Full-physics Integration
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PRISM Annual Review
October 31 & November 1, 2011
Purdue University
Calibration, validation & prediction roadmap

PRISM challenges

- Calibration and validation data from multi-devices
  - Device to device variability

- Multiple sources of uncertainty
  - In experiments and models

- Multiscale, multiphysics models
  - From electrons and atoms to devices

- Bayesian networks to calibrate, validate
- Use model form/confidence to inform predictions
Experiments and Devices Overview

- Actuation and release voltage vs. cycles
- Charging for sustained contact (Prof. Alam)
- Dynamic beam response (Prof. Raman)
- Displacement vs. voltage for property extraction
- Geometry characterization

Same fabrication process followed for all devices
Common Fabrication Process

1. Ti/Au Contacts → Silicon Oxide
   - Silicon Substrate
   - Contact Deposition

2. Silicon Nitride Dielectric
   - PECVD Nitride Deposition

3. Patterned Nitride Etch

4. Photoresist Ti/Au Seed Layer
   - Seed Layer Deposition

5. Plating Mold

6. Electroplating

7. Release

CAD Drawing

SEM Image
PRISM multi-physics integration

Contact physics
- Contact separation

Solid mechanics
- Elasticity & Creep

MD/DFT

AFM

Phase field DD

Dielectric charging
- Defects in dielectric
- Charge injection & transport

MD/DFT

Fluid damping
- Continuum & rarefied

NS+ES-BGK

Quantity of interest
Multi-physics, multiscale network

AFM
- Surface roughness

Mesoscale contact model
- Asperity properties
- Contact force-displacement
- Dielectric constant (low & high freq.)
- Trap depths
- Trap dens, barrier, eff. mass, FP freq., cross sect.

Microscopy
- Geometry \((L, h, L_d, h_d)\)
- Residual stress \((\sigma_{rs})\)
- Young’s modulus
- Creep rate coeff \((A_c)\), yield stress, hardening
- Viscosity, visc.
- Temp. exponent, molecular props., Pr

MD/DFT
- Dielectric constant constant (low & high freq.)
- Trap depths
- Trap dens, barrier, eff. mass, FP freq., cross sect.

XRD + theory

Device-level simulation
- Solid & contact mechanics
- Fluid damping
- Dielectric charging

Quantity of interest

Model, representing conditional probability
- Material property
- Input experiment
- Calibration experiment
- Validation experiment

Device parameter
GEN 5 optical measurements of pull-in voltage

- Calibration of residual stress
- Validation of membrane deformation

![Fix-fix beam](image)

**AFM**
- Surface roughness

**Asperity properties**
- Mesoscale contact model
- Contact force-displacement

**Microscopy**
- Geometry \((L, h, L_d, h_d)\)
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**XRD + theory**
- Creep rate coeff\((A_c)\), yield stress, hardening
- Viscosity, visc. Temp. exponent, molecular props., Pr

**Device-level simulation**
- Solid & contact mechanics
- Fluid damping
- Dielectric charging

**Quasistatic Pull-in voltage**

**Model, representing conditional probability**

- Material property
- Input experiment
- Calibration experiment
- Validation experiment
- Model outcome
- Device parameter

**GEN 5 optical measurements of pull-in voltage**
GEN 5 pull-in

Step 1: Calibration of residual stress

Step 2: Validate membrane deformation model
Fluid damping validation

Device-level simulation
- Solid & contact mechanics
- Fluid damping
- Dielectric charging

Geometry $(L, h, L_d, h_d)$
- Residual stress $(\sigma_{rs})$
- Young's modulus
- Creep rate coeff $(A_c)$, yield stress, hardening
- Viscosity, visc.

Trap depths
- Trap densities, barrier, effective mass, FP freq., cross sect.
- Contact force-displacement
- Dielectric constant (low & high freq.)
- MD/DFT

Asperity properties
- Surface roughness
- Mesoscale contact model

AFM
- Microscopy

MD/DFT
- XRD + theory

Quality factor?

Squeeze film damping experiments on cantilevers

Quality factor
Dielectric charging calibration

- Apply voltage & measure current vs. time

Device-level simulation
- Solid & contact mechanics
- Fluid damping
- Dielectric charging

Current vs. time

Transient current on MIM capacitor
Creep parameters calibration

**Creep parameters calibration**

- **AFM**
  - Surface roughness
- **Mesoscale contact model**
  - Asperity properties
  - Contact force-displacement
  - Dielectric constant (low & high freq.)
  - Trap depths
- **MD/DFT**
  - Trap dens, barrier, eff. mass, FP freq., cross sect.
- **Microscopy**
  - Geometry \((L, h, L_d, h_d)\)
  - Residual stress \((\sigma_{rs})\)
- **XRD + theory**
  - Young’s modulus
  - Creep rate coeff \((A_c)\), yield stress, hardening
  - Viscosity, visc.
  - Temp. exponent, molecular props., Pr
- **Device-level simulation**
  - Solid & contact mechanics
  - Fluid damping
  - Dielectric charging
  - Position vs. time
  - Varactor gap vs. time

**Calibration**

Apply a constant voltage and measure gap vs. time
Multi-physics, multiscale network

Device-level simulation
- Solid & contact mechanics
- Fluid damping
- Dielectric charging

Quantity of interest

Geometry \((L, h, L_d, h_d)\)

Residual stress \((\sigma_{rs})\)

Young’s modulus

Creep rate coeff \((A_c)\), yield stress, hardening

Viscosity, visc.
Temp. exponent, molecular props., Pr

Membrane deformation for fix-fix beam validated
Calibrated

Fluid damping validated

Calibrated

Contact force-displacement

Asperity properties

Mesoscale contact model

Trap depths

Trap dens, barrier, eff. mass, FP freq., cross sect.

Dielectric constant (low & high freq.)

Contact force-displacement

Contact force-displacement

AFM

Surface roughness

Microscopy

XRD + theory

Calibrated

MD/DFT

Calibrated

Calibrated
Pull-in voltage prediction: 500 \( \mu \text{m} \) GEN5 devices

- Residual stress calibrated using 22 devices with 400 \( \mu \text{m} \) length
- Model validated using 22 additional 400 \( \mu \text{m} \) devices
  - Confidence factor of 0.8
- Prediction for 500 \( \mu \text{m} \) vs. experimental measurements

![PDF plot with curves labeled Path 1, Path 2, and Data, along with annotations for MEMOSA, Validated predictions, and Experimental results.](image)
Remaining validation via cantilever experiments

Remaining validation tasks:
- Dielectric charging model in switch
- Contact model
- Creep model

- Pull-in and pull-out from optical measurements
  - Varying $t_{\text{close}}$ allows use to independently validate contact and charging models

- Long-time deformation for creep validation

Calibration & validation status

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Applied voltage vs. time diagram:
- $t_{\text{close}}$
- Pull-in
- Pull-out
Predictions on cantilevers

- Initial device-level predictions vs. experiments
- Models are calibrated but not validated

Applied voltage 150 V
Multiple repetitions on 7 devices
Full physics simulations of fix-fix beam
Full physics simulations of fix-fix beam

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Pull-out voltage predictions for PRISM device

Role of dielectric charging on pull-out (V=120 V)

Charging for 5 ms

Charging for 50 s