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IMPACT – Center for Advancement of MEMS/NEMS VLSI

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Summary of Research Progress

I. Mechanical Domain Characterization and Modeling

Our mechanical characterization and modeling activities emphasize the experimental investigation at the micro and nano-scale of the mechanical properties of the material parameters used in MEMS, and their accurate quantitative description in terms of models compatible with multi-physics, stochastic computational techniques for device functionality assessment and trustworthy device performance degradation analysis. The following are highlights from research accomplishments during Q2 of 2008.

Characterization of Stress Relaxation Behavior of Metal Films in RF MEMS Capacitive Switches

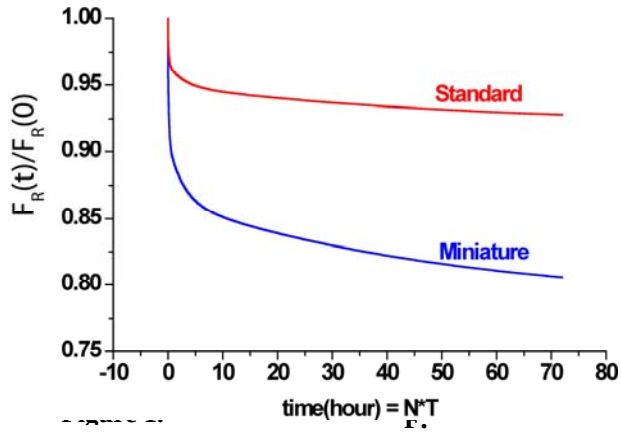
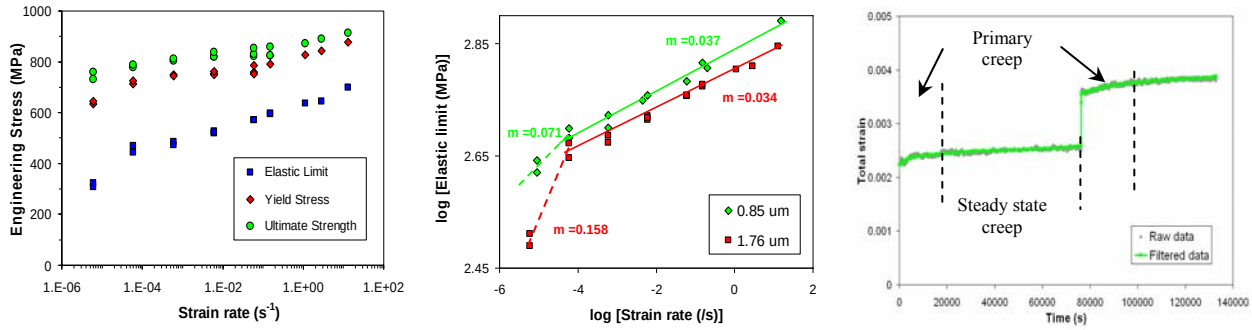


Figure 1. Demonstration of stress relaxation

This research is carried out at Lehigh under the supervision of Prof. Rick Vinci and Prof. Walter Brown, and through collaboration with Dr. Chuck Goldsmith from MEMtronics. During the past quarter we continued to characterize the anelastic relaxation behavior of pure Au films (1.2 um thick). A time-dependent elastic modulus function was established for a 72 hour period, the longest measured thus far. An analytical model for the restoring force of a typical fixed-fixed beam was developed to allow us to estimate the effect that a time-dependent modulus would have on the actual performance of a switch. The model has two stiffness terms: one that is directly dependent on the modulus of the beam material and one that is dependent on the total stress in the beam. The total stiffness of the beam is used to calculate the restoring force available to reopen an actuated switch as a function of time. The restoring force model was used to analyze two cases that represent different styles of switch, one with "Standard" beam dimensions (e.g., 280 um long) and the other with "Miniature" beam dimensions (e.g., 21 um long). The Standard switch design is highly sensitive to the value of the total stress whereas the Miniature design is more sensitive to the elastic modulus component of the restoring force. The resulting behavior, shown in the accompanying Figure, demonstrates the strong interplay between anelastic relaxation and device design. The Standard switch experiences only a 5% drop in restoring force over 72 hours whereas the Miniature switch suffers a decrease of nearly 20%.

Mechanical Response of Au Films at Fast / Slow Actuation Rates for Large Displacement MEMS

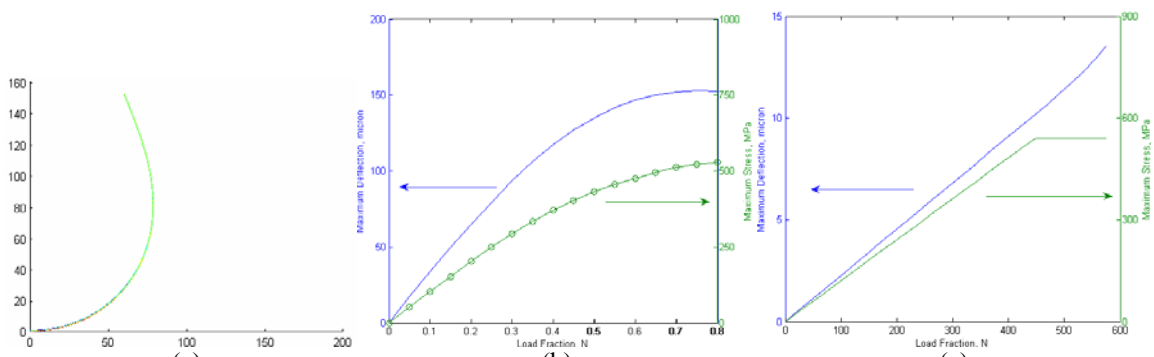
In parallel to the above mechanical characterization activity, Professor Chasiotis' group investigated the mechanical response of Au films with two different thicknesses: 830 nm and 1760 nm, fabricated by Prof. Peroulis' group at Purdue. A new experimental apparatus capable of achieving very fast loading rates (10^{-1} to 10 s^{-1}) corresponding to ms switching times was implemented for the first time. Figure 2(a) shows a summary of all experimental results for loading rates between 10^{-6} to 10 s^{-1} and 1760 nm films including the fast strain rate (fast switching) experiments conducted in the reporting period. The unusually large yield strength seen in Figure 2(a) is attributed to the very small grain size of this Au (38 nm) that does not promote dislocation-driven plasticity. Another key observation was that at the fastest loading rate, the films remained linearly elastic until the stresses reached the extraordinary amplitude of 800 MPa. Figure 2(b) shows the elastic limit (the maximum design stress) for both film thicknesses as a function of strain rate. The rate sensitivity factor, which is closely related to the dominant deformation mechanism, changes drastically between 10^{-5} and 10^{-6} s^{-1}, indicating enhanced creep at these (or below) rates. Therefore, it is expected that even nanocrystalline Au films will be subjected to creep at extended loading times (as expected for Au.)



(a) **(b)** **(c)**

Figure 2. (a) Key material properties as a function of loading/actuation rate for 1,760 nm Au films. **(b)** Elastic limit vs. strain rate for two device thicknesses. The change in slope (rate sensitivity) at 10^{-5} s^{-1} denotes strong creep at slower loading (switching) rates. **(c)** Multi-stage creep tests for 1.76 um Au films.

High resolution imaging revealed key differences in the mechanism of damage initiation/accumulation in Au at different loading/actuation rates. At slow strain rates, there was extensive plasticity and failure was characterized by void formation throughout the cross-section as well the top film surface. However, at higher strain rates, failure was also due to shear localization but void formation was concentrated only around the center of the cross-section pointing to a three-dimensional state of stress in the films, which is contrary to the approach of plane stress that is usually applied to thin film structures. In the reporting period we also developed a microscale testing apparatus for creep experiments with MEMS scale samples. We showed that the Au films suffered from extended primary creep that lasts 2-5 hours, Figure 2(c), followed by clear steady state creep. This last outcome is key in the development of Au RF-MEMS as it points out to the vital importance of fully quantifying and modeling the effect of creep so that this time dependent material response is integrated in device models to predict the evolution of device response over long periods of time and under complex loading profiles.



(a) (b) (c)

Figure 3. (a) MEMS beam deflected largely under the bending; (b) Nonlinear variation of maximum stress and deflection of free end for a large deflected beam; (c) Nonlinear variation of maximum stress and deflection of free end for a beam having elastic - perfectly plastic behavior.

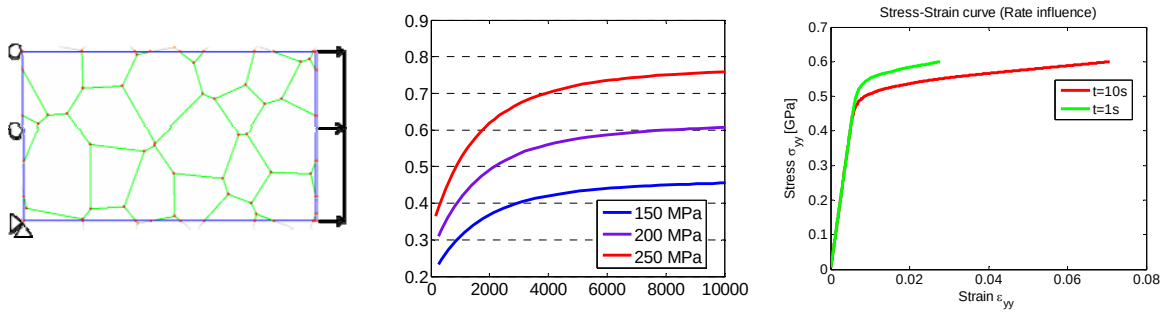
<u>Stochastic Grain-Scale Fatigue Modeling of Large-Displacement MEMS Devices</u>

At Purdue, under the supervision of Professor Farshid Sadeghi, a damage mechanics based fatigue model was developed to study the process of fatigue crack initiation and propagation in MEMS devices. Considering the high aspect ratios of MEMS cantilever beams and their low-flaw material structure, they can deliver very large deflections under bending loading with small stresses. This feature has been introduced successfully to the model employing a nonlinear elastic large deflection analysis added to the model. For this purpose, we simulated the Au cantilever beams with the length of 200 mm and thickness of 1 mm under the bending loading. Figure 3(a) shows the deflected beam under the loading and Figure 3(b) shows the nonlinear variation of maximum stress and the deflection of the beam free end with increasing the load value. On the other hand, it has been tried to apply the elastic - plastic constitutive relations to the model.

Up to this point, elastic - perfectly plastic case has been incorporated to the model. Figure 3(c) illustrates the results obtained for a Ti cantilever beam under bending loading. As seen, the maximum stress variation follows the elastic - perfectly plastic behavior provided to the model. Also, maximum deflection of beam free end varies nonlinearly after commence of plasticity in the model. The discrete element fatigue model is being modified to better account for the effects of grain anisotropy and interaction on the local stress field in an effort to develop a higher resolution fatigue life model. The model is being developed in the framework of the combined finite – discrete element method wherein each material grain is being modeled as a deformable discrete element. The grain deformability is being captured through an explicit FEA formulation while the grain interaction is being captured through the existing discrete element contact algorithms.

Multi-scale Modeling of Impact of Grannular Microstructure on MEMS Mechanical Response

The structural response of MEMS devices is often affected by the granular microstructure of the material.



(a) (b) (c)

Figure 4. (a) Geometry and boundary condition for a small ensemble of grains used to simulate creep and tensile tests; (b) Comparison between numerical and experimental results for the tensile test over 5 decades of imposed strain rate; (c) Materials properties as a function of the applied strain rate, showing the competition between the two damage mechanisms.

This is particularly true for NEMS and for micron-size features of MEMS devices (such as notches and anchors) with dimensions of the order of grain sizes. Professor Geubelle's group at the University of Illinois is pursing the development and implementation of a multi-scale numerical tool based on the finite element method to extract the effect of the granular microstructure on the constitutive and failure response of MEMS materials. The structural response of MEMS devices is often affected by the granular microstructure of the material, especially in the vicinity of micron-sized features (notches, anchors, steps, etc.) with dimensions on the order of grain sizes. The key objective of this project is to develop and implement a multi-scale numerical tool based on the finite element method to extract the effect of the granular microstructure on the constitutive and damage response of thin film metallic materials used in MEMS. Over the last three months, we have implemented and validated a multi-scale finite element model able to capture the competition between inelastic processes that can occur along grain boundaries and in the grain interior. The inter-granular processes are modeled by cohesive (interfacial) elements that account for diffusion-mediated sliding between grains and rate-dependent grain boundary opening. The intra-granular behavior is captured by a rate-dependent single crystal plasticity model that models the evolution of the various slip systems present in each grain. Figure 4(a) shows the geometric model used to simulate the creep and tensile response of a multi-grain system by grain boundary opening and sliding. The numerical results for the tensile test are presented on Figure 4(b) together with the experimental results obtained by I. Chasiotis at the University of Illinois. Figure 4(c) shows the materials properties as a function of the applied strain rate. In this figure it is possible to see the predictive capability of the numerical method (blue line) by showing the drop on the on the elastic limit for small values of the applied strain rate.

II. Electrostatic Domain Characterization and Modeling

Our electrostatic characterization and modeling activities emphasize the advancement of more accurate models for the quantitative description of dielectric charging in RF MEMS capacitive switches. The following are highlights from research activities and findings during Q2 2008.

Impact of humidity on surface dielectric charging

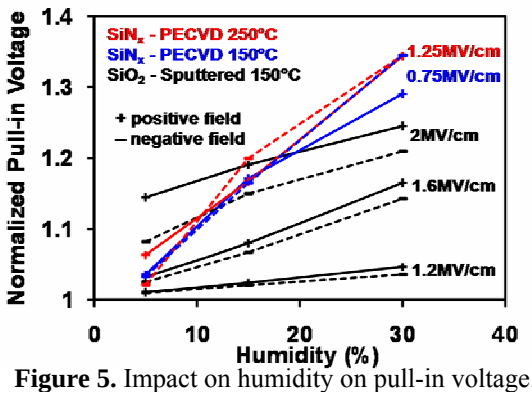


Figure 5. Impact on humidity on pull-in voltage.

Humidity has long been suspected to strongly influence dielectric charging and adhesion failure of RF MEMS capacitive switches. We now report the first systematic study of such humidity effect. The figure on the left illustrates the experimentally measured shift in pull-in voltage, which is directly proportional to the charge in the dielectric, after charging different dielectrics under different humidity levels and different fields for 25 min. In all cases, the magnitude of pull-in voltage increases, indicating charge built up on the surface instead of in the bulk of the dielectric. As expected, this surface charge increases exponentially with increasing field, whether positive or negative. Under comparable fields, SiO_2 appears to be more resistant to surface charging than SiN_x, probably because SiO_2 is hydrophobic whereas SiN_x is hydrophilic. However, it is not clear why the surface charge increases linearly with increasing humidity. Since surface charging is detrimental to RF MEMS switches, it is imperative that they are packaged in a humidity-free ambient. To this end, different packaging practices are being investigated in detail.

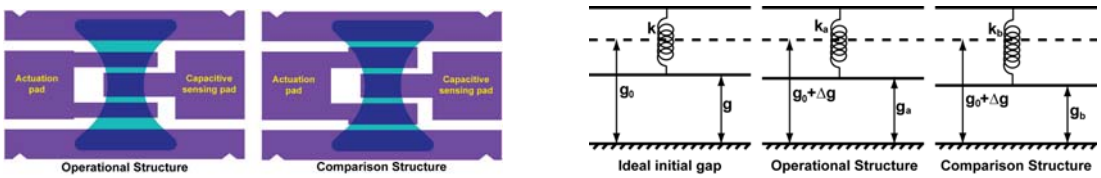
Work also continued in Prof. Papapolymerou's group at Georgia Tech, on the experimental investigation of the dependence of dielectric charging on the thickness of the dielectric layer. Fabricated RF MEMS capacitive switches with silicon nitride as the dielectric deposited at 150°C (thickness of 200 nm) where characterized under different humidity ambient at Lehigh University. Georgia Tech also fabricated nitride capacitive switches and capacitors with a PECVD deposition temperature of 250° C (the same temperature is used by Raytheon who is one of our industrial sponsors) and various thicknesses. These switches are currently being tested in terms of C-V characteristic and transients at various temperatures for extraction of charging parameters.

III. Electro Micro Metrology for In-Situ Process Characterization

Under the direction of Prof. D. Peroulis and Prof. J. Clark at Purdue, we have demonstrated that Electro Micro Metrology (EMM) can be used to quickly and accurately determine planar geometry variations for planar-actuated MEMS structures fabricated on an entire wafer. The measurements are all performed using a chip-based capacitor sensor. Since then, we have verified our measurements using a NIST-recommended Andeen Hagerling AH2700 capacitance bridge meter. We have extended EMM to the characterization of geometry variations, Δw, and pull-in gap variations, Δg, in vertically-actuated MEMS switches. Geometry variation is primarily due to tolerance in photo-lithography mask and during photoresist UV exposure, while pull-in gap variation is due to height variations of spun photoresist. Use is made of two EMM structures to determine these variations (see Fig. 6).

$$\Delta w = \frac{w_{LO}\left[m-(np)\left(\frac{\Delta C_b}{\Delta C_a}\frac{V_{P,b}^2}{V_{P,a}^2}\right)\right]}{(n+p)\left(\frac{\Delta C_b}{\Delta C_a}\frac{V_{P,b}^2}{V_{P,a}^2}\right)-(m+1)}, \quad \Delta g = \sqrt{\frac{\Delta V_{a,b}^2 \Delta C_{a,b}}{2k_b'\left(\frac{V_a^2 \Delta C_b k_b' A_a}{V_b^2 \Delta C_a k_a' A_b} - 2\frac{V_a}{V_b}\sqrt{\frac{\Delta C_b k_b' A_a}{\Delta C_a k_a' A_b}}+1\right)}} - g_0 \qquad (1)$$

The equations above make use of measurable parameters for the characterization of these variations. w_{LO} is the layout width; m, n, and p are layout dimension ratios; ΔC is the measured capacitance difference; V_P is the pull-in voltage; $\Delta V_{a,b}$ is the matching voltage between structures, $\Delta C_{a,b}$ is the capacitance difference between structures, and k_b is the spring constant of the comparison structure. Our next steps involve fabrication of the appropriated structures followed by measurements to verify the applicability of the above expressions to vertically-actuated MEMS structures. MEMS structures fabricated at Purdue University, Georgia Tech, MEMtronics, and Raytheon will be used for this purpose.



(a) (b)

Figure 6. (a) Design layout of two vertically-actuated MEMS switches. The structures differ by the actuation pad area, resulting in different responses when subjected to the same bias condition. (b) Simple spring diagram showing the separation gap difference, Δg, (see Equation (1)) that is being determined using EMM.

V. Computational Framework for Stochastic Multi-Physics Modeling

Research continued at the University of Illinois toward the advancement of modeling methodologies and computer algorithms for enhancing the accuracy and computational efficiency of performance degradation-driven, fully-coupled, electro-mechanical, stochastic modeling of electrostatically-actuated MEMS accounting for uncertainties in geometric/material properties and loading conditions. The following offers highlights of our accomplishments in this area over the past three months.

Stochastic, Coupled Electro-Mechanical Modeling

Under the leadership of Prof. N. Aluru, progress was made on two aspects in uncertainty quantification. First, we were able to compute the sensitivities of peak deflection in MEMS switches for uncertainties in material properties and gaps. We were able to show that uncertainties in gap can have a more significant influence on peak displacement and pull-in voltage of a MEMS switch compared to uncertainties in Young's modulus. Second, MEMS switches exhibit well-known instability known as electrostatic pull-in. The treatment of electrostatic pull-in in uncertainty quantification methods requires special treatment. We have developed a preliminary implementation of uncertainty quantification method to deal with electrostatic pull-in instability.

Fast Coupled Electro-Mechanical Finite Element Modeling of Electrostatically-Actuated MEMS

Under the direction of Prof. Aluru and Prof. Cangellaris work continued on enhancing the accuracy of the methodology we reported in our 2008 Q1 report for expediting the coupled electro-mechanical finite element modeling of electrostatically-actuated MEMS [3]. The new methodology eliminates the need for repeated finite element meshing and subsequent electrostatic modeling of the device during mechanical deformation. The accuracy of the enhanced approach was assessed through comparisons with finite element solution obtained using ANSYS. In all cases tested, better than 3% accuracy was observed.

Computational Framework for Thermal Transport Modeling at the Meso- and Nano-scale

Under the leadership of Prof. Jayathi Murthy, work continued at Purdue University on: (i) the development and completion of the numerical framework for solving the coupled gas-phonon thermal transport problem; (ii) the completion of the atomistic Green's function approach (AGF) for evaluating the thermal resistance of rough interfaces between phononic materials; (iii) commencement of efforts to couple mesoscale modeling of thermal transport in semiconductors and dielectrics with interface thermal resistance models obtained either from wave-packet molecular dynamics or atomistic Green's function approaches. Mesoscale modeling has been done using the particle Boltzmann transport equation (BTE), both for the gas and phonons, the former with the Ellipsoidal-Statistical (ES-BGK) framework. We have applied our models to a variety of canonical interface problems including (i) mesoscale planar interfaces between a rarefied gas (ii) gas-wire contact with constrictions, (iii) thermal transpiration flow, and (iv) phonon-phonon transport across composite interfaces. It has been found that the on scales comparable to the gas phase mean free path (~100-200 nm), the gas resistance becomes the main bottleneck to transport I the configurations considered, despite significant confinement effects in the solid. Values for the interface gas-solid resistance have been computed across the range of gas and solid Knudsen numbers, which can be used for MEMS design. Furthermore, our AGF results show that for randomly rough interfaces, the main phenomenon causing an increase in interface resistance is the destructive interference of waves; in the presence of regular interface roughness patterns, we have found that resonance effects can even decrease or saturate thermal resistance.

Modeling of Coupled Electro-Thermal Transport Between Metal Electrodes in RF MEMS Switches

Work continued under the direction of Prof. Ravaioli on the application of percolation theory to the quantitative modeling of electro-thermal transport between the electrodes in metal-to-metal contact switches. Electro-thermal effects between electrodes of RF Metal Switches have a considerable importance in the process of oxidation and erosion of metal surfaces leading to variations of the contact resistance or complete failure of the device. With this respect, our stochastic model was further enhanced to take into account the situation of contacting metal electrodes during the ON-state of a contacting device. In this scope, we created a computationally efficient predictive model of the contact resistance based on a digital reproduction of a rough metal surface based on experimentally observable parameters (Fig. 7.a and 7.b). The emphasis has been put on the ease of integration of the latter model in CAD tools of our partner companies. Additionally, our multi-scale predictive model of cavity discharges has been integrated in a highly adaptable, time efficient, and user friendly framework, offering the possibility to be deployed on the internet (Fig.7.c.). In this way, other researchers can benefit from the use our percolation based MEMS discharge simulation tool to design their devices and contribute to model refinement. Our stochastic models of electro-thermal transport between contacting and non contacting metal electrodes showed good performance in predicting physically consistent results on the statistical device lifetime, and are now ready to be validated against experimental work. Theoretical investigation of the statistical properties of discharges will be conducted in order to get a stronger understanding of the processes leading to surface erosion and oxidation.

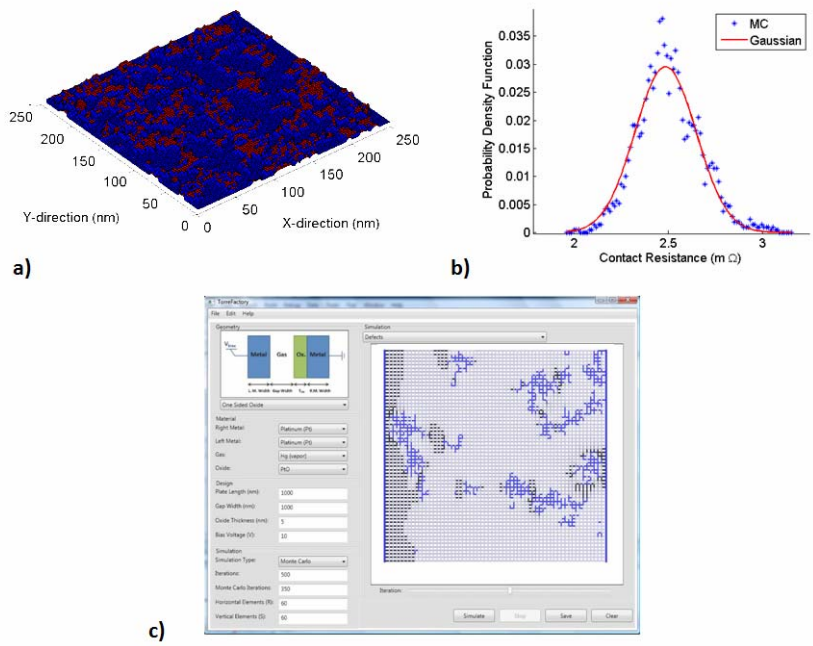


Figure 7. a) Digital model of a rough gold surface. b) Simulated statistical distribution of the device contact resistance based on the stochastic digital model. c) Snapshot of TorreFactory, the percolation based, device lifetime prediction framework.

Publications & Conference Presentations

[1] C. Palego, S. Hadler, B. Baloglu, Z. Peng, J.C.M. Hwang, H. F. Nied, D.I. Forehand, C.L. Goldsmith, "Microwave intermodulation technique for monitoring the mechanical stress in RF MEMS capacitive switches," Proc. 2008 IEEE International Microwave Symposium, pp. 29-32, Atlanta, GA, June 2008.

[2] R. Daigler, G. Papaioannou, E. Papandreou and J. Papapolymerou, "Effect of Dielectric Film Thickness on Dielectric Charging of RF MEMS Capacitive Switches," Proc. 2008 IEEE International Microwave Symposium, pp. 1275-1278, Atlanta, GA, June 2008.

[3] L. Sun and J.Y. Murthy, "Molecular Dynamics Simulation of Phonon Scattering At Rough Semiconductor Interfaces," Proc. I-Therm 2008, Orlando, Florida, May 2008.