Security Administration under contract grant no. DE-FC52-08NA28617. The author gratefully acknowledges the contributions of Professor Alejandro Strachan, Hojin Kim, and Benjamin Haley, who have made the completion of this work possible. He also extends his gratitude to Keng-Hua Lin for the deployment of this tool.

REFERENCES

- Brophy, S., Magana, A., & Strachan, A. (in press). Lectures and simulation laboratories to improve learners conceptual understanding. *Advances in Engineering Education*.
- Delrio, F. W., de Boer, M. P., Knapp, J. A., Reedy, Jr., E. D., Clews, P. J., & Dunn, M. L. (2005). The role of van der Waals forces in adhesion of micromachined surfaces. *Nature Materials*, 4, 629-634.
- Giuliano, G., & Clarke, D. R. (2006). The interrelation between adhesion, contact creep, and roughness on the life of gold contacts in radio-frequency microswitches. *Journal of Applied Physics*, 100(9), 094904.
- Goldsmith, C. L., Yao, Z., Eshelman, S., Denniston, D. (1998). Performance of low-loss RF MEMS capacitive switches. *IEEE Microwave and Guided Wave Letters*, 8(8), 269-271.
- Kalil, T., & Wadia, C. (2011). Materials genome initiative: A renaissance of American manufacturing. *White House Office of Science and Technology Policy Blog*. Retrieved from <http://www.whitehouse.gov/blog/2011/06/24/materials-genome-initiative-renaissance-american-manufacturing>
- Kam, H., Lee, D. T., Howe, R. T., & King, T.-J. (2005). A new nano-electro-mechanical field effect transistor (NEMFET) design for low-power electronics. *Electron Devices Meeting, IEDM Technical Digest*, 463-466.
- Kim, H., & Strachan, A. (2011). Molecular dynamics characterization of the contact between clean metallic surfaces with nanoscale asperities. *Physical Review B*, 83(2), 024108.
- McLennan, M. (2005). The Rappture toolkit. Retrieved from <http://rappture.org>
- Persson, B. N. J. (2006). Contact mechanics for randomly rough surfaces. *Surface Science Reports*, 61(4), 201-227.
- Rebeiz, G. M., & Muldavin, J. B. (2001). RF MEMS switches and switch circuits. *IEEE Microwave Magazine*, 2(4), 59-71.