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Summary of Research Progress

I. Mechanical Domain Characterization and Modeling

Our mechanical characterization and modeling activities emphasize the experimental investigation of 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 Q1 of 2008.

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

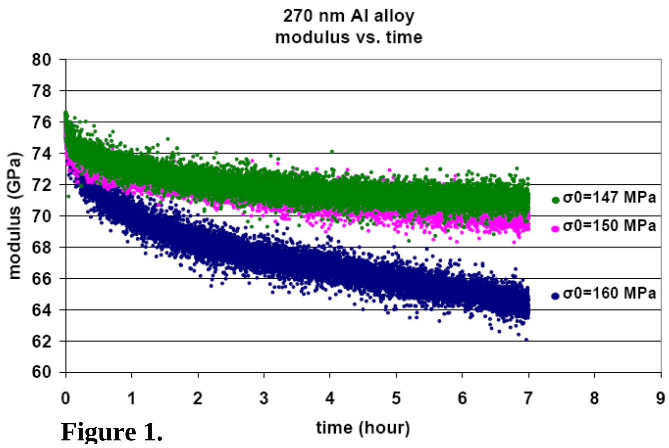


Figure 1.

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. We have begun testing the stress relaxation behavior of Al alloy films using the same gas pressure bulge tool and analysis methods we developed for testing Au films. Al alloy membranes with a thickness of 270 nm were fabricated and characterized. Three successive strain step experiments were carried out. Each consisted of the rapid application of a strain at the level of 1.2×10^{-3} followed by seven-hour stress relaxations at that constant strain state. From the results, the change of the film's effective modulus was calculated as shown in the figure above. The blue curve is the result of the first experiment, followed by the pink and then the green. We found that the residual stress in the film decreased after each stage of the experiment and the time dependence of the effective modulus was strongly dependent on the residual stress in the film. This was also true for the 1.2 um thick Au membrane film we tested earlier. This behavior indicates the existence of both viscoplasticity and viscoelasticity (a.k.a., anelasticity). However, the plasticity contribution to the relaxation was exhausted in fewer strain cycles in the Al alloy film than in the Au film. Moreover, we also found that the anelasticity in this Al alloy film is linear (i.e., independent of strain), which means that the simulation approach developed for pure Au films should work equally well for Al alloy films.

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

In parallel to the above mechanical characterization activity, Professor Ioannis Chasiotis' group at the University of Illinois, with the support by Prof. Peroulis group at Purdue, has investigated the mechanical response of Au films with three different thicknesses: 0.5 µm, 0.83 µm and 1.76 µm, over strain rates ranging from 10^{-1} s^{-1} to 10^{-6} s^{-1}, see Figure 2(a). X-ray diffraction revealed that all film thicknesses had strong <111> texture and 40 nm average grain size. Thus, differences in the mechanical response of films with different thickness are owed to the film thickness and not the grain size. As expected, the elastic modulus for the two thicker films was loading rate-independent with an average value of E= 69.1±2.1 GPa, which is 15% smaller than the modulus of bulk Au, E=78 GPa. The yield strength, elastic limit (the maximum stress the film can be used before it the onset of irreversible deformation), Figure 2(b), and ultimate strength, however, increased monotonically with increasing strain rate, while the ultimate failure strain monotonically decreased, Figure 2(c). It is noticeable that the ductility of 0.83-µm films suddenly increased to 5.8-7.0% at 10^{-5} s^{-1}, Figure 2(a). This indicates that at rates slower or equal to 10^{-5} s^{-1} (i.e. the film remains loaded for minutes) the material creep becomes very important. The mechanism responsible for increased ductility in 0.83-µm films was observed at a rate (10^{-5} s^{-1}) that was one order of magnitude faster than the rate (10^{-6} s^{-1}) at which 1.76-µm thick films demonstrated similar behavior. ***Thus, thicker Au films would be less prone to creep.*** However, ***the mechanical response of 0.5-µm films was not consistent with that of the thicker films***. The 0.5-µm Au films had significantly lower elastic modulus, E= 53 GPa. Irrespective of the reduced modulus, the thinnest specimens demonstrated significant rate sensitivity also.

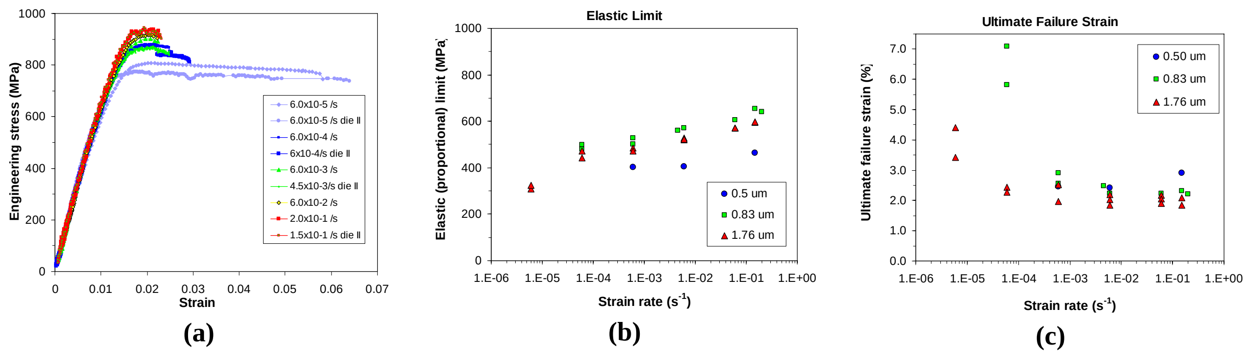


Figure 2. (a) The stress-strain curves for 0.83 μm Au films, **(b)** elastic limit for films with three thicknesses and **(c)** failure strain for films with different thickness as a function of strain rate. The trends for yield stress and ultimate strength for different thicknesses are similar to those for the elastic limit.

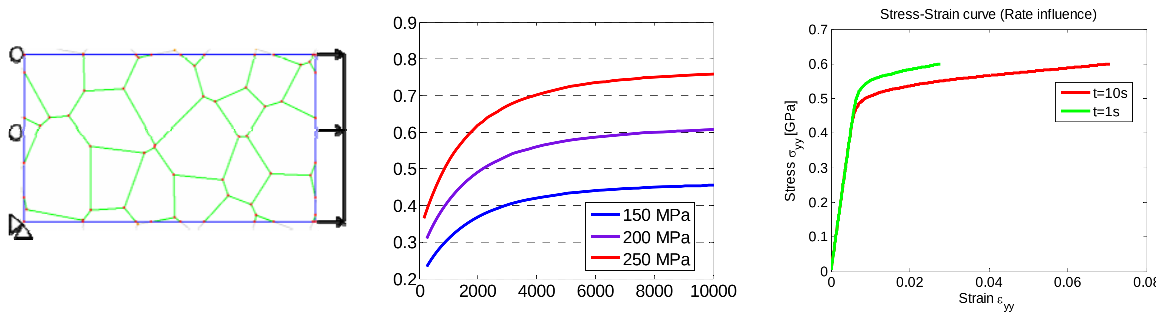
Our rate dependence studies point to the need for better understanding of the creep behavior of Au films. Further experiments at strains 1 - 10 s^{-1} are now conducted to complete the investigation at strain rates that are relevant to RF- MEMS operating over a broad range of frequencies. Subsequently, our efforts would be focused in experimental creep studies on Au films. A more detailed discussion of these findings is provided in Reference [1].

Stochastic Grain-Scale Fatigue Modeling of Large-Displacement MEMS Devices

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. The model takes into account the gradual material degradation that occurs under cyclic loading through an empirical damage evolution equation whose parameters are determined from fatigue testing of MEMS materials. The most salient features of the model include: a) the ability to predict the MEMS fatigue life over many hundreds of billions of cycles based on experimental data collected from a few million cycles; b) the ability to account for the statistical variation of material properties; and c) the ability to account for material flaws resulting from non-perfect fabrication techniques. The model was applied to a dog-bone shaped tensile specimen to investigate the effects of material heterogeneity and flaws on fatigue life. Allowing for variability of material elastic and damage properties was found to lead to a similar increase in scatter and reduction in fatigue life. Much larger reductions in life and increases in scatter occurred when initial material flaws were considered. The most detrimental conditions occurred when an initial surface void was present. The results of this work were submitted to the *Journal of Microelectromechanical Systems* for review for publication (see Reference [2]).

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

The structural response of MEMS devices is often affected by the granular microstructure of the material. 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. More specifically, the project is focused on creep response of nano-crystalline metallic films. Over the last three months, finite element models have been developed to capture the competition between inelastic processes that can occur along grain boundaries and in the grain interior. The intergranular 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 3(a) shows the geometric model used to simulate the creep response of a multigrain system by grain boundary opening and sliding. The resulting creep curves obtained for different stress levels are presented on Figure 3(b). Figure 3(c) shows the stress strain-strain curve of a single crystal subject to loads applied at different strain rates. As is apparent in Fig. 3(b) and 3(c), the implemented models are able to capture the key time- and rate-dependent phenomena of interest. A multi-scale finite element model that includes both models is under development.



(a) (b) (c)

Figure 3. (a) Geometry and boundary condition for a small ensemble of grains used to simulate creep tests; (b) Computed creep strain-time curves at different load levels; (c) Stress-strain curves for a single crystal subjected to different load rates.

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 Q1 2008.

Dependence of Dielectric Charging on Applied Electric Field

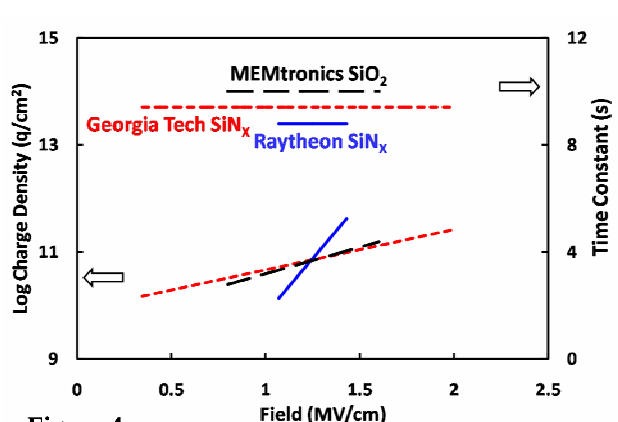


Figure 4.

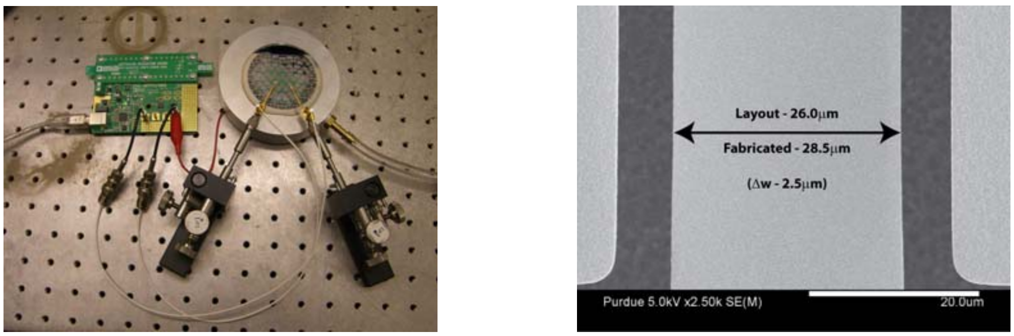
Work continued in Prof. James Hwang's group on the investigation of the dependence of dielectric charging on applied electric field. The same methodology of quantifying dielectric charging previously applied to MEMtronics and Georgia Tech devices has been extended to Raytheon devices, which contain 280-nm silicon-nitride dielectric formed by plasma-enhanced chemical vapor deposition. As shown in the figure on the left, transient currents measured on metal-insulator-metal (MIM) capacitors yielded comparable charge densities and time constants as that of MEMtronics and Georgia Tech devices, except that the charge density of Raytheon devices appears to have a stronger field dependence. More samples will be characterized to confirm the field dependence and to extend the field range. Packaged and unpackaged Raytheon switches are also being characterized under different ambient to determine whether they suffer from charging of the surface or the bulk of the dielectric, and in the latter case, correlate their charging tendency with that of the MIM capacitors.

Experimental Investigation of Dielectric Layer Thickness on Dielectric Charging

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. The characterization included a variety of capacitive RF MEMS switches and MIM capacitors fabricated at Georgia Tech, as well as RF MEMS switches obtained from Raytheon and MEMtronics. An Appendix to this report, attached as a PDF document, discusses further preliminary results from this investigation. For the Georgia Tech switches and MIM capacitors the dielectric material used was Si_xN_y while the electrode was Au. In both cases an increase of dielectric charging with dielectric layer thickness was observed. In the next quarter emphasis will be placed on correlating measured C-V data with specific nitride deposition conditions.

III. Test Devices for In-Situ Process Characterization

Under the direction of Prof. D. Peroulis and Prof. J. Clark at Purdue, the first experimental results were demonstrated of a new process, called *Electro-Micro Metrology* (EMM) for quantifying process variations related to material and geometrical properties. This newly proposed EMM Measurement Protocol (EMM MP) measures changes in capacitance of electro-actuated comb structures. The fabrication of MEMS test structure for EMM MP is a two-mask process. A wafer is first oxidized and patterned. A 25-μm thick photoresist mold is then applied and patterned so a 20-μm thick Nickel-plated MEMS structure can be formed. The structure is then released by etching the silicon substrate below it with XeF_2 gas. The setup consists of an Agilent 6645A (170V) power supply for electrostatic actuation and an Analog Devices AD7746 low-capacitance evaluation IC. The AD7746 has a 4fF to 21pF range with 32aF resolution.



(a) (b)

Figure 5. a) A typical low-capacitance measurement setup using the Analog Devices AD7746 without EMI shielding. b) Scanning electro beam microscope image of a comb finger. Optical inspection method was used to measure the geometry change so as to verify the integrity of EMM capacitive measurement.

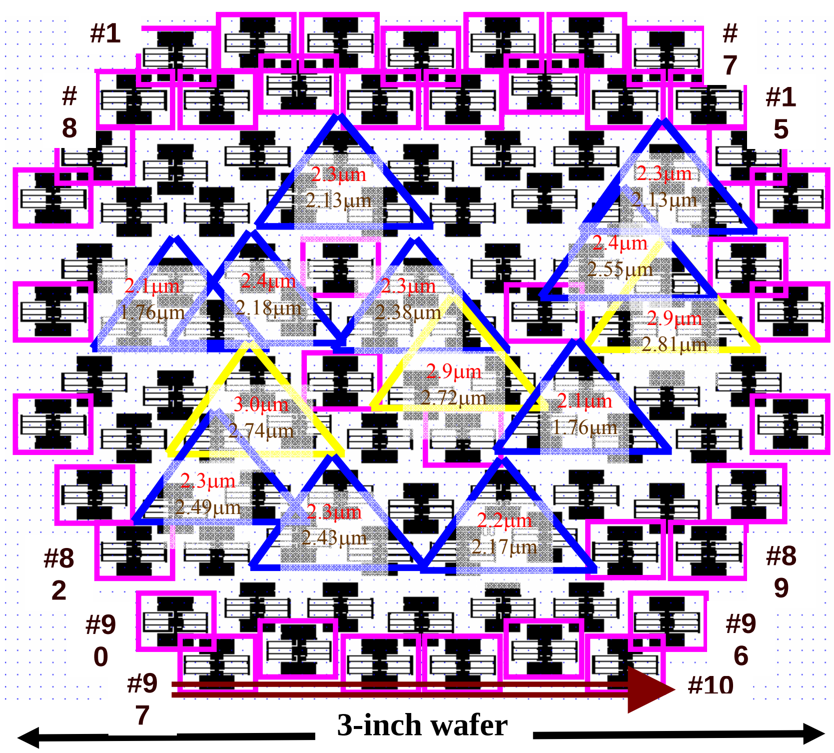


Figure 6. Map of 3-inch wafer showing the groups of test structures measured for geometry change. Red text shows the geometry change measured using scanning electron beam microscope. Brown text shows geometry change measured using EMM MP.

A minimum of two EMM structures are required to determine geometry and material properties. The difference between the EMM structures is the width of the spring arms. All other dimensions are kept the same. The fabricated structures were first optically inspected using a scanning beam microscope. Geometrical variations of the spring arm width were between 1-3 μm; with the SEM having 10% uncertainty (this will further improved with higher resolution images in our next run). Low-capacitance measurements on the same structures show between 1-3 μm change. Current capacitance measured is in the tens of fF and uncertainty is less than 10 fF. The measured uncertainty is high due to the lack of appropriate EMI shielding. Figure 5a shows the spatial layout of the arrays of test structures on a three-inch wafer and the comparison of geometry change between optical and electro measurement. Figure 5b shows a typical SEM image, while Figure 6 presents an overview of the collected results. In the next quarter we will further improve the quality of EMM measurements and focus on extending the EMM technique to capturing material properties variations.

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

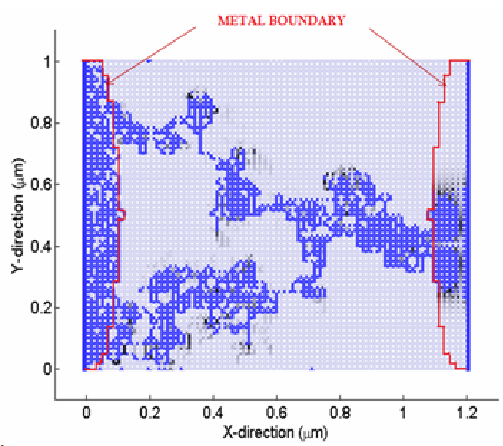
Under the leadership of Prof. N. Aluru, the stochastic electrostatic code was coupled with the stochastic mechanics code based on generalized polynomial chaos (GPC), to handle uncertain coupled electromechanical interaction, arising from variations in material properties and geometrical parameters such as gap between the microstructures, applicable to the static analysis of electrostatic MEMS. The stochastic framework comprises of two components – a stochastic mechanical analysis, which quantifies the uncertainty associated with the deformation of MEM structures due to the variations in material properties and/or applied traction, and a stochastic electrostatic analysis to quantify the uncertainty in the electrostatic pressure due to variations in geometrical parameters or uncertain deformation of the conductors. The stochastic analysis is based on a stochastic Lagrangian approach, where, in addition to uncertain input parameters and unknown field variables, the random deformed configuration is expanded in terms of GPC basis functions. The spectral modes for the unknown field variables are finally obtained using Galerkin projection in the space spanned by GPC basis functions. The stochastic mechanical and electrostatic analyses are performed in a self-consistent manner to obtain the random deformation of the MEM structures. Various numerical examples are presented to study the effect of uncertain parameters on performance of various MEMS devices. The results, obtained using the newly developed method, were verified using rigorous Monte Carlo simulations. It was shown that the proposed method accurately predicts the statistics and probability density functions of various relevant parameters at a computational cost two orders of magnitude smaller than that of Monte Carlo.

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

Under the direction of Prof. Aluru and Prof. Cangellaris a methodology was developed and demonstrated 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. This is achieved by defining an auxiliary boundary value problem that involves the device geometry in the absence of actuation with modified boundary conditions for the electrostatic potential. The modification in the boundary conditions is such that the solution of the auxiliary problem for the electrostatic pressure on the movable electrode matches closely the one obtained from the solution for the electrostatic potential in the deformed geometry during actuation. The proposed methodology was demonstrated through its application to the modeling of four MEMS devices with varying length-to-gap ratios, multiple dielectrics and complicated geometries. The accuracy of the proposed methodology was confirmed through comparisons of its results with results obtained using both analytical solutions and finite element solutions obtained using ANSYS.

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. Electrical discharges between electrodes of RF metal-to-metal contact switches have a considerable importance in the process of oxidation and erosion of metal surfaces leading to modification of the contact resistance or complete failure of the device. It has been further suggested that the discharge process may be used in order to repair highly oxidized surfaces. Our former multi-scale predictive model of cavity discharges has been extended to account for coupled local thermal and electrical transport in both the metal electrodes and the gas. Stochastic approximations have been connected to elements of discharge physics. Additionally, non linearity of the surface has been included in the model. With this respect, the current approach, based on percolation theory, is used to predict the statistical time to discharge when a static bias is applied between electrodes (Fig 7.a). Results appear physically consistent and reflect high local temperatures at the cathode-gas interface capable of vaporizing the metal in the gas (Fig. 7.b). As a consequence, the simulation may be used to engineer the electrode shape, material, and the constituents of the gas in order to achieve optimal time to breakdown for a given bias. In this scope, results are expected to be tested against experimental work reported in the literature in the near future. Further theoretical investigation of the statistical properties of the discharge will also be conducted in order to get a stronger understanding of the processes leading to surface erosion and oxidation.



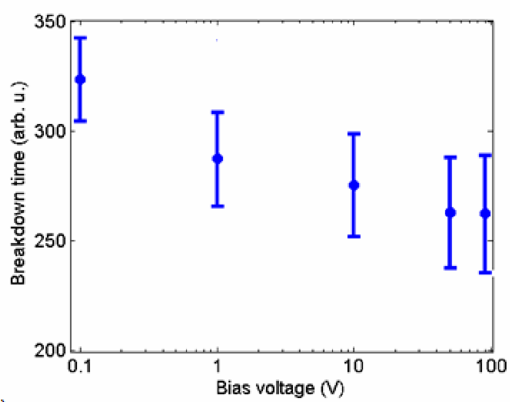


Figure 7. a) Appearance of high local current (blue elements) between 1μm non-linear metal plates under a static 1V applied bias. b) Simulated statistical distribution of the device failure time under increasing bias.

Patents

None

Publications & Conference Presentations

[1] N. Karanjgaokar at al, “Mechanical behavior of nanocrystalline Au films as a function of strain rate and film thickness,” *Proc. of the Society for Experimental Mechanics (SEM) XI International Congress & Exposition on Experimental and Applied Mechanics Conference Theme: Experimental Mechanics Applied to Damage: Detection, Analysis and Mitigation*, Rosen Plaza Hotel, Orlando, Florida USA, June 2 - 5, 2008. (**PDF attached to this report**)

[2] T. Slack, F. Sadeghi, D. Peroulis, “A discrete damage mechanics models for fatigue of MEMS devices,” *Journal of Microelectromechanical Systems*, under review. (**PDF attached to this report**)

[3] P. S. Sumant, N. R. Aluru, and A. C. Cangellaris, “A Methodology for Fast Finite Element Modeling of Electrostatically-Actuated MEMS,” *Int. J. Numerical Methods in Engineering*, accepted for publication. (**PDF attached to this report**)

Appendix

J. Papapolymerou, Investigation of Dependence of Dielectric Charging on Thickness of Dielectric Layer. (**PDF attached to this report**)