IMPACT - Center for Advancement of MEMS/NEMS VLSI

2007 Q1 Quarterly R&D Status Report

Prepared by:

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Executive Summary

The Year 1 objectives of the research activities in the Center include: a) The experimental investigation and characterization of the individual physical domains (electrical, thermal and mechanical) that govern the functionality of the MEMS devices under consideration in the Center; b) The development of the computational framework for the stochastic, fully-coupled, multi-domain physics modeling of MEMS devices. Toward these objectives, our 2007 Q1 activities and accomplishments included:

Mechanical Domain Characterization and Modeling

- The design, fabrication, and preliminary characterization of the first set of test structures used for the experimental characterization of the mechanical properties and behavior of the metallic membranes used in capacitive RF MEMS switches.
- The design, fabrication, and preliminary characterization of a set of samples used for stress-strain characterization for large-displacement bimorph actuators.
- The development of finite element models that incorporate the constitutive behavior obtained from mechanical measurements to demonstrate the effects of viscoelasticity on membrane response during pull-down and release.
- The development and implementation of the tools needed to discretize actual micrographs of the MEMS material, accounting for the presence of micro-structural features, in order create realistic representative volume elements (RVE). Subsequent, multi-scale modeling of the RVE will provide for the quantitative, description of the elasto-plastic response of the material.
- Preliminary demonstration of the application of the Discrete Element Method (DEM) that accounts for the discontinuities introduced by micro-structural features in the prediction of the mechanical behavior of the material under loading.

Electrostatic Domain Characterization and Modeling

- A set of test structures, including both switches and MIM capacitors of various sizes and geometries, were designed and fabricated for the purposes of this experimental investigation of dielectric charging. Characterization of the MIM capacitors commenced at Lehigh.

- A switch capacitance model was developed at Memtronics that accounts for the surface roughness of the dielectric. This model is important in understanding the actual "active" area of the MEMS switch that is subject to dielectric charging.
- An electro-quasi-static model was developed to serve as a unifying modeling framework for the incorporation in the multi-physics modeling of RF-MEMS switches of the various physical attributes and processes known to impact dielectric charging.

Thermal Domain Characterization and Modeling

- Test structures were designed and fabricated for the characterization of the thermal properties of thin film Au and SiO_2 films.
- A general purpose computational framework has been established for solving phonon and electron transport at both continuum and sub-continuum scales. Results obtained from the hierarchy of models supported in this framework are compared with measured data to identify the level of detail needed for thermal modeling of MEMS devices as a function of material properties and feature size.

Computational Framework for Stochastic Multi-Physics Modeling

- A general framework was developed and demonstrated through preliminary numerical studies for the quantification of the impact of uncertainty in geometric parameters on the electrostatic behavior of the MEMS device.
- Layout and masks were produced necessary for the first generation of the process characterization test structures which will be used to extract statistical description of process-induced uncertainty on geometric and material parameters.

These accomplishments are discussed in more detail in the next section.

During Q1 2007 we completed the formation of our Center's Scientific Advisory Board (SAB). Our SAB members are:

- John (Jack) Ebel — Air Force Research Lab
- Anantha Krishnan — Lawrence Livermore Lab
- Art Morris — wiSpry, Inc.
- Chris Nordquist — Sandia National Lab
- Dev Palmer — Army Research Office
- Barry Perlman — US Army RDECOM
- Daniel Powell — NASA

Finally, on April 20 our Spring Industrial Affiliates meeting was held at Georgia Tech. A number of the Center's SAB members participated in the meeting. William Snowden and Chris Ma were the DARPA representatives attending the meeting. During the meeting our Center's activities to date were presented. Feedback was provided by our industrial affiliates and SAB members on several issues including a) critical assessment of the research focus and direction in the Center; b) ways in which to strengthen our collaboration with our industry members; c) ways in which our industry partners can help us with the recruitment of MEMS CAD tool developers in the Center.

Mechanical Domain Characterization and Modeling

Our mechanical characterization 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. Our research activities in this area involve complementary tasks at Lehigh (Vinci, Neid, Brown), Georgia Tech (Papapolymerou), Memtronics (Goldsmith), Purdue University (Peroulis, Sadeghi), and the University of Illinois (Chasiotis, Geubelle).

During Q1 of 2007 a set of test structures were designed at Georgia Tech and Lehigh for the characterization of the mechanical behavior of the RF MEMS switch membranes. For the mechanical characterization, rectangular windows with a size of 12mm×2mm were designed on top of a silicon wafer (see Fig. 1). These windows are etched from the back in order to allow access to the pressure tool at Lehigh University that will perform the mechanical testing. Metal is deposited on the front side on top of a very thin nitride membrane that serves as an etch mask and stop layer for the silicon etching. Initial fabrication runs were done at Georgia Tech with gold evaporated metal.

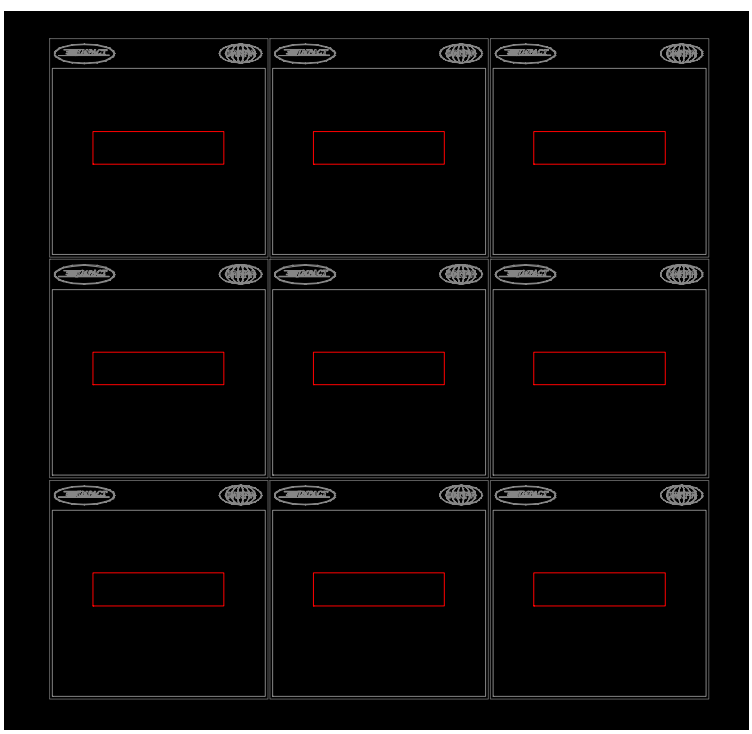

Figure 1: Mask for mechanical testing of the metallic switch membrane.

A unique Bulge Testing tool at Lehigh has been modified to enable high resolution thin film stress relaxation measurements (i.e., stress changes over time at constant strain). Using the mechanical test structures, preliminary room temperature measurements of

Lehigh gold/silicone nitride membranes have been carried out and the results have been put in a mathematical form suitable for use in Finite Element Modeling. We have demonstrated that pure gold films approximately 0.5 μm thick display linear viscoelastic behavior at small strains. This behavior is characterized by rapid stress relaxation over a period of seconds followed by continuing relaxation over at least 11 hours. This relaxation represents a reduction in the restoring force available to open a switch when the actuating voltage is switched off.

In parallel, for the purpose of stress-strain characterization for large-displacement bimorph actuators, a micro-tension apparatus was developed by Chasiotis' group at the University of Illinois that allows for mechanical testing at strain rates (loading rates) in the range of 10^{-6} s^{-1} and 10^{1} s^{-1}. The method, based on high-speed optical microscopy and digital image correlation, provides the material response between dead-load conditions to those loading rates encountered during fast MEMS switching. The first experiments were conducted in the strain rate range of 10^{-6} - 10^{-3} s^{-1} by using Pt MEMS-scale specimens 400 nm in thickness and 100 microns in width. These Pt specimens were fabricated at ARL. The elastic modulus and Poisson's ratio were found to be very close to those of bulk and as expected they were independent of the rate of loading. However, the strength of these thin films was significantly larger than bulk and dependent on the rate of loading. An important outcome was the realization that the elastic behavior of the Pt films was controlled by the strain rate. The elastic limit (when deviation from the elastic behavior occurs) was found to decrease by 10% for a decrease in the strain rate by one order of magnitude. Thus, the elastic response of Pt extended to 1,000 MPa stress at 10^{-3} s^{-1} strain rate but it decreased to below 700 MPa at 10^{-6} s^{-1} strain rate. This rate sensitive behavior is controlled by material creep and it is expected to be more pronounced in Au films whose mechanical response is a long-term objective of the experimental component of this project. Thus, depending on the stress amplitude, the application of constant forces on metallic MEMS may lead to issues of long-term stability. Experiments at faster strain rates and the mechanical behavior of Au films of various thicknesses fabricated by Prof. D. Peroulis at Purdue University will be explored in the next months.

In parallel to these experimental activities, modeling activities at Lehigh, Purdue and University of Illinois focused on the pursuit of enhanced methodologies and models for the mechanical domain that include the new knowledge about material parameters contributed by our experimental investigation.

At Lehigh University, finite element meshes have been created for a simple, test-structure geometry and for several realistic switch geometries. Constitutive behavior from mechanical measurements has been used in combination with the simple 3-D structure mesh to demonstrate the effects of viscoelasticity on membrane response during pull-down and release. Furthermore, linear elasticity has been applied to the meshes of six realistic switch geometries to determine the following properties: static displacements; the minimum force determined to keep a switch in the ON (i.e., deflected) position; Von-Mises Stress for different switch shapes; modal analysis; natural frequencies; the first four fundamental mode shapes; and dynamic oscillatory behavior upon sudden release of a switch.

Toward the investigation and modeling of deflection, fatigue, and fracture of large displacement MEMS actuators the modeling groups at the University of Illinois (Geubelle) and Purdue (Sadeghi) have been devising new ways in which micro-structural features, such as grain boundaries, can be taken into account in such modeling. This capability becomes essential as MEMS/NEMS device feature sizes shrink down to the sub-micron regime.

The emphasis at the University of Illinois is on the development and demonstration of a multi-scale modeling capability that will provide for a probabilistic model for the mechanical properties at the material level. Such a model, which independent of the specific MEMS device, makes possible the predictive assessment of the probability of device degradation under the specific loading conditions pertinent to its desirable operation. During Q1 of 2007 the emphasis has been on the development and implementation of the tools needed to discretize actual micrographs of the MEMS material and create realistic representative volume elements (RVE). These RVE will then be used in multi-scale finite element studies of the evolving nonlinear response of the MEMS microstructure to be used in the device-level multi-physics simulations of the MEMS performance. Based on micrographs obtained by Prof. Chasiotis, we have combined various image processing and coloring software (in collaboration with the Visualization Lab. at the UIUC Beckman Institute) with an open-source, grain-level automatic mesh generation software made available by NIST. We are in the process of using the resulting FE models of the microstructure with an in-house multi-scale framework to extract the elasto-plastic response of the heterogeneous material.

At Purdue University, Sadeghi's group has been pursuing the application of the Discrete Element Method (DEM) to account for the discontinuities associated with the aforementioned micro-structural features. In this approach the material is represented as a discontinuous assemblage of elements that interact at their boundaries through springs. The equations of motion for each element are integrated in time to obtain the response of the system. The elements consist of randomly generated Voronoi polygons that will be used to represent the grains of a polycrystalline material. To corroborate the model with continuum based approaches a 10 (μm) by 100 (μm) cantilever beam has been modeled using square elements. A 30 (μN) point load was applied to the free end and the resulting deflection and maximum normal stress were compared against those obtained from beam theory. Both end deflection and the maximum normal stress were within 3% error of those values obtained using beam theory. The model is currently being modified to investigate the fatigue process in single and bimorph, micro-cantilever beams.

Electrostatic Domain Characterization and Modeling

Our electrostatic characterization and modeling activities emphasize the advancement of more accurate models for dielectric charging in RF MEMS switches and rely on closely-coordinated, collaborative research activities at Lehigh (Huang), Georgia Tech

(Papapolymerou), Memtronics (Goldsmith), and the University of Illinois (Aluru, Cangellaris).

During Q1 2007 a mask for the study of dielectric charging in RF MEMS switches was designed. The design included both switches and MIM capacitors of various sizes and geometries (see Fig. 2). Initial fabrication runs at Georgia Tech were performed on high resistivity silicon wafers with PECVD nitride as the dielectric and electroplated gold as switch membrane.

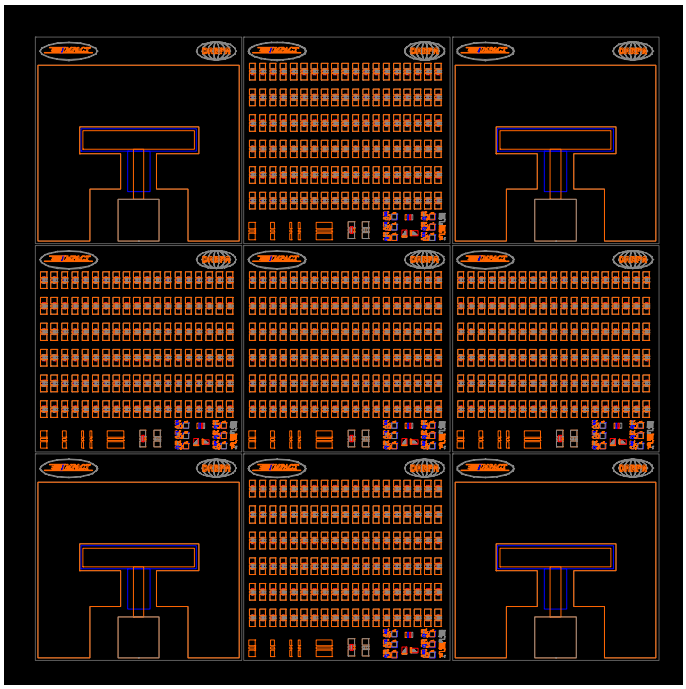

Fig. 2 Mask for the study of dielectric charging in RF MEMS switches.

The electrical characterization of contacting MEMS at Lehigh concentrated on 500µm x 500µm Au/SiN/Ti capacitor test structures that were fabricated alongside the Georgia Tech MEMS switches. The SiN was 0.45µm thick and was deposited by plasma-enhanced chemical vapor deposition. The methodology previously developed under the DARPA HERMIT program appears to be applicable here. Transient charging/discharging currents in the femto-ampere range were characterized between −50 and 50 V and fitted with two exponential functions of increasing time constants. Similar to what was found under the HERMIT program the time constants are independent of the voltage, while the saturated charge densities increase exponentially with voltage. The magnitudes of the time constants and steady-state charge densities are within the range of that of the HERMIT program.

The uniformity and scalability of the capacitors were quickly surveyed. The charging current was found to be uniform within ±10% across the 4” wafer. The charging current of the 100µm × 100µm capacitors was found to scale well with that of the 500µm ×

500μm capacitors. Since the 100μm × 100μm capacitors have approximately the same size of contact area as the MEMS switches, this implies that the charging model extracted from the 500μm × 500μm capacitors is potentially applicable to the MEMS switches. The charging current of the smallest capacitors, at 50μm × 50μm, also scales with that of the 500μm × 500μm capacitors, except that the data obtained on the 50μm × 50μm capacitor are noisier. During the next quarter, the charging model extracted from the capacitors will be used to predict the actuation-voltage shift of MEMS switches and compared with the measured actuation-voltage shift of the switches.

In parallel to these activities, a switch capacitance model was developed at Memtronics that accounts for the surface roughness of the dielectric. The model, called the wavy-plate model, is based on previous experience in MEMS technology and builds upon a previously developed 2-D analytical model for the surface roughness. This numerical model incorporates a 3-D approximation to the shape of the dielectric surface (based on characterization of the lower electrode surface morphology) and provides an estimate of the expected MEMS switch on-capacitance. This model is important in understanding the actual "active" area of the MEMS switch that is subject to dielectric charging. Once the initial round of switches has been completed, we will conduct appropriate measurements and experiments to verify the accuracy of the model.

In an effort to provide for a unifying modeling framework for the incorporation of the various physical attributes and processes known to impact dielectric charging, an electro-quasi-static model was developed at the University of Illinois for the macroscopic, quantitative description of the process of dielectric charging in RF MEMS capacitive switches. The model allows for the specific conduction mechanism in the dielectric to be taken into account in the model. In addition, it provides for the impact of the imperfect contact at the metal-dielectric interface, which is due to surface roughness, to be incorporated in the model. The proposed model relies on experimental input for the definition of several of the parameters used. More specifically, these parameters can be extracted through experiments involving surface roughness characterization and capacitance and conductivity measurements as a function of applied voltage.

Thermal Characterization and Modeling

The thermal characterization and modeling activities are carried out through close collaboration between researchers at Purdue University (Murthy, Peroulis) and the University of Illinois (Ravaioli). An important objective in this effort is to identify the appropriate level of sophistication in thermal modeling, depending on the types of materials used and the device feature sizes, required for accurate thermal analysis of MEMS devices.

During Q1 2007 test structures were designed, fabricated and tested appropriate for the characterization of the thermal properties of thin film Au and SiO_2 films. These structures included long and thin (varying from 0.2 to 1 μm) Au lines printed on Si/SiO_2 wafers. These lines were excited with dc currents so joule heating would raise their temperatures. The temperature was recorded with a thermal camera. The available information will be

compared with data obtained through a hierarchy of models of increasing detail and modeling sophistication, as discussed in more detail in the following paragraphs, to identify the level of modeling detail needed in the thermal modeling of the MEMS devices under investigation in our Center.

On the modeling side, the focus of our effort over the past few months has been on the development of general purpose frameworks for solving phonon and electron transport at both continuum and sub-continuum scales. In semiconductors and dielectrics, thermal transport is mainly by phonons, which are quanta of lattice vibrations. When the mean free path of phonons, approximately 300 nm in silicon at room temperature, becomes comparable to the length scale of the device under consideration, sub-continuum effects such as ballistic transport and boundary scattering become dominant. These effects can be addressed through approaches using the phonon Boltzmann transport equation (BTE) as long as phase coherence effects can be neglected. In metals, thermal transport is primarily through electrons, and for low-voltage conditions, an electron Boltzmann transport equation may be formulated. We have developed an unstructured finite volume solver which can address both these classes of physics and tested and validated it against available experimental data and theoretical results for thin films and nano-constrictions. At continuum scales, the same finite volume methodology is used to solve Fourier conduction, with electro-thermal coupling being addresses through the introduction of Joule heating terms.

In addition to the development of Boltzmann solvers, we have also completed work on the evaluation of contact resistance at nanoscale interfaces through the use of three techniques: (i) an atomistic Green's function approach which can capture wave and confinement effects, (ii) a wave-packet molecular dynamics technique which can extract mode-specific transmissivities of interfaces, and (iii) a phonon Boltzmann transport equation which can capture ballistic and scattering effects at interfaces. These techniques are being applied to the evaluation of contact and constriction resistance in canonical geometries.

Computational Framework for Stochastic Multi-Physics Modeling

The advancement of a computational framework for stochastic, multi-physics modeling of MEMS is pursued under the coordination of the University of Illinois (Aluru).

During Q1 2007 we developed a general framework to quantify the impact of uncertainty arising from geometrical variations on the electrostatic behavior of MEMS. The uncertainty associated with geometry is modeled as a random field, which is first expanded using either polynomial chaos or Karhunen-Loeve expansion in terms of independent random variables. The random field is then treated as a random displacement applied to the conductors defined by the mean geometry, to derive the stochastic Lagrangian boundary integral equation. The surface charge density is modeled as a random field, and is discretized both in the random dimension and space using polynomial chaos and classical boundary element method, respectively.

We have investigated several numerical examples – a single line over a ground plane, a double line over a ground plane, cantilever and fixed-fixed structures and comb-drive structures – to study the effect of uncertain geometry on relevant parameters such as capacitance and net electrostatic force. We have validated the results obtained using our proposed method with rigorous but computationally much slower, Monte Carlo simulations. We have shown that our proposed method and implementation accurately predicts the statistics and probability density functions of various relevant parameters.

In order to start demonstrating the application of this capability utilizing statistical data about fabrication process-induced variations in geometry and material parameters, the layout and masks necessary for the first generation of the process characterization test structures were developed at Purdue (Peroulis). The fabrication of these structures will begin in May 2007 and it is expected to be concluded by the end of the same month. The first measurement data are expected to be available in June 2007.

Patents

None

Publications

1. G. Papaioannou and J. Papapolymerou, "Dielectric charging mechanisms in RF-MEMS capacitive switches," *submitted to the 2007 IEEE European Microwave Conference.*
2. P. Sumant, A. C. Cangellaris and N. Aluru, "Modeling of dielectric charging in RF-MEMS switches," *Center for Computational Electromagnetics and the Electromagnetics Laboratory Report*, ECE Department, University of Illinois, Urbana-Champaign, April 2007.
3. T. Wang and J.Y. Murthy, " Solution of the Phonon Boltzmann Transport Equation Employing Rigorous Implementation of Phonon Conservation Rules," Presented at IMECE 2006; in preparation for submission to *Journal of Applied Physics*, 2007.